

VAMP, Version 1.0: Vegas AMPlified: Anisotropy, Multi-channel sampling and Parallelization

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Abstract

We present an new implementation of the classic Vegas algorithm for adaptive multi-dimensional Monte Carlo integration in Fortran95. This implementation improves the performance for a large class of integrands, supporting stratified sampling in higher dimensions through automatic identification of the directions of largest variation. This implementation also supports multi channel sampling with individual adaptive grids. Sampling can be performed in parallel on workstation clusters and other parallel hardware. Note that for maintenance of the code, and especially its usage within the event generator WHIZARD, some features of Fortran2003 have been added.

Revision Control

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Program Summary:

- **Title of program:** VAMP, Version 1.0 (October 1999)
- **Program obtainable** by anonymous `ftp` from the host `crunch.ikp.physik.th-darmstadt.de` in the directory `pub/ohl/vamp`.
- **Licensing provisions:** Free software under the GNU General Public License.
- **Programming language used:** From version 2.2.0 of the program: Fortran2003 [8] Until version 2.1.x of the program: Fortran95 [9] (Fortran90 [7] and F [14] versions available as well)
- **Number of program lines in distributed program, including test data, etc.:** ≈ 4300 (excluding comments)
- **Computer/Operating System:** Any with a Fortran95 (or Fortran90 or F) programming environment.
- **Memory required to execute with typical data:** Negligible on the scale of typical applications calling the library.
- **Typical running time:** A small fraction (typically a few percent) of the running time of applications calling the library.
- **Purpose of program:**
- **Nature of physical problem:**
- **Method of solution:**
- **Keywords:** adaptive integration, event generation, parallel processing

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INTRODUCTION

We present a reimplementation of the classic Vegas [1, 2] algorithm for adaptive multi-dimensional integration in Fortran95 [9, 13]¹ (Note that for the maintenance of the program and especially its usage within the event generator WHIZARD parts of the program have been adapted to Fortran2003). The purpose of this reimplementation is two-fold: for pedagogical reasons it is useful to employ Fortran95 features (in particular the array language) together with literate programming [4] for expressing the algorithm more concisely and more transparently. On the other hand we use a Fortran95 abstract type to separate the state from the functions. This allows multiple instances of Vegas with different adaptations to run in parallel and in paves the road for a more parallelizable implementation.

The variable names are more in line with [1] than with [2] or with [17, 18, 19], which is almost identical to [2].

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```

¹Fully functional versions conforming to preceeding Fortran standard [7], High Performance Fortran (HPF) [10, 11, 15], and to the Fortran90 subset F [14] are available as well. A translation to the obsolete FORTRAN77 standard [6] is possible in principle, but extremely tedious and error prone if the full functionality shall be preserved.

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—2— ALGORITHMS

 The notation has to be synchronized with [3]!

We establish some notation to allow a concise discussion. Notation:

$$\text{expectation: } E(f) = \frac{1}{|\mathcal{D}|} \int_{\mathcal{D}} dx f(x) \quad (2.1a)$$

$$\text{variance: } V(f) = E(f^2) - (E(f))^2 \quad (2.1b)$$

$$\text{estimate of expectation (average): } \langle X|f \rangle = \frac{1}{|X|} \sum_{x \in X} f(x) \quad (2.1c)$$

$$\text{estimate of variance: } \sigma_X^2(f) = \frac{1}{|X| - 1} (\langle X|f^2 \rangle - \langle X|f \rangle^2) \quad (2.1d)$$

Where $|X|$ is the size of the point set and $|\mathcal{D}| = \int_{\mathcal{D}} dx$ the size of the integration region. If $\mathcal{E}(\langle f \rangle)$ denotes the ensemble average of $\langle X|f \rangle$ over random point sets X with $|X| = N$, we have for expectation and variance

$$\mathcal{E}(\langle f \rangle) = E(f) \quad (2.2a)$$

$$\mathcal{E}(\sigma^2(f)) = V(f) \quad (2.2b)$$

and the ensemble variance of the expectation is also given by the variance

$$\mathcal{V}(\langle f \rangle) = \frac{1}{N} V(f) \quad (2.2c)$$

Therefore, it can be estimated from $\sigma_X^2(f)$. Below, we will also use the notation \mathcal{E}_g for the ensemble average over random point sets X_g with probability distribution g . We will write $E_g(f) = E(fg)$ as well.

2.1 Importance Sampling

If, instead of uniformly distributed points X , we use points X_g distributed according to a probability density g , we can easily keep the expectation constant

$$\mathcal{E}_g(\langle f \rangle) = E_g \left(\frac{f}{g} \right) = E(f) \quad (2.3)$$

while the variance transforms non-trivially

$$\mathcal{V}_g(\langle f \rangle) = \frac{1}{N} V_g \left(\frac{f}{g} \right) = \frac{1}{N} \left(E_g \left(\frac{f^2}{g^2} \right) - \left(E_g \left(\frac{f}{g} \right) \right)^2 \right) \quad (2.4)$$

and the error is minimized when f/g is constant, i.e. g is a good approximation of f . The non-trivial problem is to find a g that can be generated efficiently and is a good approximation at the same time.

One of the more popular approaches is to use a mapping ϕ of the integration domain

$$\begin{aligned} \phi : \mathcal{D} &\rightarrow \Delta \\ x &\mapsto \xi = \phi(x) \end{aligned} \quad (2.5)$$

In the new coordinates, the distribution is multiplied by the Jacobian of the inverse map ϕ^{-1} :

$$\int_{\mathcal{D}} dx f(\phi(x)) = \int_{\Delta} d\xi J_{\phi^{-1}}(\xi) f(\xi) \quad (2.6)$$

A familiar example is given by the map

$$\begin{aligned} \phi : [0, 1] &\rightarrow \mathbf{R} \\ x &\mapsto \xi = x^0 + a \cdot \tan \left(\left(x - \frac{1}{2} \right) \pi \right) \end{aligned} \quad (2.7)$$

with the inverse $\phi^{-1}(\xi) = \text{atan}((\xi - x_0)/a)/\pi + 1/2$ and the corresponding Jacobian reproducing a resonance

$$J_{\phi^{-1}}(\xi) = \frac{d\phi^{-1}(\xi)}{d\xi} = \frac{a}{\pi} \frac{1}{(\xi - x^0)^2 + a^2} \quad (2.8)$$

Obviously, this works only for a few special distributions. Fortunately, we can combine several of these mappings to build efficient integration algorithms, as will be explained in section 2.4 below. Another approach is to construct the approximation numerically, by appropriate binning of the integration domain (cf. [1, 2, 20]). The most popular technique for this will be discussed below in section 2.3.

2.2 Stratified Sampling

The technique of importance sampling concentrates the sampling points in the region where the contribution to the integrand is largest. Alternatively we can also concentrate the sampling points in the region where the contribution to the variance is largest.

If we divide the sampling region \mathcal{D} into n disjoint subregions \mathcal{D}^i

$$\mathcal{D} = \bigcup_{i=1}^n \mathcal{D}^i, \quad \mathcal{D}^i \cap \mathcal{D}^j = \emptyset \quad (i \neq j) \quad (2.9)$$

a new estimator is

 Bzzzt! Wrong. These multi-channel formulae are incorrect for partitionings and must be fixed.

$$\overline{\langle X|f \rangle} = \sum_{i=1}^n \frac{N_i}{N} \langle X_{\theta_i} | f \rangle \quad (2.10)$$

where

$$\theta_i(x) = \begin{cases} 1 & \text{for } x \in \mathcal{D}^i \\ 0 & \text{for } x \notin \mathcal{D}^i \end{cases} \quad (2.11)$$

and

$$\sum_{i=1}^n N_i = N \quad (2.12)$$

since the expectation is linear

$$\mathcal{E}(\overline{\langle f \rangle}) = \sum_{i=1}^n \frac{N_i}{N} \mathcal{E}_{\theta_i}(\langle f \rangle) = \sum_{i=1}^n \frac{N_i}{N} E_{\theta_i}(f) = \sum_{i=1}^n \frac{N_i}{N} E(f\theta_i) = E(f) \quad (2.13)$$

On the other hand, the variance of the estimator $\overline{\langle X|f \rangle}$ is

$$\mathcal{V}(\overline{\langle f \rangle}) = \sum_{i=1}^n \frac{N_i}{N} \mathcal{V}_{\theta_i}(\langle f \rangle) \quad (2.14)$$

This is minimized for

$$N_i \propto \sqrt{V(f \cdot \theta_{\mathcal{D}^i})} \quad (2.15)$$

as a simple variation of $\mathcal{V}(\overline{\langle f \rangle})$ shows.



Figure 2.1: **vegas** grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.



Figure 2.2: One-dimensional illustration of the **vegas** grid structure for pseudo stratified sampling, which is used in high dimensions.

2.3 Vegas

Under construction!

2.3.1 Vegas' Inflexibility

The classic implementation of the Vegas algorithm [1, 2] treats all dimensions alike. This constraint allows a very concise FORTRAN77-style coding of the algorithm, but there is no theoretical reason for having the same number of divisions in each direction. On the contrary, under these circumstances, even a dimension in which the integrand is rather smooth will contribute to the exponential blow-up of cells for stratified sampling. It is obviously beneficial to use a finer grid in those directions in which the fluctuations are stronger, while a coarser grid will suffice in the other directions.

One small step along this line is implemented in Version 5.0 of the package `BASES/SPRING` [20], where one set of “wild” variables is separated from “smooth” variables [21].

The present reimplementaion of the Vegas algorithm allows the application to choose the number of divisions in each direction freely. The routines that reshape the grid accept an integer array with the number of divisions as an optional argument `num_div`. It is easy to construct examples in which the careful use of this feature reduces the variance significantly.

Currently, no attempt is made for automatic optimization of the number of divisions. One reasonable approach is to monitor Vegas’ grid adjustments and to increase the number of division in those directions where Vegas’ keeps adjusting because of fluctuations. For each direction, a numerical measure of these fluctuations is given by the spread in the m_i . The total number of cells can be kept constant by reducing the number of divisions in the other directions appropriately. Thus

$$n_{\text{div},j} \rightarrow \frac{Q_j n_{\text{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\text{dim}}}} \quad (2.16)$$

where we have used the damped standard deviation

$$Q_j = \left(\sqrt{\text{Var}(\{m\}_j)}\right)^\alpha \quad (2.17)$$

instead of the spread.

2.3.2 Vegas’ Dark Side



Under construction!

A partial solution of this problem will be presented in section 2.5.

2.4 Multi Channel Sampling

Even if Vegas performs well for a large class of integrands, many important applications do not lead to a factorizable distribution. The class of integrands that can be integrated efficiently by Vegas can be enlarged substantially by using multi channel methods. The new class will include almost all integrals appearing in high energy physics simulations.



The first version of this section is now obsolete. Consult [3] instead.

2.5 *Revolving*



Under construction!

2.6 *Parallelization*

Traditionally, parallel processing has not played a large rôle in simulations for high energy physics. A natural and trivial method of utilizing many processors will run many instances of the same (serial) program with different values of the input parameters in parallel. Typical matrix elements and phase space integrals offer few opportunities for small scale parallelization.

On the other hand, parameter fitting has become possible recently for observables involving a phase space integration. In this case, fast evaluation of the integral is essential and parallel execution becomes an interesting option.

A different approach to parallelizing Vegas has been presented recently [22].

2.6.1 *Multilinear Structure of the Sampling Algorithm*

In order to discuss the problems with parallelizing adaptive integration algorithms and to present solutions, it helps to introduce some mathematical notation. A sampling S is a map from the space π of point sets and the space F of functions to the real (or complex) numbers

$$\begin{aligned} S : \pi \times F &\rightarrow \mathbf{R} \\ (p, f) &\mapsto I = S(p, f) \end{aligned}$$

For our purposes, we have to be more specific about the nature of the point set. In general, the point set will be characterized by a sequence of pseudo random numbers $\rho \in R$ and by one or more grids $G \in \Gamma$ used for importance or stratified sampling. A simple sampling

$$\begin{aligned} S_0 : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} &\rightarrow R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} \\ (\rho, G, a, f, \mu_1, \mu_2) &\mapsto (\rho', G, a', f, \mu'_1, \mu'_2) = S_0(\rho, G, a, f, \mu_1, \mu_2) \end{aligned} \tag{2.18}$$

estimates the n -th moments $\mu'_n \in \mathbf{R}$ of the function $f \in F$. The integral and its standard deviation can be derived easily from the moments

$$I = \mu_1 \tag{2.19a}$$

$$\sigma^2 = \frac{1}{N-1} (\mu_2 - \mu_1^2) \tag{2.19b}$$

while the latter are more convenient for the following discussion. In addition, S_0 collects auxiliary information to be used in the grid refinement, denoted by $a \in A$. The unchanged arguments G and f have been added to the result of S_0 in (2.18), so that S_0 has identical domain and codomain and can therefore be iterated. Previous estimates μ_n may be used in the estimation of μ'_n , but a particular S_0 is free to ignore them as well. Using a little notational freedom, we augment \mathbf{R} and A with a special value \cdot , which will always be discarded by S_0 .

In an adaptive integration algorithm, there is also a refinement operation $r : \Gamma \times A \rightarrow \Gamma$ that can be extended naturally to the codomain of S_0

$$\begin{aligned} r : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} &\rightarrow R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} \\ (\rho, G, a, f, \mu_1, \mu_2) &\mapsto (\rho, G', a, f, \mu_1, \mu_2) = r(\rho, G, a, f, \mu_1, \mu_2) \end{aligned} \quad (2.20)$$

so that $S = rS_0$ is well defined and we can specify n -step adaptive sampling as

$$S_n = S_0(rS_0)^n \quad (2.21)$$

Since, in a typical application, only the estimate of the integral and the standard deviation are used, a projection can be applied to the result of S_n :

$$\begin{aligned} P : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} &\rightarrow \mathbf{R} \times \mathbf{R} \\ (\rho, G, a, f, \mu_1, \mu_2) &\mapsto (I, \sigma) \end{aligned} \quad (2.22)$$

Then

$$(I, \sigma) = PS_0(rS_0)^n(\rho, G_0, \cdot, f, \cdot, \cdot) \quad (2.23)$$

and a good refinement prescription r , such as Vegas, will minimize the σ .

For parallelization, it is crucial to find a division of S_n or any part of it into *independent* pieces that can be evaluated in parallel. In order to be effective, r has to be applied to *all* of a and therefore a synchronization of G before and after r is appropriately. Furthermore, r usually uses only a tiny fraction of the CPU time and it makes little sense to invest a lot of effort into parallelizing it beyond what the Fortran compiler can infer from array notation. On the other hand, S_0 can be parallelized naturally, because all operations are linear, including the computation of a . We only have to make sure that the cost of communicating the results of S_0 and r back and forth during the computation of S_n do not offset any performance gain from parallel processing.

When we construct a decomposition of S_0 and prove that it does not change the results, i.e.

$$S_0 = \iota S_0 \phi \quad (2.24)$$

where ϕ is a forking operation and ι is a joining operation, we are faced with the technical problem of a parallel random number source ρ . As made explicit in (2.18), S_0 changes the state of the random number general ρ , demanding *identical* results therefore imposes a strict ordering on the operations and defeats parallelization. It is possible to devise implementations of S_0 and ρ that circumvent this problem by distributing subsequences of ρ in such a way among processes that results do not depend on the number of parallel processes.

However, a reordering of the random number sequence will only change the result by the statistical error, as long as the scale of the allowed reorderings is *bounded* and much smaller than the period of the random number generator¹ Below, we will therefore use the notation $x \approx y$ for “equal for an appropriate finite reordering of the ρ used in calculating x and y ”. For our purposes, the relation $x \approx y$ is strong enough and allows simple and efficient implementations.

Since S_0 is essentially a summation, it is natural to expect a linear structure

$$\bigoplus_i S_0(\rho_i, G_i, a_i, f, \mu_{1,i}, \mu_{2,i}) \approx S_0(\rho, G, a, f, \mu_1, \mu_2) \quad (2.25a)$$

where

$$\rho = \bigoplus_i \rho_i \quad (2.25b)$$

$$G = \bigoplus_i G_i \quad (2.25c)$$

$$a = \bigoplus_i a_i \quad (2.25d)$$

$$\mu_n = \bigoplus_i \mu_{n,i} \quad (2.25e)$$

for appropriate definitions of “ \oplus ”. For the moments, we have standard addition

$$\mu_{n,1} \oplus \mu_{n,2} = \mu_{n,1} + \mu_{n,2} \quad (2.26)$$

and since we only demand equality up to reordering, we only need that the ρ_i are statistically independent. This leaves us with G and a and we have to discuss importance sampling and stratified sampling separately.

¹Arbitrary reorderings on the scale of the period of the random number generators could select constant sequences and have to be forbidden.

Importance Sampling

In the case of naive Monte Carlo and importance sampling the natural decomposition of G is to take j copies of the same grid G/j which is identical to G , each with one j -th of the total sampling points. As long as the a are linear themselves, we can add them up just like the moments

$$a_1 \oplus a_2 = a_1 + a_2 \quad (2.27)$$

and we have found a decomposition (2.25). In the case of Vegas, the a_i are sums of function values at the sampling points. Thus they are obviously linear and this approach is applicable to Vegas in the importance sampling mode.

Stratified Sampling

The situation is more complicated in the case of stratified sampling. The first complication is that in pure stratified sampling there are only two sampling points per cell. Splitting the grid in two pieces as above provide only a very limited amount of parallelization. The second complication is that the a are no longer linear, since they correspond to a sampling of the variance per cell and no longer of function values themselves.

However, as long as the samplings contribute to disjoint bins only, we can still “add” the variances by combining bins. The solution is therefore to divide the grid into disjoint bins along the divisions of the stratification grid and to assign a set of bins to each processor.

Finer decompositions will incur higher communications costs and other resource utilization. An implementation based on PVM is described in [22], which minimizes the overhead by running identical copies of the grid G on each processor. Since most of the time is usually spent in function evaluations, it makes sense to run a full S_0 on each processor, skipping function evaluations everywhere but in the region assigned to the processor. This is a neat trick, which is unfortunately tied to the computational model of message passing systems such as PVM and MPI [12]. More general paradigms can not be supported since the separation of the state for the processors is not explicit (it is implicit in the separated address space of the PVM or MPI processes).

However, it is possible to implement (2.25) directly in an efficient manner. This is based on the observation that the grid G used by Vegas is factorized into divisions D^j for each dimension

$$G = \bigotimes_{j=1}^{n_{\text{dim}}} D^j \quad (2.28)$$

and decompositions of the D^j induce decompositions of G

$$\begin{aligned} G_1 \oplus G_2 &= \left(\bigotimes_{j=1}^{i-1} D^j \otimes D_1^i \otimes \bigotimes_{i=j+1}^{n_{\text{dim}}} D^j \right) \oplus \left(\bigotimes_{j=1}^{i-1} D^j \otimes D_2^i \otimes \bigotimes_{i=j+1}^{n_{\text{dim}}} D^j \right) \\ &= \bigotimes_{j=1}^{i-1} D^j \otimes (D_1^i \oplus D_2^i) \otimes \bigotimes_{j=i+1}^{n_{\text{dim}}} D^j \quad (2.29) \end{aligned}$$

We can translate (2.29) directly to code that performs the decomposition $D^i = D_1^i \oplus D_2^i$ discussed below and simply duplicates the other divisions $D^{j \neq i}$. A decomposition along multiple dimensions is implemented by a recursive application of (2.29).

In Vegas, the auxiliary information a inherits a factorization similar to the grid (2.28)

$$a = (d^1, \dots, d^{n_{\text{dim}}}) \quad (2.30)$$

but not a multilinear structure. Instead, *as long as the decomposition respects the stratification grid*, we find the in place of (2.29)

$$a_1 \oplus a_2 = (d_1^1 + d_2^1, \dots, d_1^i \oplus d_2^i, \dots, d_1^{n_{\text{dim}}} + d_2^{n_{\text{dim}}}) \quad (2.31)$$

with “+” denoting the standard addition of the bin contents and “ \oplus ” denoting the aggregation of disjoint bins. If the decomposition of the division would break up cells of the stratification grid (2.31) would be incorrect, because, as discussed above, the variance is not linear.

Now it remains to find a decomposition

$$D^i = D_1^i \oplus D_2^i \quad (2.32)$$

for both the pure stratification mode and the pseudo stratification mode of vegas (cf. figure 2.1). In the pure stratification mode, the stratification grid is strictly finer than the adaptive grid and we can decompose along either of them immediately. Technically, a decomposition along the coarser of the two is straightforward. Since the adaptive grid already has more than 25 bins, a decomposition along the stratification grid makes no practical sense and the decomposition along the adaptive grid has been implemented. The sampling algorithm S_0 can be applied *unchanged* to the individual grids resulting from the decomposition.

For pseudo stratified sampling (cf. figure 2.2), the situation is more complicated, because the adaptive and the stratification grid do not share bin boundaries. Since Vegas does *not* use the variance in this mode, it would be theoretically possible to decompose along the adaptive grid and to mimic the



Figure 2.3: Forking one dimension d of a grid into three parts $ds(1)$, $ds(2)$, and $ds(3)$. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 2.2).

incomplete bins of the stratification grid in the sampling algorithm. However, this would be a technical complication, destroying the universality of S_0 . Therefore, the adaptive grid is subdivided in a first step in

$$\text{lcm} \left(\frac{\text{lcm}(n_f, n_g)}{n_f}, n_x \right) \quad (2.33)$$

bins,² such that the adaptive grid is strictly finer than the stratification grid. This procedure is shown in figure 2.3.

2.6.2 State and Message Passing

2.6.3 Random Numbers

In the parallel example sitting on top of MPI [12] takes advantage of the ability of Knuth's generator [16] to generate statistically independent subse-

²The coarsest grid covering the division of n_g bins into n_f forks has $n_g / \gcd(n_f, n_g) = \text{lcm}(n_f, n_g) / n_f$ bins per fork.

quences. However, since the state of the random number generator is explicit in all procedure calls, other means of obtaining subsequences can be implemented in a trivial wrapper.

The results of the parallel example will depend on the number of processors, because this effects the subsequences being used. Of course, the variation will be compatible with the statistical error. It must be stressed that the results are deterministic for a given number of processors and a given set of random number generator seeds. Since parallel computing environments allow to fix the number of processors, debugging of exceptional conditions is possible.

2.6.4 Practice

In this section we show three implementations of S_n : one serial, and two parallel, based on HPF [10, 11, 15] and MPI [12], respectively. From these examples, it should be obvious how to adapt VAMP to other parallel computing paradigms.

Serial

Here is a bare bones serial version of S_n , for comparison with the parallel versions below. The real implementation of `vamp_sample_grid` in the module `vamp` includes some error handling, diagnostics and the projection P (cf. (2.22)):

```
14  $\langle$ Serial implementation of  $S_n = S_0(rS_0)^n$  14 $\rangle \equiv$ 
  subroutine vamp_sample_grid (rng, g, iterations, func)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: iterations
     $\langle$ Interface declaration for func 22 $\rangle$ 
    integer :: iteration
    iterate: do iteration = 1, iterations
      call vamp_sample_grid0 (rng, g, func)
      call vamp_refine_grid (g)
    end do iterate
  end subroutine vamp_sample_grid
```

HPF

The HPF version of S_n is based on decomposing the grid `g` as described in section 2.6.1 and lining up the components in an array `gs`. The elements of `gs` can then be processed in parallel. This version can be compiled with any

Fortran compiler and a more complete version of this procedure (including error handling, diagnostics and the projection P) is included with VAMP as `vamp_sample_grid_parallel` in the module `vamp`. This way, the algorithm can be tested on a serial machine, but there will obviously be no performance gain.

Instead of one random number generator state `rng`, it takes an array consisting of one state per processor. These `rng(:)` are assumed to be initialized, such that the resulting sequences are statistically independent. For this purpose, Knuth's random number generator [16] is most convenient and is included with VAMP (see the example on page 16). Before each S_0 , the procedure `vamp_distribute_work` determines a good decomposition of the grid `d` into `size(rng)` pieces. This decomposition is encoded in the array `d` where `d(1,:)` holds the dimensions along which to split the grid and `d(2,:)` holds the corresponding number of divisions. Using this information, the grid is decomposed by `vamp_fork_grid`. The HPF compiler will then distribute the `!hpf$ independent` loop among the processors. Finally, `vamp_join_grid` gathers the results.

```

15 <Parallel implementation of  $S_n = S_0(rS_0)^n$  (HPF) 15>≡
  subroutine vamp_sample_grid_hpf (rng, g, iterations, func)
    type(tao_random_state), dimension(:), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: iterations
    <Interface declaration for func 22>
    type(vamp_grid), dimension(:), allocatable :: gs, gx
    !hpf$ processors p(number_of_processors())
    !hpf$ distribute gs(cyclic(1)) onto p
    integer, dimension(:,:), pointer :: d
    integer :: iteration, num_workers
    iterate: do iteration = 1, iterations
      call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
      num_workers = max (1, product (d(2,:)))
      if (num_workers > 1) then
        allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
        call vamp_create_empty_grid (gs)
        call vamp_fork_grid (g, gs, gx, d)
        !hpf$ independent
        do i = 1, num_workers
          call vamp_sample_grid0 (rng(i), gs(i), func)
        end do
        call vamp_join_grid (g, gs, gx, d)
        call vamp_delete_grid (gs)
        deallocate (gs, gx)
      end if
    end do
  end subroutine

```



```

        else
            call vamp_sample_grid0 (rng(1), g, func)
        end if
        call vamp_refine_grid (g)
    end do iterate
end subroutine vamp_sample_grid_hpf

```

Since `vamp_sample_grid0` performs the bulk of the computation, an almost linear speedup with the number of processors can be achieved, if `vamp_distribute_work` finds a good decomposition of the grid. The version of `vamp_distribute_work` distributed with VAMP does a good job in most cases, but will not be able to use all processors if their number is a prime number larger than the number of divisions in the stratification grid. Therefore it can be beneficial to tune `vamp_distribute_work` to specific hardware. Furthermore, using a finer stratification grid can improve performance.

For definiteness, here is an example of how to set up the array of random number generators for HPF. Note that this simple seeding procedure only guarantees statistically independent sequences with Knuth's random number generator [16] and will fail with other approaches.

```

16 <Parallel usage of  $S_n = S_0(rS_0)^n$  (HPF) 16>≡
    type(tao_random_state), dimension(:), allocatable :: rngs
    !hpf$ processors p(number_of_processors())
    !hpf$ distribute gs(cyclic(1)) onto p
    integer :: i, seed
    ! ...
    allocate (rngs(number_of_processors()))
    seed = 42 ! can be read from a file, of course ...
    !hpf$ independent
    do i = 1, size (rngs)
        call tao_random_create (rngs(i), seed + i)
    end do
    ! ...
    call vamp_sample_grid_hpf (rngs, g, 6, func)
    ! ...

```

MPI

The MPI version is more low level, because we have to keep track of message passing ourselves. Note that we have made this synchronization points explicit with three `if ... then ... else ... end if` blocks: forking, sampling, and joining. These blocks could be merged (without any performance gain) at the expense of readability. We assume that `rng` has been initialized

in each process such that the sequences are again statistically independent.

17 \langle Parallel implementation of $S_n = S_0(rS_0)^n$ (MPI) 17 $\rangle \equiv$

```

subroutine vamp_sample_grid_mpi (rng, g, iterations, func)
  type(tao_random_state), dimension(:), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: iterations
   $\langle$ Interface declaration for func 22 $\rangle$ 
  type(vamp_grid), dimension(:), allocatable :: gs, gx
  integer, dimension(:,:), pointer :: d
  integer :: num_proc, proc_id, iteration, num_workers
  call mpi90_size (num_proc)
  call mpi90_rank (proc_id)
  iterate: do iteration = 1, iterations
    if (proc_id == 0) then
      call vamp_distribute_work (num_proc, vamp_rigid_divisions (g), d)
      num_workers = max (1, product (d(2,:)))
    end if
    call mpi90_broadcast (num_workers, 0)
    if (proc_id == 0) then
      allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
      call vamp_create_empty_grid (gs)
      call vamp_fork_grid (g, gs, gx, d)
      do i = 2, num_workers
        call vamp_send_grid (gs(i), i-1, 0)
      end do
    else if (proc_id < num_workers) then
      call vamp_receive_grid (g, 0, 0)
    end if
    if (proc_id == 0) then
      if (num_workers > 1) then
        call vamp_sample_grid0 (rng, gs(1), func)
      else
        call vamp_sample_grid0 (rng, g, func)
      end if
    else if (proc_id < num_workers) then
      call vamp_sample_grid0 (rng, g, func)
    end if
    if (proc_id == 0) then
      do i = 2, num_workers
        call vamp_receive_grid (gs(i), i-1, 0)
      end do
      call vamp_join_grid (g, gs, gx, d)
      call vamp_delete_grid (gs)
    end if
  end do
end subroutine vamp_sample_grid_mpi

```

```

        deallocate (gs, gx)
        call vamp_refine_grid (g)
    else if (proc_id < num_workers) then
        call vamp_send_grid (g, 0, 0)
    end if
end do iterate
end subroutine vamp_sample_grid_mpi

```

A more complete version of this procedure is included with VAMP as well, this time as `vamp_sample_grid` in the MPI support module `vampi`.

—3—

DESIGN TRADE OFFS

There have been three competing design goals for vegas, that are not fully compatible and had to be reconciled with compromises:

- *Ease-Of-Use*: few procedures, few arguments.
- *Parallelizability*: statelessness
- *Performance and Flexibility*: rich interface, functionality.

In fact, parallelizability and ease-of-use are complementary. A parallelizable implementation has to expose *all* the internal state. In our case, this includes the state of the random number generator and the adaptive grid. A simple interface would hide such details from the user.

The modern language features introduced to Fortran in 1990 [7] allows to reconcile these competing goals. Two abstract data types `vamp.state` and `tao.random.state` hide the details of the implementation from the user and encapsulate the two states in just two variables.

Another problem with parallelizability arised from the lack of a general exception mechanism in Fortran. The Fortran90 standard [9] forbids *any* input/output (even to the terminal) as well as `stop` statements in parallelizable (`pure`) procedures. This precludes simple approaches to monitoring and error handling. In Vegas we use a simple hand crafted exception mechanism (see chapter B) for communicating error conditions to the out layers of the applications. Unfortunately this requires the explicit passing of state in argument lists.

An unfortunate consequence of the similar approach to monitoring is that monitoring is *not* possible during execution. Instead, intermediate results can only be examined after a parallelized section of code has completed.

3.1 *Programming Language*

We have chosen to implement VAMP in Fortran90/95, which some might consider a questionable choice today. Nevertheless, we are convinced that Fortran90/95 (with all its weaknesses) is, by a wide margin, the right tool for the job.

Let us consider the alternatives

- FORTRAN77 is still the dominant language in high energy physics and all running experiment's software environments are based on it. However, the standard [6] is obsolete now and the successors [7, 9] have added many desirable features, while retaining almost all of FORTRAN77 as a subset.
- C/C++ appears to be the most popular programming language in industry and among young high energy physicists. Large experiments have taken a bold move and are basing their software environment on C++.
- Typed higher order functional programming languages (ML, Haskell, etc.) are a very promising development. Unfortunately, there is not yet enough industry support for high performance optimizing compilers. While the performance penalty of these languages is not as high as commonly believed (research compilers, which do not perform extensive processor specific optimizations, result in code that runs by a factor of two or three slower than equivalent Fortran code), it is relevant for long running, computing intensive applications. In addition, these languages are syntactically and idiomatically very different from Fortran and C. Another implementation of VAMP in ML will be undertaken for research purposes to investigate new algorithms that can only be expressed awkwardly in Fortran, but we do not expect it to gain immediate popularity.

—4— USAGE

4.1 Basic Usage

`type(vamp_grid)`

`subroutine vamp_create_grid (g, domain [, num_calls] [, exc])`

Create a fresh grid for the integration domain

$$\mathcal{D} = [D_{1,1}, D_{2,1}] \times [D_{1,2}, D_{2,2}] \times \dots \times [D_{1,n}, D_{2,n}] \quad (4.1)$$

dropping all accumulated results. This function *must not* be called twice on the first argument, without an intervening

`vamp_delete_grid`. Iff the variable `num_calls` is given, it will be the number of sampling points per iteration for the call to `vamp_sample_grid`.

`subroutine vamp_delete_grid (g [, exc])`

`subroutine vamp_discard_integral (g [, num_calls] [, exc])`

Keep the current optimized grid, but drop the accumulated results for the integral (value and errors). Iff the variable `num_calls` is given, it will be the new number of sampling points per iteration for the calls to `vamp_sample_grid`.

`subroutine vamp_reshape_grid (g [, num_calls] [, exc])`

Keep the current optimized grid and the accumulated results for the integral (value and errors). The variable `num_calls` is the new number of sampling points per iteration for the calls to `vamp_sample_grid`.

`subroutine vamp_sample_grid (rng, g, func, iterations
[, integral] [, std_dev] [, avg_chi2] [, exc] [, history])`

Sample the function `func` using the grid `g` for `iterations` iterations and optimize the grid after each iteration. The results are returned in `integral`, `std_dev` and `avg_chi2`. The random number generator uses and updates the state stored in `rng`. The explicit random number state is inconvenient, but required for parallelizability.

```
subroutine vamp_integrate (rng, g, func, calls [, integral]
[, std_dev] [, avg_chi2] [, exc] [, history])
```

This is a wrapper around the above routines, that is steered by a integer, dimension(2,:) array `calls`. For each `i`, there will be `calls(1,i)` iterations with `calls(2,i)` sampling points.

```
subroutine vamp_integrate (rng, domain, func, calls
[, integral] [, std_dev] [, avg_chi2] [, exc] [, history])
```

A second specific form of `vamp_integrate`. This one keeps a private grid and provides the shortest—and most inflexible—calling sequence.

```
22 <Interface declaration for func 22>≡ (14 15 17 86a 94c 103b 113 115 120b 135c 136c 139–42 169d 175c 182
interface
  function func (xi, data, weights, channel, grids) result (f)
    use kinds
    use vamp_grid_type !NODEP!
    import vamp_data_t
    real(kind=default), dimension(:), intent(in) :: xi
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: f
  end function func
end interface
```

4.1.1 Basic Example

In Fortran95, the function to be sampled *must* be pure, i.e. have no side effects to allow parallelization. The optional arguments `weights` and `channel` *must* be declared to allow the compiler to verify the interface, but they are ignored during basic use. Their use for multi channel sampling will be explained below. Here’s a Gaussian

$$f(x) = e^{-\frac{1}{2} \sum_i x_i^2} \quad (4.2)$$

```

23a <basic.f90 23a>≡
    module basic_fct
        use kinds
        implicit none
        private
        public :: fct
    contains
        function fct (x, weights, channel) result (f_x)
            real(kind=default), dimension(:), intent(in) :: x
            real(kind=default), dimension(:), intent(in), optional :: weights
            integer, intent(in), optional :: channel
            real(kind=default) :: f_x
            f_x = exp (-0.5 * sum (x*x))
        end function fct
    end module basic_fct
23b >

```

In the main program, we need to import five modules. The customary module `kinds` defines `double` as the kind for double precision floating point numbers. The model `exceptions` provides simple error handling support (parallelizable routines are not allowed to issue error messages themselves, but must pass them along). The module `tao_random_numbers` hosts the random number generator used and `vamp` is the adaptive iteration module proper. Finally, the application module `basic_fct` has to be imported as well.

```

23b <basic.f90 23a>+≡
    program basic
        use kinds
        use exceptions
        use tao_random_numbers
        use vamp
        use basic_fct
        implicit none
23c <23a 23c>

```

Then we define four variables for an error message, the random number generator state and the adaptive integration grid. We also declare a variable for holding the integration domain and variables for returning the result. In this case we integrate the 7-dimensional hypercube.

```

23c <basic.f90 23a>+≡
    type(exception) :: exc
    type(tao_random_state) :: rng
    type(vamp_grid) :: grid
    real(kind=default), dimension(2,7) :: domain
    real(kind=default) :: integral, error, chi2
    domain(1,:) = -1.0
    domain(2,:) = 1.0
23b <23b 24a>

```


Initialize and seed the random number generator. Initialize the grid for 10 000 sampling points.

```
24a <basic.f90 23a>+≡ <23c 24b>
    call tao_random_create (rng, seed=0)
    call clear_exception (exc)
    call vamp_create_grid (grid, domain, num_calls=10000, exc=exc)
    call handle_exception (exc)
```

Warm up the grid in six low statistics iterations. Clear the error status before and check it after the sampling.

```
24b <basic.f90 23a>+≡ <24a 24c>
    call clear_exception (exc)
    call vamp_sample_grid (rng, grid, fct, 6, exc=exc)
    call handle_exception (exc)
```

Throw away the intermediate results and reshape the grid for 100 000 sampling points—keeping the adapted grid—and do four iterations of a higher statistics integration

```
24c <basic.f90 23a>+≡ <24b>
    call clear_exception (exc)
    call vamp_discard_integral (grid, num_calls=100000, exc=exc)
    call handle_exception (exc)
    call clear_exception (exc)
    call vamp_sample_grid (rng, grid, fct, 4, integral, error, chi2, exc=exc)
    call handle_exception (exc)
    print *, "integral = ", integral, "+/-", error, " (chi^2 = ", chi2, ")"
end program basic
```

Since this is the most common use, there is a convenience routine available and the following code snippet is equivalent:

```
24d <Alternative to basic.f90 24d>≡
    integer, dimension(2,2) :: calls
    calls(:,1) = (/ 6, 10000 /)
    calls(:,2) = (/ 4, 100000 /)
    call clear_exception (exc)
    call vamp_integrate (rng, domain, fct, calls, integral, error, chi2, exc=exc)
    call handle_exception (exc)
```

4.2 Advanced Usage



Caveat emptor: no magic of literate programming can guarantee that the following remains in sync with the implementation. This has to be maintained manually.

All `real` variables are declared as `real(kind=default)` in the source and the variable `double` is imported from the module `kinds` (see appendix A.1). The representation of real numbers can therefore be changed by changing `double` in `kinds`.

4.2.1 Types

```
type(vamp_grid)
type(vamp_grids)
type(vamp_history)
type(exception)
  (from module exceptions)
```

4.2.2 Shared Arguments

Arguments keep their name across procedures, in order to make the Fortran90 keyword interface consistent.

```
real, intent(in) :: accuracy
```

Terminate S_n after $n' < n$ iterations, if relative error is smaller than `accuracy`. Specifically, the termination condition is

$$\frac{\text{std_dev}}{\text{integral}} < \text{accuracy} \quad (4.3)$$

```
real, intent(out) :: avg_chi2
```

The average χ^2 of the iterations.

```
integer, intent(in) :: channel
```

Call `func` with this optional argument. Multi channel sampling uses this to emulate arrays of functions

```
logical, intent(in) :: covariance
```

Collect covariance data.

```
type(exception), intent(inout) :: exc
```

Exceptional conditions are reported in `exc`.

```
type(vamp_grid), intent(inout) :: g
```

Unless otherwise noted, `g` denotes the active sampling grid in the documentation below.

```
type(vamp_histories), dimension(:), intent(inout) ::  
  histories
```

Diagnostic information for multi channel sampling.

```
type(vamp_history), dimension(:), intent(inout) ::  
  history
```

Diagnostic information for single channel sampling or summary of multi channel sampling.

```
real, intent(out) :: integral
```

The current best estimate of the integral.

```
integer, intent(in) :: iterations
```

```
real, dimension(:,:), intent(in) :: map
```

```
integer, intent(in) :: num_calls
```

The number of sampling points.

```
integer, dimension(:), intent(in) :: num_div
```

Number of divisions of the adaptive grid in each dimension.

```
logical, intent(in) :: quadrupole
```

Allow “quadrupole oscillations” of the sampling grid (cf. section 2.3.1).

```
type(tao_random_state), intent(inout) :: rng
```

Unless otherwise noted, `rng` denotes the source of random numbers used for sampling in the documentation below.

```
real, intent(out) :: std_dev
```

The current best estimate of the error on the integral.

```
logical, intent(in) :: stratified
```

Try to use stratified sampling.

```
real(kind=default), dimension(:), intent(in) :: weights
```

```
...
```

4.2.3 Single Channel Procedures

```
subroutine vamp_create_grid (g, domain, num_calls
    [, quadrupole] [, stratified] [, covariance] [, map] [, exc])

    real, dimension(:, :), intent(in) :: domain

subroutine vamp_create_empty_grid (g)

subroutine vamp_discard_integral (g [, num_calls]
    [, stratified] [, quadrupole] [, covariance] [, exc])

subroutine vamp_reshape_grid (g [, num_calls] [, num_div]
    [, stratified] [, quadrupole] [, covariance] [, exc])

subroutine vamp_sample_grid (rng, g, func, iterations
    [, integral] [, std_dev] [, avg_chi2] [, accuracy] [, channel]
    [, weights] [, exc] [, history])

    func

     $S_n$  with  $n = \text{iterations}$ 

subroutine vamp_sample_grid0 (rng, g, func, [, channel]
    [, weights] [, exc])

    func

     $S_0$ 

subroutine vamp_refine_grid (g, [, exc])

    r

subroutine vamp_average_iterations (g, iteration, integral,
    std_dev, avg_chi2)

    integer, intent(in) :: iteration
    Number of iterations so far (needed for  $\chi^2$ ).

subroutine vamp_integrate (g, func, calls [, integral]
    [, std_dev] [, avg_chi2] [, accuracy] [, covariance])

    type(vamp_grid), intent(inout) :: g
    func
```

```

integer, dimension(:,:), intent(in) :: calls

subroutine vamp_integratex (region, func, calls [, integral]
[, std_dev] [, avg_chi2] [, stratified] [, accuracy] [, pancake]
[, cigar])

real, dimension(:,:), intent(in) :: region
func
integer, dimension(:,:), intent(in) :: calls
integer, intent(in) :: pancake
integer, intent(in) :: cigar

subroutine vamp_copy_grid (lhs, rhs)

type(vamp_grid), intent(inout) :: lhs
type(vamp_grid), intent(in) :: rhs

subroutine vamp_delete_grid (g)

type(vamp_grid), intent(inout) :: g

```

4.2.4 Inout/Output and Marshling

```

subroutine vamp_write_grid (g, [, ...])

type(vamp_grid), intent(inout) :: g

subroutine vamp_read_grid (g, [, ...])

type(vamp_grid), intent(inout) :: g

subroutine vamp_write_grids (g, [, ...])

type(vamp_grids), intent(inout) :: g

subroutine vamp_read_grids (g, [, ...])

type(vamp_grids), intent(inout) :: g

pure subroutine vamp_marshall_grid (g, integer_buffer,
double_buffer)

```

```

type(vamp_grid), intent(in) :: g
integer, dimension(:), intent(inout) ::
    integer_buffer
real(kind=default), dimension(:), intent(inout)
    :: double_buffer

```

Marshal the grid `g` in the integer array `integer_buffer` and the real array `double_buffer`, which must have at least the sizes obtained from call `vamp_marshall_grid_size (g, integer_size, double_size)`.



Note that we can not use the `transfer` intrinsic function for marshalling types that contain pointers that substitute for allocatable array components. `transfer` would copy the pointers in this case and not where they point to!

```

pure subroutine vamp_marshall_grid_size (g, integer_size,
    double_size)

```

```

type(vamp_grid), intent(in) :: g
integer :: words

```

Compute the sizes of the arrays required for marshaling the grid `g`.

```

pure subroutine vamp_unmarshal_grid (g, integer_buffer,
    double_buffer)

```

```

type(vamp_grid), intent(inout) :: g
integer, dimension(:), intent(in) ::
    integer_buffer
real(kind=default), dimension(:), intent(in) ::
    double_buffer

```

Marshaling and unmarshaling need to use two separate buffers for integers and floating point numbers. In a homogeneous network, the intrinsic procedure `transfer` could be used to store the floating point numbers in the integer array. In a heterogenous network this will fail. However, message passing environments provide methods for sending floating point numbers. For example, here's how to send a grid from process 0 to process 1 in MPI [12]

```

29 <MPI communication example 29>≡
    call vamp_marshall_grid_size (g, isize, dsize)

```

```

allocate (ibuf(isize), dbuf(dsize))
call mpi_comm_rank (MPI_COMM_WORLD, proc_id, errno)
select case (proc_id)
  case (0)
    call vamp_marshall_grid (g, ibuf, dbuf)
    call mpi_send (ibuf, size (ibuf), MPI_INTEGER, &
                  1, 1, MPI_COMM_WORLD, errno)
    call mpi_send (dbuf, size (dbuf), MPI_DOUBLE_PRECISION, &
                  1, 2, MPI_COMM_WORLD, errno)
  case (1)
    call mpi_recv (ibuf, size (ibuf), MPI_INTEGER, &
                  0, 1, MPI_COMM_WORLD, status, errno)
    call mpi_recv (dbuf, size (dbuf), MPI_DOUBLE_PRECISION, &
                  0, 2, MPI_COMM_WORLD, status, errno)
    call vamp_unmarshal_grid (g, ibuf, dbuf)
end select

```

assuming that double is such that MPI_DOUBLE_PRECISION corresponds to real(kind=default). The module `vampi` provides two high level functions `vamp_send_grid` and `vamp_receive_grid` that handle the low level details:

```

30  <MPI communication example' 30>≡
    call mpi_comm_rank (MPI_COMM_WORLD, proc_id, errno)
    select case (proc_id)
      case (0)
        call vamp_send_grid (g, 1, 0)
      case (1)
        call vamp_receive_grid (g, 0, 0)
    end select

    subroutine vamp_marshall_history_size (g, [, ...])

      type(vamp_grid), intent(inout) :: g

    subroutine vamp_marshall_history (g, [, ...])

      type(vamp_grid), intent(inout) :: g

    subroutine vamp_unmarshal_history (g, [, ...])

      type(vamp_grid), intent(inout) :: g

```

4.2.5 Multi Channel Procedures

$$g \circ \phi_i = \left| \frac{\partial \phi_i}{\partial x} \right|^{-1} \left(\alpha_i g_i + \sum_{\substack{j=1 \\ j \neq i}}^{N_c} \alpha_j (g_j \circ \pi_{ij}) \left| \frac{\partial \pi_{ij}}{\partial x} \right| \right). \quad (4.4)$$

31a \langle Interface declaration for phi 31a $\rangle \equiv$ (113 115 116b 136c 182c)

```
interface
  pure function phi (xi, channel) result (x)
    use kinds
    real(kind=default), dimension(:), intent(in) :: xi
    integer, intent(in) :: channel
    real(kind=default), dimension(size(xi)) :: x
  end function phi
end interface
```

31b \langle Interface declaration for ihp 31b $\rangle \equiv$ (113b)

```
interface
  pure function ihp (x, channel) result (xi)
    use kinds
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: channel
    real(kind=default), dimension(size(x)) :: xi
  end function ihp
end interface
```

31c \langle Interface declaration for jacobian 31c $\rangle \equiv$ (113)

```
interface
  pure function jacobian (x, data, channel) result (j)
    use kinds
    use vamp_grid_type !NODEP!
    import vamp_data_t
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: channel
    real(kind=default) :: j
  end function jacobian
end interface
```

```
function vamp_multi_channel (func, phi, ihp, jacobian, x,
  weights1, grids)
```

```
  real(kind=default), dimension(:), intent(in) :: x
```



```

real(kind=default), dimension(:), intent(in) ::
    weights
integer, intent(in) :: channel
type(vamp_grid), dimension(:), intent(in) :: grids

function vamp_multi_channel0 (func, phi, jacobian, x,
    weights1)

    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in) ::
        weights
    integer, intent(in) :: channel

subroutine vamp_check_jacobian (rng, n, channel, region,
    delta, [, x_delta])

    type(tao_random_state), intent(inout) :: rng
    integer, intent(in) :: n
    integer, intent(in) :: channel
    real(kind=default), dimension(:,:), intent(in) ::
        region
    real(kind=default), intent(out) :: delta
    real(kind=default), dimension(:), intent(out),
        optional :: x_delta

```

Verify that

$$g(\phi(x)) = \frac{1}{\left| \frac{\partial \phi}{\partial x} \right| (x)} \quad (4.5)$$

```

subroutine vamp_copy_grids (lhs, rhs)

    type(vamp_grids), intent(inout) :: lhs
    type(vamp_grids), intent(in) :: rhs

subroutine vamp_delete_grids (g)

    type(vamp_grids), intent(inout) :: g

```

```

subroutine vamp_create_grids (g, domain, num_calls, weights
[, maps] [, stratified])

    type(vamp_grids), intent(inout) :: g
    real, dimension(:,:), intent(in) :: domain
    integer, intent(in) :: num_calls
    real, dimension(:), intent(in) :: weights
    real, dimension(:,:,:), intent(in) :: maps

subroutine vamp_create_empty_grids (g)

    type(vamp_grids), intent(inout) :: g

subroutine vamp_discard_integrals (g [, num_calls]
[, stratified])

    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: num_calls

subroutine vamp_refine_weights (g [, power)

    type(vamp_grids), intent(inout) :: g
    real, intent(in) :: power

subroutine vamp_update_weights (g, weights [, num_calls]
[, stratified])

    type(vamp_grids), intent(inout) :: g
    real, dimension(:), intent(in) :: weights
    integer, intent(in) :: num_calls

subroutine vamp_reshape_grids (g, num_calls [, stratified])

    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: num_calls

subroutine vamp_reduce_channels (g, [, ...])

    type(vamp_grid), intent(inout) :: g

```

```

subroutine vamp_sample_grids (g, func, iterations [, integral]
    [, std_dev] [, accuracy] [, covariance] [, variance])

    type(vamp_grids), intent(inout) :: g
    func
    integer, intent(in) :: iterations

function vamp_sum_channels (x, weights, func)

    real, dimension(:), intent(in) :: x
    real, dimension(:), intent(in) :: weights
    func

```

4.2.6 Event Generation

```

subroutine vamp_next_event (g, [, ...])

subroutine vamp_warmup_grid (g, [, ...])

    type(vamp_grid), intent(inout) :: g
    func
    integer, intent(in) :: iterations

subroutine vamp_warmup_grids (g, [, ...])

    type(vamp_grids), intent(inout) :: g
    func
    integer, intent(in) :: iterations

```

4.2.7 Parallelization

```

subroutine vamp_fork_grid (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_join_grid (g, [, ...])

    type(vamp_grid), intent(inout) :: g

```

```

subroutine vamp_fork_grid_joints (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_sample_grid_parallel (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_distribute_work (g, [, ...])

    type(vamp_grid), intent(inout) :: g

```

4.2.8 Diagnostics

```

subroutine vamp_create_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_copy_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_delete_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_terminate_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_get_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_get_history_single (g, [, ...])

    type(vamp_grid), intent(inout) :: g

subroutine vamp_print_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g

```

 Discuss why the value of the integral in each channel differs.

4.2.9 *Other Procedures*

```
subroutine vamp_rigid_divisions (g, [, ...])  
    type(vamp_grid), intent(inout) :: g  
function vamp_get_covariance (g, [, ...])  
    type(vamp_grid), intent(inout) :: g  
subroutine vamp_nullify_covariance (g, [, ...])  
    type(vamp_grid), intent(inout) :: g  
function vamp_get_variance (g, [, ...])  
    type(vamp_grid), intent(inout) :: g  
subroutine vamp_nullify_variance (g, [, ...])  
    type(vamp_grid), intent(inout) :: g
```

4.2.10 *(Currently) Undocumented Procedures*

```
subroutine (... , [, ...])  
function (... , [, ...])
```

—5—

IMPLEMENTATION

5.1 *The Abstract Datatype `division`*

```
37a <divisions.f90 37a>≡
! divisions.f90 --
<Copyleft notice 1>
module divisions
  use kinds
  use exceptions
  use vamp_stat
  use utils
  use iso_fortran_env
  implicit none
  private
  <Declaration of divisions procedures 38a>
  <Interfaces of divisions procedures 61a>
  <Variables in divisions 46a>
  <Declaration of divisions types 37b>
  <Constants in divisions 64b>
contains
  <Implementation of divisions procedures 38b>
end module divisions
```



`vamp_apply_equivalences` from `vamp` accesses %variance ...

```
37b <Declaration of divisions types 37b>≡ (37a) 57e>
type, public :: division_t
! private
!!! Avoiding a g95 bug
real(kind=default), dimension(:), pointer :: x => null ()
real(kind=default), dimension(:), pointer :: integral => null ()
```

```

real(kind=default), dimension(:), pointer &
                                :: variance => null ()
!                                public :: variance => null ()
! real(kind=default), dimension(:), pointer :: efficiency => null ()
real(kind=default) :: x_min, x_max
real(kind=default) :: x_min_true, x_max_true
real(kind=default) :: dx, dxg
integer :: ng = 0
logical :: stratified = .true.
end type division_t

```

5.1.1 Creation, Manipulation & Injection

38a *<Declaration of divisions procedures 38a>*≡ (37a) 43a>

```

public :: create_division, create_empty_division
public :: copy_division, delete_division
public :: set_rigid_division, reshape_division

```

38b *<Implementation of divisions procedures 38b>*≡ (37a) 39a>

```

elemental subroutine create_division &
    (d, x_min, x_max, x_min_true, x_max_true)
type(division_t), intent(out) :: d
real(kind=default), intent(in) :: x_min, x_max
real(kind=default), intent(in), optional :: x_min_true, x_max_true
allocate (d%x(0:1), d%integral(1), d%variance(1))
! allocate (d%efficiency(1))
d%x(0) = 0.0
d%x(1) = 1.0
d%x_min = x_min
d%x_max = x_max
d%dx = d%x_max - d%x_min
d%stratified = .false.
d%ng = 1
d%dxg = 1.0 / d%ng
if (present (x_min_true)) then
    d%x_min_true = x_min_true
else
    d%x_min_true = x_min
end if
if (present (x_max_true)) then
    d%x_max_true = x_max_true
else
    d%x_max_true = x_max

```

```

end if
end subroutine create_division

```

39a *⟨Implementation of divisions procedures 38b⟩*+≡ (37a) <38b 39b>

```

elemental subroutine create_empty_division (d)
  type(division_t), intent(out) :: d
  nullify (d%x, d%integral, d%variance)
! nullify (d%efficiency)
end subroutine create_empty_division

```

39b *⟨Implementation of divisions procedures 38b⟩*+≡ (37a) <39a 39c>

```

elemental subroutine set_rigid_division (d, ng)
  type(division_t), intent(inout) :: d
  integer, intent(in) :: ng
  d%stratified = ng > 1
  d%ng = ng
  d%dxg = real (ubound (d%x, dim=1), kind=default) / d%ng
end subroutine set_rigid_division

```

$$dxg = \frac{n_{div}}{n_g} \quad (5.1)$$

such that $0 < \text{cell} \cdot dxg < n_{div}$

39c *⟨Implementation of divisions procedures 38b⟩*+≡ (37a) <39b 43b>

```

elemental subroutine reshape_division (d, max_num_div, ng, use_variance)
  type(division_t), intent(inout) :: d
  integer, intent(in) :: max_num_div
  integer, intent(in), optional :: ng
  logical, intent(in), optional :: use_variance
  real(kind=default), dimension(:), allocatable :: old_x, m
  integer :: num_div, equ_per_adap
  if (present (ng)) then
    if (max_num_div > 1) then
      d%stratified = ng > 1
    else
      d%stratified = .false.
    end if
  else
    d%stratified = .false.
  end if
  if (d%stratified) then
    d%ng = ng
    ⟨Initialize stratified sampling 42⟩

```



```

else
    num_div = max_num_div
    d%ng = 1
end if
d%dxg = real (num_div, kind=default) / d%ng
allocate (old_x(0:ubound(d%x,dim=1)), m(ubound(d%x,dim=1)))
old_x = d%x
⟨Set m to (1,1,...) or to rebinning weights from d%variance 40a⟩
⟨Resize arrays, iff necessary 40b⟩
d%x = rebin (m, old_x, num_div)
deallocate (old_x, m)
end subroutine reshape_division

```

40a ⟨Set m to (1,1,...) or to rebinning weights from d%variance 40a⟩≡ (39c)

```

if (present (use_variance)) then
    if (use_variance) then
        m = rebinning_weights (d%variance)
    else
        m = 1.0
    end if
else
    m = 1.0
end if

```

40b ⟨Resize arrays, iff necessary 40b⟩≡ (39c)

```

if (ubound (d%x, dim=1) /= num_div) then
    deallocate (d%x, d%integral, d%variance)
    ! deallocate (d%efficiency)
    allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
    ! allocate (d%efficiency(num_div))
end if

```

Genuinely stratified sampling will superimpose an equidistant grid on the adaptive grid, as shown in figure 5.2. Obviously, this is only possible when the number of cells of the stratification grid is large enough, specifically when $n_g \geq n_{\text{div}}^{\min} = n_{\text{div}}^{\max}/2 = 25$. This condition can be met by a high number of sampling points or by a low dimensionality of the integration region (cf. table 5.1).

For a low number of sampling points and high dimensions, genuinely stratified sampling is impossible, because we would have to reduce the number n_{div} of adaptive divisions too far. Instead, we keep `stratified` false which will tell the integration routine not to concentrate the grid in the regions where the contribution to the error is largest, but to use importance sampling,



Figure 5.1: **vegas** grid structure for non-stratified sampling. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.



Figure 5.2: **vegas** grid structure for genuinely stratified sampling, which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.

| n_{dim} | $N_{\text{calls}}^{\text{max}}(n_g = 25)$ |
|------------------|-------------------------------------------|
| 2 | $1 \cdot 10^3$ |
| 3 | $3 \cdot 10^4$ |
| 4 | $8 \cdot 10^5$ |
| 5 | $2 \cdot 10^7$ |
| 6 | $5 \cdot 10^8$ |

Table 5.1: To stratify or not to stratify.

i. e. concentrating the grid in the regions where the contribution to the value is largest.

In this case, the rigid grid is much coarser than the adaptive grid and furthermore, the boundaries of the cells overlap in general. The interplay of the two grids during the sampling process is shown in figure 5.3. First we determine the (integer) number k of equidistant divisions of an adaptive cell for at most $n_{\text{div}}^{\text{max}}$ divisions of the adaptive grid

$$k = \left\lfloor \frac{n_g}{n_{\text{div}}^{\text{max}}} \right\rfloor + 1 \quad (5.2a)$$

and the corresponding number n_{div} of adaptive divisions

$$n_{\text{div}} = \left\lfloor \frac{n_g}{k} \right\rfloor \quad (5.2b)$$

Finally, adjust n_g to an exact multiple of n_{div}

$$n_g = k \cdot n_{\text{div}} \quad (5.2c)$$

42 *⟨Initialize stratified sampling 42⟩*≡ (39c)

```

if (d%ng >= max_num_div / 2) then
  d%stratified = .true.
  equ_per_adap = d%ng / max_num_div + 1
  num_div = d%ng / equ_per_adap
  if (num_div < 2) then
    d%stratified = .false.
    num_div = 2
    d%ng = 1
  else if (mod (num_div,2) == 1) then
    num_div = num_div - 1
    d%ng = equ_per_adap * num_div
  else
    d%ng = equ_per_adap * num_div

```



Figure 5.3: One-dimensional illustration of the **vegas** grid structure for pseudo stratified sampling, which is used in high dimensions.

```

    end if
  else
    d%stratified = .false.
    num_div = max_num_div
    d%ng = 1
  end if

```

Figure 5.3 on page 43 is a one-dimensional illustration of the sampling algorithm. In each cell of the rigid equidistant grid, two random points are selected (or N_{calls} in the not stratified case). For each point, the corresponding cell and relative coordinate in the adaptive grid is found, *as if the adaptive grid was equidistant* (upper arrow). Then this point is mapped according to the adapted grid (lower arrow) and the proper Jacobians are applied to the weight.

$$\prod_{j=1}^n (x_i^j - x_{i-1}^j) \cdot N^n = \text{Vol}(\text{cell}') \cdot \frac{1}{\text{Vol}(\text{cell})} = \frac{1}{p(x_i^j)} \quad (5.3)$$

```

43a  <Declaration of divisions procedures 38a>+≡ (37a) <38a 44c>
      public :: inject_division, inject_division_short

43b  <Implementation of divisions procedures 38b>+≡ (37a) <39c 44b>
      elemental subroutine inject_division (d, r, cell, x, x_mid, idx, wgt)
        type(division_t), intent(in) :: d
        real(kind=default), intent(in) :: r
        integer, intent(in) :: cell
        real(kind=default), intent(out) :: x, x_mid
        integer, intent(out) :: idx
        real(kind=default), intent(out) :: wgt
        real(kind=default) :: delta_x, xi
        integer :: i
        xi = (cell - r) * d%dxg + 1.0
        <Set i, delta_x, x, and wgt from xi 44a>

```

```

    idx = i
    x_mid = d%x_min + 0.5 * (d%x(i-1) + d%x(i)) * d%dx
end subroutine inject_division

```

44a \langle Set i, delta_x, x, and wgt from xi 44a $\rangle \equiv$ (43b 44b)

```

    i = max (min (int (xi), ubound (d%x, dim=1)), 1)
    delta_x = d%x(i) - d%x(i-1)
    x = d%x_min + (d%x(i-1) + (xi - i) * delta_x) * d%dx
    wgt = delta_x * ubound (d%x, dim=1)

```

44b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 43b 44d \rangle

```

    elemental subroutine inject_division_short (d, r, x, idx, wgt)
    type(division_t), intent(in) :: d
    real(kind=default), intent(in) :: r
    integer, intent(out) :: idx
    real(kind=default), intent(out) :: x, wgt
    real(kind=default) :: delta_x, xi
    integer :: i
    xi = r * ubound (d%x, dim=1) + 1.0
     $\langle$ Set i, delta_x, x, and wgt from xi 44a $\rangle$ 
    idx = i
end subroutine inject_division_short

```

5.1.2 Grid Refinement

44c \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 43a 45c \rangle

```

    public :: record_integral, record_variance, clear_integral_and_variance
    ! public :: record_efficiency

```

44d \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 44b 44e \rangle

```

    elemental subroutine record_integral (d, i, f)
    type(division_t), intent(inout) :: d
    integer, intent(in) :: i
    real(kind=default), intent(in) :: f
    d%integral(i) = d%integral(i) + f
    if (.not. d%stratified) then
        d%variance(i) = d%variance(i) + f*f
    end if
end subroutine record_integral

```

44e \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 44d 45b \rangle

```

    elemental subroutine record_variance (d, i, var_f)

```

```

type(division_t), intent(inout) :: d
integer, intent(in) :: i
real(kind=default), intent(in) :: var_f
if (d%stratified) then
    d%variance(i) = d%variance(i) + var_f
end if
end subroutine record_variance

```

45a \langle Implementation of divisions procedures (removed from WHIZARD) 45a $\rangle \equiv$ 60b \rangle

```

elemental subroutine record_efficiency (d, i, eff)
    type(division_t), intent(inout) :: d
    integer, intent(in) :: i
    real(kind=default), intent(in) :: eff
    ! d%efficiency(i) = d%efficiency(i) + eff
end subroutine record_efficiency

```

45b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 44e 45d \rangle

```

elemental subroutine clear_integral_and_variance (d)
    type(division_t), intent(inout) :: d
    d%integral = 0.0
    d%variance = 0.0
    ! d%efficiency = 0.0
end subroutine clear_integral_and_variance

```

45c \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 44c 47a \rangle

```

public :: refine_division

```

45d \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 45b 46b \rangle

```

elemental subroutine refine_division (d)
    type(division_t), intent(inout) :: d
    character(len=*), parameter :: FN = "refine_division"
    d%x = rebin (rebinning_weights (d%variance), d%x, size (d%variance))
end subroutine refine_division

```

Smooth the $d_i = \bar{f}_i \Delta x_i$

$$\begin{aligned}
 d_1 &\rightarrow \frac{1}{2}(d_1 + d_2) \\
 d_2 &\rightarrow \frac{1}{3}(d_1 + d_2 + d_3) \\
 &\dots \\
 d_{n-1} &\rightarrow \frac{1}{3}(d_{n-2} + d_{n-1} + d_n) \\
 d_n &\rightarrow \frac{1}{2}(d_{n-1} + d_n)
 \end{aligned} \tag{5.4}$$

As long as the initial `num_div` ≥ 6 , we know that `num_div` ≥ 3 .

46a *<Variables in divisions 46a>* \equiv (37a) 59a>
`integer, private, parameter :: MIN_NUM_DIV = 3`

Here the Fortran90 array notation really shines, but we have to handle the cases `nd` ≤ 2 specially, because the `quadrupole` option can lead to small `nds`. The equivalent Fortran77 code [2] is orders of magnitude less obvious ¹ Also protect against vanishing d_i that will blow up the logarithm.

$$m_i = \left(\frac{\frac{\bar{f}_i \Delta x_i}{\sum_j \bar{f}_j \Delta x_j} - 1}{\ln \left(\frac{\bar{f}_i \Delta x_i}{\sum_j \bar{f}_j \Delta x_j} \right)} \right)^\alpha \quad (5.5)$$

46b *<Implementation of divisions procedures 38b>* \equiv (37a) <45d 47c>
`pure function rebinning_weights (d) result (m)`
`real(kind=default), dimension(:), intent(in) :: d`
`real(kind=default), dimension(size(d)) :: m`
`real(kind=default), dimension(size(d)) :: smooth_d`
`real(kind=default), parameter :: ALPHA = 1.5`
`integer :: nd`
`<Bail out if any (d == NaN) 47b>`
`nd = size (d)`
`if (nd > 2) then`
`smooth_d(1) = (d(1) + d(2)) / 2.0`
`smooth_d(2:nd-1) = (d(1:nd-2) + d(2:nd-1) + d(3:nd)) / 3.0`
`smooth_d(nd) = (d(nd-1) + d(nd)) / 2.0`
`else`
`smooth_d = d`
`end if`
`if (all (smooth_d < tiny (1.0_default))) then`
`m = 1.0_default`
`else`
`smooth_d = smooth_d / sum (smooth_d)`
`where (smooth_d < tiny (1.0_default))`
`smooth_d = tiny (1.0_default)`
`end where`
`where (smooth_d /= 1._default)`
`m = ((smooth_d - 1.0) / (log (smooth_d)))**ALPHA`
`elsewhere`
`m = 1.0_default`
`endwhere`
`end if`
`end function rebinning_weights`

¹Some old timers call this a feature, however.

47a \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \triangleleft 45c 47d \triangleright
 private :: rebinning_weights



The NaN test is probably not portable:

47b \langle Bail out if any (d == NaN) 47b $\rangle \equiv$ (46b)
 if (any (d /= d)) then
 m = 1.0
 return
 end if

Take a binning x and return a new binning with num_div bins with the m homogeneously distributed:

47c \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 46b 48c \triangleright
 pure function rebin (m, x, num_div) result (x_new)
 real(kind=default), dimension(:), intent(in) :: m
 real(kind=default), dimension(0:), intent(in) :: x
 integer, intent(in) :: num_div
 real(kind=default), dimension(0:num_div) :: x_new
 integer :: i, k
 real(kind=default) :: step, delta
 step = sum (m) / num_div
 k = 0
 delta = 0.0
 x_new(0) = x(0)
 do i = 1, num_div - 1
 \langle Increment k until $\sum m_k \geq \Delta$ and keep the surplus in δ 47e \rangle
 \langle Interpolate the new x_i from x_k and δ 48a \rangle
 end do
 x_new(num_div) = 1.0
 end function rebin

47d \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \triangleleft 47a 48b \triangleright
 private :: rebin

We increment k until another Δ (a.k.a. step) of the integral has been accumulated (cf. figure 5.4). The mismatch will be corrected below.

47e \langle Increment k until $\sum m_k \geq \Delta$ and keep the surplus in δ 47e $\rangle \equiv$ (47c)
 do
 if (step <= delta) then
 exit
 end if
 k = k + 1
 delta = delta + m(k)
 end do
 delta = delta - step

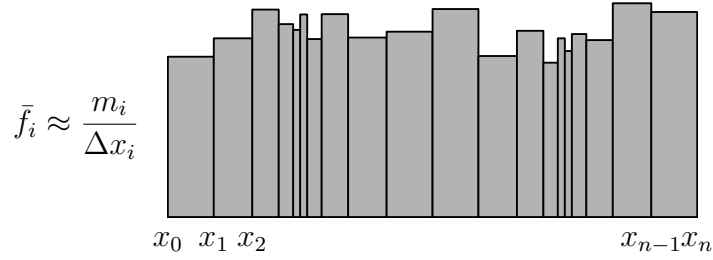


Figure 5.4: Typical weights used in the rebinning algorithm.

$$48a \quad \langle \text{Interpolate the new } x_i \text{ from } x_k \text{ and } \delta \text{ 48a} \rangle \equiv \quad (47c)$$

$$\mathbf{x_new}(i) = \mathbf{x}(k) - (\mathbf{x}(k) - \mathbf{x}(k-1)) * \mathbf{delta} / \mathbf{m}(k)$$

5.1.3 Probability Density

$$48b \quad \langle \text{Declaration of divisions procedures 38a} \rangle \equiv \quad (37a) \quad \langle 47d \quad 49a \rangle$$

$$\text{public} :: \text{probability}$$

$$\xi = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \in [0, 1] \quad (5.6)$$

and

$$\int_{x_{\min}}^{x_{\max}} dx p(x) = 1 \quad (5.7)$$

$$48c \quad \langle \text{Implementation of divisions procedures 38b} \rangle \equiv \quad (37a) \quad \langle 47c \quad 49b \rangle$$

```

elemental function probability (d, x) result (p)
  type(division_t), intent(in) :: d
  real(kind=default), intent(in) :: x
  real(kind=default) :: p
  real(kind=default) :: xi
  integer :: hi, mid, lo
  xi = (x - d%x_min) / d%dx
  if ((xi >= 0) .and. (xi <= 1)) then
    lo = lbound (d%x, dim=1)
    hi = ubound (d%x, dim=1)
    bracket: do
      if (lo >= hi - 1) then
        p = 1.0 / (ubound (d%x, dim=1) * d%dx * (d%x(hi) - d%x(hi-1)))
        return
      end if
      mid = (hi + lo) / 2
      if (xi > d%x(mid)) then

```

```

        lo = mid
    else
        hi = mid
    end if
end do bracket
else
    p = 0
end if
end function probability

```

5.1.4 *Quadrupole*

- 49a *<Declaration of divisions procedures 38a>+≡* (37a) <48b 49c>
 public :: **quadrupole_division**
- 49b *<Implementation of divisions procedures 38b>+≡* (37a) <48c 49d>
 elemental function **quadrupole_division** (d) result (q)
 type(**division_t**), intent(in) :: d
 real(kind=default) :: q
 !!! q = **value_spread_percent** (**rebinning_weights** (d%variance))
 q = **standard_deviation_percent** (**rebinning_weights** (d%variance))
 end function **quadrupole_division**

5.1.5 *Forking and Joining*

The goal is to split a division in such a way, that we can later sample the pieces separately and combine the results.

- 49c *<Declaration of divisions procedures 38a>+≡* (37a) <49a 54b>
 public :: **fork_division**, **join_division**, **sum_division**



Caveat emptor: splitting divisions can lead to **num_div** < 3 and the application *must not* try to refine such grids before merging them again!

- 49d *<Implementation of divisions procedures 38b>+≡* (37a) <49b 50>
 pure **subroutine fork_division** (d, ds, sum_calls, **num_calls**, exc)
 type(**division_t**), intent(in) :: d
 type(**division_t**), dimension(:), intent(inout) :: ds
 integer, intent(in) :: sum_calls
 integer, dimension(:), intent(inout) :: **num_calls**
 type(**exception**), intent(inout), optional :: exc
 character(len=*), parameter :: FN = "**fork_division**"
 integer, dimension(size(ds)) :: n0, n1
 integer, dimension(0:size(ds)) :: n, ds_ng

```

integer :: i, j, num_div, num_forks, nx
real(kind=default), dimension(:), allocatable :: d_x, d_integral, d_variance
! real(kind=default), dimension(:), allocatable :: d_efficiency
num_div = ubound (d%x, dim=1)
num_forks = size (ds)
if (d%ng == 1) then
    ⟨Fork an importance sampling division 51a⟩
else if (num_div >= num_forks) then
    if (modulo (d%ng, num_div) == 0) then
        ⟨Fork a pure stratified sampling division 51d⟩
    else
        ⟨Fork a pseudo stratified sampling division 53⟩
    end if
else
    if (present (exc)) then
        call raise_exception (exc, EXC_FATAL, FN, "internal error")
    end if
    num_calls = 0
end if
end subroutine fork_division

```

50 *⟨Implementation of divisions procedures 38b⟩*+≡ (37a) <49d 54c>

```

pure subroutine join_division (d, ds, exc)
type(division_t), intent(inout) :: d
type(division_t), dimension(:), intent(in) :: ds
type(exception), intent(inout), optional :: exc
character(len=*), parameter :: FN = "join_division"
integer, dimension(size(ds)) :: n0, n1
integer, dimension(0:size(ds)) :: n, ds_ng
integer :: i, j, num_div, num_forks, nx
real(kind=default), dimension(:), allocatable :: d_x, d_integral, d_variance
! real(kind=default), dimension(:), allocatable :: d_efficiency
num_div = ubound (d%x, dim=1)
num_forks = size (ds)
if (d%ng == 1) then
    ⟨Join importance sampling divisions 51b⟩
else if (num_div >= num_forks) then
    if (modulo (d%ng, num_div) == 0) then
        ⟨Join pure stratified sampling divisions 52a⟩
    else
        ⟨Join pseudo stratified sampling divisions 54a⟩
    end if
else
    if (present (exc)) then

```

```

        call raise_exception (exc, EXC_FATAL, FN, "internal error")
    end if
end if
end subroutine join_division

```

Importance Sampling

Importance sampling ($d\%ng == 1$) is trivial, since we can just sample `size(ds)` copies of the same grid with (almost) the same number of points

51a \langle Fork an importance sampling division 51a $\rangle \equiv$ (49d)

```

    if (d%stratified) then
        call raise_exception (exc, EXC_FATAL, FN, &
            "ng == 1 incompatible w/ stratification")
    else
        call copy_division (ds, d)
        num_calls(2:) = ceiling (real (sum_calls) / num_forks)
        num_calls(1) = sum_calls - sum (num_calls(2:))
    end if

```

and sum up the results in the end:

51b \langle Join importance sampling divisions 51b $\rangle \equiv$ (50)

```

    call sum_division (d, ds)

```

Note, however, that this is only legitimate as long as $d\%ng == 1$ implies $d\%stratified == .false.$, because otherwise the sampling code would be incorrect (cf. `var_f` on page 89).

Stratified Sampling

For stratified sampling, we have to work a little harder, because there are just two points per cell and we have to slice along the lines of the stratification grid. Actually, we are slicing along the adaptive grid, since it has a reasonable size. Slicing along the stratification grid could be done using the method below. However, in this case *very* large adaptive grids would be shipped from one process to the other and the communication costs will outweigh the gains from parallel processing.

51c \langle Setup to fork a pure stratified sampling division 51c $\rangle \equiv$ (51d 52a)

```

    n = (num_div * (/ (j, j=0,num_forks) /)) / num_forks
    n0(1:num_forks) = n(0:num_forks-1)
    n1(1:num_forks) = n(1:num_forks)

```

51d \langle Fork a pure stratified sampling division 51d $\rangle \equiv$ (49d)

```

     $\langle$ Setup to fork a pure stratified sampling division 51c $\rangle$ 
    do i = 1, num_forks

```

```

    call copy_array_pointer (ds(i)%x, d%x(n0(i):n1(i)), lb = 0)
    call copy_array_pointer (ds(i)%integral, d%integral(n0(i)+1:n1(i)))
    call copy_array_pointer (ds(i)%variance, d%variance(n0(i)+1:n1(i)))
    ! call copy_array_pointer (ds(i)%efficiency, d%efficiency(n0(i)+1:n1(i)))
    ds(i)%x = (ds(i)%x - ds(i)%x(0)) / (d%x(n1(i)) - d%x(n0(i)))
end do
ds%x_min = d%x_min + d%dx * d%x(n0)
ds%x_max = d%x_min + d%dx * d%x(n1)
ds%dx = ds%x_max - ds%x_min
ds%x_min_true = d%x_min_true
ds%x_max_true = d%x_max_true
ds%stratified = d%stratified
ds%ng = (d%ng * (n1 - n0)) / num_div
num_calls = sum_calls ! this is a misnomer, it remains "calls per cell" here
ds%dxg = real (n1 - n0, kind=default) / ds%ng

```

Joining is the exact inverse, but we're only interested in `d%integral` and `d%variance` for the grid refinement:

52a \langle Join pure stratified sampling divisions 52a $\rangle \equiv$ (50)
 \langle Setup to fork a pure stratified sampling division 51c \rangle
do i = 1, num_forks
 d%integral(n0(i)+1:n1(i)) = ds(i)%integral
 d%variance(n0(i)+1:n1(i)) = ds(i)%variance
 ! d%efficiency(n0(i)+1:n1(i)) = ds(i)%efficiency
end do

Pseudo Stratified Sampling

The coarsest grid covering the division of n_g bins into n_f forks has $n_g / \gcd(n_f, n_g) = \text{lcm}(n_f, n_g) / n_f$ bins per fork. Therefore, we need

$$\text{lcm} \left(\frac{\text{lcm}(n_f, n_g)}{n_f}, n_x \right) \quad (5.8)$$

divisions of the adaptive grid (if n_x is the number of bins in the original adaptive grid).

Life would be much easier, if we knew that n_f divides n_g . However, this is hard to maintain in real life applications. We can try to achieve this if possible, but the algorithms must be prepared to handle the general case.

52b \langle Setup to fork a pseudo stratified sampling division 52b $\rangle \equiv$ (53 54a)
nx = lcm (d%ng / gcd (num_forks, d%ng), num_div)
ds_ng = (d%ng * (/ (j, j=0,num_forks) /)) / num_forks
n = (nx * ds_ng) / d%ng



Figure 5.5: Forking one dimension d of a grid into three parts $ds(1)$, $ds(2)$, and $ds(3)$. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 5.3).

```

n0(1:num_forks) = n(0:num_forks-1)
n1(1:num_forks) = n(1:num_forks)

53  ⟨Fork a pseudo stratified sampling division 53⟩≡ (49d)
    ⟨Setup to fork a pseudo stratified sampling division 52b⟩
    allocate (d_x(0:nx), d_integral(nx), d_variance(nx))
    ! allocate (d_efficiency(nx))
    call subdivide (d_x, d%x)
    call distribute (d_integral, d%integral)
    call distribute (d_variance, d%variance)
    ! call distribute (d_efficiency, d%efficiency)
    do i = 1, num_forks
        call copy_array_pointer (ds(i)%x, d_x(n0(i):n1(i)), lb = 0)
        call copy_array_pointer (ds(i)%integral, d_integral(n0(i)+1:n1(i)))
        call copy_array_pointer (ds(i)%variance, d_variance(n0(i)+1:n1(i)))
        ! call copy_array_pointer (ds(i)%efficiency, d_efficiency(n0(i)+1:n1(i)))
        ds(i)%x = (ds(i)%x - ds(i)%x(0)) / (d_x(n1(i)) - d_x(n0(i)))
    end do
    ds%x_min = d%x_min + d%dx * d_x(n0)
    ds%x_max = d%x_min + d%dx * d_x(n1)

```

```

ds%dx = ds%x_max - ds%x_min
ds%x_min_true = d%x_min_true
ds%x_max_true = d%x_max_true
ds%stratified = d%stratified
ds%ng = ds_ng(1:num_forks) - ds_ng(0:num_forks-1)
num_calls = sum_calls ! this is a misnomer, it remains "calls per cell" here
ds%dxg = real (n1 - n0, kind=default) / ds%ng
deallocate (d_x, d_integral, d_variance)
! deallocate (d_efficiency)

54a <Join pseudo stratified sampling divisions 54a>≡ (50)
    <Setup to fork a pseudo stratified sampling division 52b>
    allocate (d_x(0:nx), d_integral(nx), d_variance(nx))
    ! allocate (d_efficiency(nx))
    do i = 1, num_forks
        d_integral(n0(i)+1:n1(i)) = ds(i)%integral
        d_variance(n0(i)+1:n1(i)) = ds(i)%variance
        ! d_efficiency(n0(i)+1:n1(i)) = ds(i)%efficiency
    end do
    call collect (d%integral, d_integral)
    call collect (d%variance, d_variance)
    ! call collect (d%efficiency, d_efficiency)
    deallocate (d_x, d_integral, d_variance)
    ! deallocate (d_efficiency)

54b <Declaration of divisions procedures 38a>+≡ (37a) <49c 55c>
    private :: subdivide
    private :: distribute
    private :: collect

54c <Implementation of divisions procedures 38b>+≡ (37a) <50 54d>
    pure subroutine subdivide (x, x0)
        real(kind=default), dimension(0:), intent(inout) :: x
        real(kind=default), dimension(0:), intent(in) :: x0
        integer :: i, n, n0
        n0 = ubound (x0, dim=1)
        n = ubound (x, dim=1) / n0
        x(0) = x0(0)
        do i = 1, n
            x(i:n) = x0(0:n0-1) * real (n - i) / n + x0(1:n0) * real (i) / n
        end do
    end subroutine subdivide

54d <Implementation of divisions procedures 38b>+≡ (37a) <54c 55a>
    pure subroutine distribute (x, x0)
        real(kind=default), dimension(:), intent(inout) :: x

```

```

    real(kind=default), dimension(:), intent(in) :: x0
    integer :: i, n
    n = ubound (x, dim=1) / ubound (x0, dim=1)
    do i = 1, n
        x(i:n) = x0 / n
    end do
end subroutine distribute

```

55a *<Implementation of divisions procedures 38b>+≡* (37a) <54d 55b>

```

pure subroutine collect (x0, x)
    real(kind=default), dimension(:), intent(inout) :: x0
    real(kind=default), dimension(:), intent(in) :: x
    integer :: i, n, n0
    n0 = ubound (x0, dim=1)
    n = ubound (x, dim=1) / n0
    do i = 1, n0
        x0(i) = sum (x((i-1)*n+1:i*n))
    end do
end subroutine collect

```

Trivia

55b *<Implementation of divisions procedures 38b>+≡* (37a) <55a 55d>

```

pure subroutine sum_division (d, ds)
    type(division_t), intent(inout) :: d
    type(division_t), dimension(:), intent(in) :: ds
    integer :: i
    d%integral = 0.0
    d%variance = 0.0
    ! d%efficiency = 0.0
    do i = 1, size (ds)
        d%integral = d%integral + ds(i)%integral
        d%variance = d%variance + ds(i)%variance
        ! d%efficiency = d%efficiency + ds(i)%efficiency
    end do
end subroutine sum_division

```

55c *<Declaration of divisions procedures 38a>+≡* (37a) <54b 56b>

```

public :: debug_division
public :: dump_division

```

55d *<Implementation of divisions procedures 38b>+≡* (37a) <55b 56a>

```

subroutine debug_division (d, prefix)
    type(division_t), intent(in) :: d
    character(len=*), intent(in) :: prefix

```



```

print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%x: ", &
    lbound(d%x,dim=1), d%x(lbound(d%x,dim=1)), &
    " ... ", &
    ubound(d%x,dim=1), d%x(ubound(d%x,dim=1))
print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%i: ", &
    lbound(d%integral,dim=1), d%integral(lbound(d%integral,dim=1)), &
    " ... ", &
    ubound(d%integral,dim=1), d%integral(ubound(d%integral,dim=1))
print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%v: ", &
    lbound(d%variance,dim=1), d%variance(lbound(d%variance,dim=1)), &
    " ... ", &
    ubound(d%variance,dim=1), d%variance(ubound(d%variance,dim=1))
! print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%e: ", &
!     lbound(d%efficiency,dim=1), d%efficiency(lbound(d%efficiency,dim=1)), &
!     " ... ", &
!     ubound(d%efficiency,dim=1), d%efficiency(ubound(d%efficiency,dim=1))
end subroutine debug_division

```

56a *<Implementation of divisions procedures 38b>+≡* (37a) *<55d 56c>*

```

subroutine dump_division (d, prefix)
    type(division_t), intent(in) :: d
    character(len=*), intent(in) :: prefix
! print "(2(1x,a),100(1x,f10.7))", prefix, ":x: ", d%x
    print "(2(1x,a),100(1x,f10.7))", prefix, ":x: ", d%x(1:)
    print "(2(1x,a),100(1x,e10.3))", prefix, ":i: ", d%integral
    print "(2(1x,a),100(1x,e10.3))", prefix, ":v: ", d%variance
! print "(2(1x,a),100(1x,e10.3))", prefix, ":e: ", d%efficiency
end subroutine dump_division

```

5.1.6 Inquiry

Trivial, but necessary for making divisions an abstract data type:

56b *<Declaration of divisions procedures 38a>+≡* (37a) *<55c 57f>*

```

public :: inside_division, stratified_division
public :: volume_division, rigid_division, adaptive_division

```

56c *<Implementation of divisions procedures 38b>+≡* (37a) *<56a 57a>*

```

elemental function inside_division (d, x) result (theta)
    type(division_t), intent(in) :: d
    real(kind=default), intent(in) :: x
    logical :: theta
    theta = (x >= d%x_min_true) .and. (x <= d%x_max_true)
end function inside_division

```

57a \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 56c 57b \rangle
 elemental function **stratified_division** (d) result (yorn)
 type(**division_t**), intent(in) :: d
 logical :: yorn
 yorn = d%**stratified**
 end function **stratified_division**

57b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57a 57c \rangle
 elemental function **volume_division** (d) result (vol)
 type(**division_t**), intent(in) :: d
 real(kind=default) :: vol
 vol = d%**dx**
 end function **volume_division**

57c \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57b 57d \rangle
 elemental function **rigid_division** (d) result (n)
 type(**division_t**), intent(in) :: d
 integer :: n
 n = d%**ng**
 end function **rigid_division**

57d \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57c 57g \rangle
 elemental function **adaptive_division** (d) result (n)
 type(**division_t**), intent(in) :: d
 integer :: n
 n = ubound (d%**x**, dim=1)
 end function **adaptive_division**

5.1.7 Diagnostics

57e \langle Declaration of divisions types 37b $\rangle + \equiv$ (37a) \langle 37b \rangle
 type, public :: **div_history**
 private
 logical :: **stratified**
 integer :: **ng**, **num_div**
 real(kind=default) :: x_min, x_max, x_min_true, x_max_true
 real(kind=default) :: &
 spread_f_p, **stddev_f_p**, **spread_p**, **stddev_p**, **spread_m**, **stddev_m**
 end type **div_history**

57f \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 56b 58a \rangle
 public :: **copy_history**, **summarize_division**

57g \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57d 58b \rangle
 elemental function **summarize_division** (d) result (s)
 type(**division_t**), intent(in) :: d

```

type(div_history) :: s
real(kind=default), dimension(:), allocatable :: p, m
allocate (p(ubound(d%x,dim=1)), m(ubound(d%x,dim=1)))
p = probabilities (d%x)
m = rebinning_weights (d%variance)
s%ng = d%ng
s%num_div = ubound (d%x, dim=1)
s%stratified = d%stratified
s%x_min = d%x_min
s%x_max = d%x_max
s%x_min_true = d%x_min_true
s%x_max_true = d%x_max_true
s%spread_f_p = value_spread_percent (d%integral)
s%stddev_f_p = standard_deviation_percent (d%integral)
s%spread_p = value_spread_percent (p)
s%stddev_p = standard_deviation_percent (p)
s%spread_m = value_spread_percent (m)
s%stddev_m = standard_deviation_percent (m)
deallocate (p, m)
end function summarize_division

```

58a *<Declaration of divisions procedures 38a>+≡* (37a) <57f 59b>
private :: **probabilities**

58b *<Implementation of divisions procedures 38b>+≡* (37a) <57g 58c>
pure function **probabilities** (x) result (p)
real(kind=default), dimension(0:), intent(in) :: x
real(kind=default), dimension(ubound(x,dim=1)) :: p
integer :: **num_div**
num_div = ubound (x, dim=1)
p = 1.0 / (x(1:**num_div**) - x(0:**num_div**-1))
p = p / sum(p)
end function **probabilities**

58c *<Implementation of divisions procedures 38b>+≡* (37a) <58b 58d>
subroutine print_history (h, tag)
type(**div_history**), dimension(:), intent(in) :: h
character(len=*), intent(in), optional :: tag
call **write_history** (output_unit, h, tag)
flush (output_unit)
end **subroutine print_history**

58d *<Implementation of divisions procedures 38b>+≡* (37a) <58c 61b>
subroutine write_history (u, h, tag)
integer, intent(in) :: u
type(**div_history**), dimension(:), intent(in) :: h

```

character(len=*), intent(in), optional :: tag
character(len=BUFFER_SIZE) :: pfx
character(len=1) :: s
integer :: i
if (present (tag)) then
    pfx = tag
else
    pfx = "[vamp]"
end if
if ((minval (h%x_min) == maxval (h%x_min)) &
    .and. (minval (h%x_max) == maxval (h%x_max))) then
    write (u, "(1X,A11,1X,2X,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
        h(1)%x_min, " <= ", h(1)%x_min_true, &
        " < x < ", h(1)%x_max_true, " <= ", h(1)%x_max
else
    do i = 1, size (h)
        write (u, "(1X,A11,1X,I2,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
            i, h(i)%x_min, " <= ", h(i)%x_min_true, &
            " < x < ", h(i)%x_max_true, " <= ", h(i)%x_max
    end do
end if
write (u, "(1X,A11,1X,A2,2(1X,A3),A1,6(1X,A8))") pfx, &
    "it", "nd", "ng", "", &
    "spr(f/p)", "dev(f/p)", "spr(m)", "dev(m)", "spr(p)", "dev(p)"
iterations: do i = 1, size (h)
    if (h(i)%stratified) then
        s = "*"
    else
        s = ""
    end if
    write (u, "(1X,A11,1X,I2,2(1X,I3),A1,6(1X,F7.2,A1))") pfx, &
        i, h(i)%num_div, h(i)%ng, s, &
        h(i)%spread_f_p, "%", h(i)%stddev_f_p, "%", &
        h(i)%spread_m, "%", h(i)%stddev_m, "%", &
        h(i)%spread_p, "%", h(i)%stddev_p, "%"
end do iterations
flush (u)
end subroutine write_history

```

59a *<Variables in divisions 46a>*+≡ (37a) <46a 62a>

```
integer, private, parameter :: BUFFER_SIZE = 50
```

59b *<Declaration of divisions procedures 38a>*+≡ (37a) <58a 60f>

```
public :: print_history, write_history
```

60a *<Declaration of divisions procedures (removed from WHIZARD) 60a>*≡
 public :: **division_x**, **division_integral**
 public :: **division_variance**, **division_efficiency**

60b *<Implementation of divisions procedures (removed from WHIZARD) 45a>*+≡ <45a 60c>
 pure **subroutine division_x** (x, d)
 real(kind=default), dimension(:), pointer :: **x**
 type(**division_t**), intent(in) :: d
 call **copy_array_pointer** (x, d%x, 0)
 end **subroutine division_x**

60c *<Implementation of divisions procedures (removed from WHIZARD) 45a>*+≡ <60b 60d>
 pure **subroutine division_integral** (**integral**, d)
 real(kind=default), dimension(:), pointer :: **integral**
 type(**division_t**), intent(in) :: d
 call **copy_array_pointer** (**integral**, d%**integral**)
 end **subroutine division_integral**

60d *<Implementation of divisions procedures (removed from WHIZARD) 45a>*+≡ <60c 60e>
 pure **subroutine division_variance** (**variance**, d)
 real(kind=default), dimension(:), pointer :: **variance**
 type(**division_t**), intent(in) :: d
 call **copy_array_pointer** (**variance**, d%**variance**, 0)
 end **subroutine division_variance**

60e *<Implementation of divisions procedures (removed from WHIZARD) 45a>*+≡ <60d
 pure **subroutine division_efficiency** (**eff**, d)
 real(kind=default), dimension(:), pointer :: **eff**
 type(**division_t**), intent(in) :: d
 call **copy_array_pointer** (**eff**, d%**efficiency**, 0)
 end **subroutine division_efficiency**

5.1.8 I/O

60f *<Declaration of divisions procedures 38a>*+≡ (37a) <59b 66b>
 public :: **write_division**
 private :: **write_division_unit**, **write_division_name**
 public :: **read_division**
 private :: **read_division_unit**, **read_division_name**
 public :: **write_division_raw**
 private :: **write_division_raw_unit**, **write_division_raw_name**
 public :: **read_division_raw**
 private :: **read_division_raw_unit**, **read_division_raw_name**

61a \langle Interfaces of divisions procedures 61a $\rangle \equiv$ (37a)

```

interface write_division
    module procedure write_division_unit, write_division_name
end interface
interface read_division
    module procedure read_division_unit, read_division_name
end interface
interface write_division_raw
    module procedure write_division_raw_unit, write_division_raw_name
end interface
interface read_division_raw
    module procedure read_division_raw_unit, read_division_raw_name
end interface

```

It makes no sense to read or write `d%integral`, `d%variance`, and `d%efficiency`, because they are only used during sampling.

61b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 58d 62b \rangle

```

subroutine write_division_unit (d, unit, write_integrals)
    type(division_t), intent(in) :: d
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    logical :: write_integrals0
    integer :: i
    write_integrals0 = .false.
    if (present(write_integrals)) write_integrals0 = write_integrals
    write (unit = unit, fmt = descr_fmt) "begin type(division_t) :: d"
    write (unit = unit, fmt = integer_fmt) "ubound(d%x,1) = ", ubound (d%x, dim=1)
    write (unit = unit, fmt = integer_fmt) "d%ng = ", d%ng
    write (unit = unit, fmt = logical_fmt) "d%stratified = ", d%stratified
    write (unit = unit, fmt = double_fmt) "d%dx = ", d%dx
    write (unit = unit, fmt = double_fmt) "d%dxg = ", d%dxg
    write (unit = unit, fmt = double_fmt) "d%x_min = ", d%x_min
    write (unit = unit, fmt = double_fmt) "d%x_max = ", d%x_max
    write (unit = unit, fmt = double_fmt) "d%x_min_true = ", d%x_min_true
    write (unit = unit, fmt = double_fmt) "d%x_max_true = ", d%x_max_true
    write (unit = unit, fmt = descr_fmt) "begin d%x"
    do i = 0, ubound (d%x, dim=1)
        if (write_integrals0 .and. i/=0) then
            write (unit = unit, fmt = double_array_fmt) &
                i, d%x(i), d%integral(i), d%variance(i)
        else
            write (unit = unit, fmt = double_array_fmt) i, d%x(i)
        end if
    end do
end do

```

```

        write (unit = unit, fmt = descr_fmt) "end d%x"
        write (unit = unit, fmt = descr_fmt) "end type(division_t)"
    end subroutine write_division_unit
62a  <Variables in divisions 46a>+≡ (37a) <59a
        character(len=*), parameter, private :: &
            descr_fmt =      "(1x,a)", &
            integer_fmt =    "(1x,a15,1x,i15)", &
            logical_fmt =    "(1x,a15,1x,l1)", &
            double_fmt =     "(1x,a15,1x,e30.22)", &
            double_array_fmt = "(1x,i15,1x,3(e30.22))"
62b  <Implementation of divisions procedures 38b>+≡ (37a) <61b 63b>
        subroutine read_division_unit (d, unit, read_integrals)
            type(division_t), intent(inout) :: d
            integer, intent(in) :: unit
            logical, intent(in), optional :: read_integrals
            logical :: read_integrals0
            integer :: i, idum, num_div
            character(len=80) :: chdum
            read_integrals0 = .false.
            if (present(read_integrals)) read_integrals0 = read_integrals
            read (unit = unit, fmt = descr_fmt) chdum
            read (unit = unit, fmt = integer_fmt) chdum, num_div
            <Insure that ubound (d%x, dim=1) == num_div 63a>
            read (unit = unit, fmt = integer_fmt) chdum, d%ng
            read (unit = unit, fmt = logical_fmt) chdum, d%stratified
            read (unit = unit, fmt = double_fmt) chdum, d%dx
            read (unit = unit, fmt = double_fmt) chdum, d%dxg
            read (unit = unit, fmt = double_fmt) chdum, d%x_min
            read (unit = unit, fmt = double_fmt) chdum, d%x_max
            read (unit = unit, fmt = double_fmt) chdum, d%x_min_true
            read (unit = unit, fmt = double_fmt) chdum, d%x_max_true
            read (unit = unit, fmt = descr_fmt) chdum
            do i = 0, ubound (d%x, dim=1)
                if (read_integrals0 .and. i/=0) then
                    read (unit = unit, fmt = double_array_fmt) &
                        & idum, d%x(i), d%integral(i), d%variance(i)
                else
                    read (unit = unit, fmt = double_array_fmt) idum, d%x(i)
                end if
            end do
            read (unit = unit, fmt = descr_fmt) chdum
            read (unit = unit, fmt = descr_fmt) chdum
            if (.not.read_integrals0) then

```

```

        d%integral = 0.0
        d%variance = 0.0
!       d%efficiency = 0.0
    end if
end subroutine read_division_unit

```



What happened to d%efficiency?

- 63a *<Insure that ubound (d%x, dim=1) == num_div 63a>≡* (62b 64c 67b)
- ```

 if (associated (d%x)) then
 if (ubound (d%x, dim=1) /= num_div) then
 deallocate (d%x, d%integral, d%variance)
! deallocate (d%efficiency)
 allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
! allocate (d%efficiency(num_div))
 end if
 else
 allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
! allocate (d%efficiency(num_div))
 end if

```
- 63b *<Implementation of divisions procedures 38b>+≡* (37a) <62b 63c>
- ```

subroutine write_division_name (d, name, write_integrals)
    type(division_t), intent(in) :: d
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: write_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "write", status = "replace", file = name)
    call write_division_unit (d, unit, write_integrals)
    close (unit = unit)
end subroutine write_division_name

```
- 63c *<Implementation of divisions procedures 38b>+≡* (37a) <63b 64a>
- ```

subroutine read_division_name (d, name, read_integrals)
 type(division_t), intent(inout) :: d
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: read_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", file = name)
 call read_division_unit (d, unit, read_integrals)
 close (unit = unit)
end subroutine read_division_name

```



64a *<Implementation of divisions procedures 38b>+≡* (37a) <63c 64c>

```

subroutine write_division_raw_unit (d, unit, write_integrals)
 type(division_t), intent(in) :: d
 integer, intent(in) :: unit
 logical, intent(in), optional :: write_integrals
 logical :: write_integrals0
 integer :: i
 write_integrals0 = .false.
 if (present(write_integrals)) write_integrals0 = write_integrals
 write (unit = unit) MAGIC_DIVISION_BEGIN
 write (unit = unit) ubound (d%x, dim=1)
 write (unit = unit) d%ng
 write (unit = unit) d%stratified
 write (unit = unit) d%dx
 write (unit = unit) d%dxg
 write (unit = unit) d%x_min
 write (unit = unit) d%x_max
 write (unit = unit) d%x_min_true
 write (unit = unit) d%x_max_true
 do i = 0, ubound (d%x, dim=1)
 if (write_integrals0 .and. i/=0) then
 write (unit = unit) d%x(i), d%integral(i), d%variance(i)
 else
 write (unit = unit) d%x(i)
 end if
 end do
 write (unit = unit) MAGIC_DIVISION_END
end subroutine write_division_raw_unit

```

64b *<Constants in divisions 64b>≡* (37a)

```

integer, parameter, private :: MAGIC_DIVISION = 11111111
integer, parameter, private :: MAGIC_DIVISION_BEGIN = MAGIC_DIVISION + 1
integer, parameter, private :: MAGIC_DIVISION_END = MAGIC_DIVISION + 2

```

64c *<Implementation of divisions procedures 38b>+≡* (37a) <64a 65>

```

subroutine read_division_raw_unit (d, unit, read_integrals)
 type(division_t), intent(inout) :: d
 integer, intent(in) :: unit
 logical, intent(in), optional :: read_integrals
 logical :: read_integrals0
 integer :: i, num_div, magic
 character(len=*), parameter :: FN = "read_division_raw_unit"
 read_integrals0 = .false.
 if (present(read_integrals)) read_integrals0 = read_integrals
 read (unit = unit) magic

```

```

if (magic /= MAGIC_DIVISION_BEGIN) then
 print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_BEGIN, &
 ", found ", magic
 stop
end if
read (unit = unit) num_div
<Insure that ubound (d%x, dim=1) == num_div 63a>
read (unit = unit) d%ng
read (unit = unit) d%stratified
read (unit = unit) d%dx
read (unit = unit) d%dxg
read (unit = unit) d%x_min
read (unit = unit) d%x_max
read (unit = unit) d%x_min_true
read (unit = unit) d%x_max_true
do i = 0, ubound (d%x, dim=1)
 if (read_integrals0 .and. i/=0) then
 read (unit = unit) d%x(i), d%integral(i), d%variance(i)
 else
 read (unit = unit) d%x(i)
 end if
end do
if (.not.read_integrals0) then
 d%integral = 0.0
 d%variance = 0.0
! d%efficiency = 0.0
end if
read (unit = unit) magic
if (magic /= MAGIC_DIVISION_END) then
 print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_END, &
 ", found ", magic
 stop
end if
end subroutine read_division_raw_unit

```

65 <Implementation of divisions procedures 38b>+≡ (37a) <64c 66a>

```

subroutine write_division_raw_name (d, name, write_integrals)
 type(division_t), intent(in) :: d
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: write_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", &
 form = "unformatted", file = name)

```

```

 call write_division_unit (d, unit, write_integrals)
 close (unit = unit)
 end subroutine write_division_raw_name
66a <Implementation of divisions procedures 38b>+≡ (37a) <65 66c>
 subroutine read_division_raw_name (d, name, read_integrals)
 type(division_t), intent(inout) :: d
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: read_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", &
 form = "unformatted", file = name)
 call read_division_unit (d, unit, read_integrals)
 close (unit = unit)
 end subroutine read_division_raw_name

```

### 5.1.9 Marshaling

Note that we can not use the transfer intrinsic function for marshalling types that contain pointers that substitute for allocatable array components. transfer will copy the pointers in this case and not where they point to!

```

66b <Declaration of divisions procedures 38a>+≡ (37a) <60f 67c>
 public :: marshal_division_size, marshal_division, unmarshal_division
66c <Implementation of divisions procedures 38b>+≡ (37a) <66a 67a>
 pure subroutine marshal_division (d, ibuf, dbuf)
 type(division_t), intent(in) :: d
 integer, dimension(:), intent(inout) :: ibuf
 real(kind=default), dimension(:), intent(inout) :: dbuf
 integer :: num_div
 num_div = ubound (d%x, dim=1)
 ibuf(1) = d%ng
 ibuf(2) = num_div
 if (d%stratified) then
 ibuf(3) = 1
 else
 ibuf(3) = 0
 end if
 dbuf(1) = d%x_min
 dbuf(2) = d%x_max
 dbuf(3) = d%x_min_true
 dbuf(4) = d%x_max_true
 dbuf(5) = d%dx
 end subroutine marshal_division

```

```

 dbuf(6) = d%dxg
 dbuf(7:7+num_div) = d%x
 dbuf(8+ num_div:7+2*num_div) = d%integral
 dbuf(8+2*num_div:7+3*num_div) = d%variance
 ! dbuf(8+3*num_div:7+4*num_div) = d%efficiency
end subroutine marshal_division

```

67a *<Implementation of divisions procedures 38b>+≡* (37a) <66c 67b>

```

pure subroutine marshal_division_size (d, iwords, dwords)
 type(division_t), intent(in) :: d
 integer, intent(out) :: iwords, dwords
 iwords = 3
 dwords = 7 + 3 * ubound (d%x, dim=1)
 ! dwords = 7 + 4 * ubound (d%x, dim=1)
end subroutine marshal_division_size

```

67b *<Implementation of divisions procedures 38b>+≡* (37a) <67a 67d>

```

pure subroutine unmarshal_division (d, ibuf, dbuf)
 type(division_t), intent(inout) :: d
 integer, dimension(:), intent(in) :: ibuf
 real(kind=default), dimension(:), intent(in) :: dbuf
 integer :: num_div
 d%ng = ibuf(1)
 num_div = ibuf(2)
 d%stratified = ibuf(3) /= 0
 d%x_min = dbuf(1)
 d%x_max = dbuf(2)
 d%x_min_true = dbuf(3)
 d%x_max_true = dbuf(4)
 d%dx = dbuf(5)
 d%dxg = dbuf(6)
 <Insure that ubound (d%x, dim=1) == num_div 63a>
 d%x = dbuf(7:7+num_div)
 d%integral = dbuf(8+ num_div:7+2*num_div)
 d%variance = dbuf(8+2*num_div:7+3*num_div)
 ! d%efficiency = dbuf(8+3*num_div:7+4*num_div)
end subroutine unmarshal_division

```

67c *<Declaration of divisions procedures 38a>+≡* (37a) <66b  
 public :: marshal\_div\_history\_size, marshal\_div\_history, unmarshal\_div\_history

67d *<Implementation of divisions procedures 38b>+≡* (37a) <67b 68a>

```

pure subroutine marshal_div_history (h, ibuf, dbuf)
 type(div_history), intent(in) :: h
 integer, dimension(:), intent(inout) :: ibuf
 real(kind=default), dimension(:), intent(inout) :: dbuf

```

```

 ibuf(1) = h%ng
 ibuf(2) = h%num_div
 if (h%stratified) then
 ibuf(3) = 1
 else
 ibuf(3) = 0
 end if
 dbuf(1) = h%x_min
 dbuf(2) = h%x_max
 dbuf(3) = h%x_min_true
 dbuf(4) = h%x_max_true
 dbuf(5) = h%spread_f_p
 dbuf(6) = h%stddev_f_p
 dbuf(7) = h%spread_p
 dbuf(8) = h%stddev_p
 dbuf(9) = h%spread_m
 dbuf(10) = h%stddev_m
end subroutine marshal_div_history
68a <Implementation of divisions procedures 38b>+≡ (37a) <67d 68b>
pure subroutine marshal_div_history_size (h, iwords, dwords)
 type(div_history), intent(in) :: h
 integer, intent(out) :: iwords, dwords
 iwords = 3
 dwords = 10
end subroutine marshal_div_history_size
68b <Implementation of divisions procedures 38b>+≡ (37a) <68a 69a>
pure subroutine unmarshal_div_history (h, ibuf, dbuf)
 type(div_history), intent(inout) :: h
 integer, dimension(:), intent(in) :: ibuf
 real(kind=default), dimension(:), intent(in) :: dbuf
 h%ng = ibuf(1)
 h%num_div = ibuf(2)
 h%stratified = ibuf(3) /= 0
 h%x_min = dbuf(1)
 h%x_max = dbuf(2)
 h%x_min_true = dbuf(3)
 h%x_max_true = dbuf(4)
 h%spread_f_p = dbuf(5)
 h%stddev_f_p = dbuf(6)
 h%spread_p = dbuf(7)
 h%stddev_p = dbuf(8)
 h%spread_m = dbuf(9)
 h%stddev_m = dbuf(10)

```

end subroutine unmarshal\_div\_history

### 5.1.10 Boring Copying and Deleting of Objects

69a  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$  (37a)  $\langle$ 68b 69b $\rangle$

```

elemental subroutine copy_division (lhs, rhs)
 type(division_t), intent(inout) :: lhs
 type(division_t), intent(in) :: rhs
 if (associated (rhs%x)) then
 call copy_array_pointer (lhs%x, rhs%x, lb = 0)
 else if (associated (lhs%x)) then
 deallocate (lhs%x)
 end if
 if (associated (rhs%integral)) then
 call copy_array_pointer (lhs%integral, rhs%integral)
 else if (associated (lhs%integral)) then
 deallocate (lhs%integral)
 end if
 if (associated (rhs%variance)) then
 call copy_array_pointer (lhs%variance, rhs%variance)
 else if (associated (lhs%variance)) then
 deallocate (lhs%variance)
 end if
 ! if (associated (rhs%efficiency)) then
 ! call copy_array_pointer (lhs%efficiency, rhs%efficiency)
 ! else if (associated (lhs%efficiency)) then
 ! deallocate (lhs%efficiency)
 ! end if
 lhs%dx = rhs%dx
 lhs%dxg = rhs%dxg
 lhs%x_min = rhs%x_min
 lhs%x_max = rhs%x_max
 lhs%x_min_true = rhs%x_min_true
 lhs%x_max_true = rhs%x_max_true
 lhs%ng = rhs%ng
 lhs%stratified = rhs%stratified
end subroutine copy_division

```

69b  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$  (37a)  $\langle$ 69a 70a $\rangle$

```

elemental subroutine delete_division (d)
 type(division_t), intent(inout) :: d
 if (associated (d%x)) then
 deallocate (d%x, d%integral, d%variance)
 end if

```

```

! deallocate (d%efficiency)
 end if
end subroutine delete_division
70a <Implementation of divisions procedures 38b>+≡ (37a) <69b
 elemental subroutine copy_history (lhs, rhs)
 type(div_history), intent(out) :: lhs
 type(div_history), intent(in) :: rhs
 lhs%stratified = rhs%stratified
 lhs%ng = rhs%ng
 lhs%num_div = rhs%num_div
 lhs%x_min = rhs%x_min
 lhs%x_max = rhs%x_max
 lhs%x_min_true = rhs%x_min_true
 lhs%x_max_true = rhs%x_max_true
 lhs%spread_f_p = rhs%spread_f_p
 lhs%stddev_f_p = rhs%stddev_f_p
 lhs%spread_p = rhs%spread_p
 lhs%stddev_p = rhs%stddev_p
 lhs%spread_m = rhs%spread_m
 lhs%stddev_m = rhs%stddev_m
 end subroutine copy_history

```

## 5.2 The Abstract Datatype *vamp\_grid*

```

70b <vamp.f90 70b>≡ 70c>
! vamp.f90 --
<Copyleft notice 1>

```



NAG f95 requires this split. Check with the Fortran community, if it is really necessary, or a bug! The problem is that this split forces us to expose the components of **vamp\_grid**.

**NB:** with the introduction of **vamp\_equivalences**, this question has (probably) become academic.

```

70c <vamp.f90 70b>+≡ <70b 71a>
 module vamp_grid_type
 use kinds
 use divisions
 private
 <Declaration of vamp_grid_type types 76a>
 end module vamp_grid_type

```



By WK for WHIZARD.

```

71a <vamp.f90 70b>+≡ <70c 75a>
 module vamp_equivalences
 use kinds
 use divisions
 use vamp_grid_type !NODEP!
 implicit none
 private
 <Declaration of vamp_equivalences procedures 72a>
 <Constants in vamp_equivalences 71d>
 <Declaration of vamp_equivalences types 71b>
 contains
 <Implementation of vamp_equivalences procedures 71e>
 end module vamp_equivalences

71b <Declaration of vamp_equivalences types 71b>≡ (71a) 71c>
 type, public :: vamp_equivalence_t
 integer :: left, right
 integer, dimension(:), allocatable :: permutation
 integer, dimension(:), allocatable :: mode
 end type vamp_equivalence_t

71c <Declaration of vamp_equivalences types 71b>+≡ (71a) <71b
 type, public :: vamp_equivalences_t
 type(vamp_equivalence_t), dimension(:), allocatable :: eq
 integer :: n_eq, n_ch
 integer, dimension(:), allocatable :: pointer
 logical, dimension(:), allocatable :: independent
 integer, dimension(:), allocatable :: equivalent_to_ch
 integer, dimension(:), allocatable :: multiplicity
 integer, dimension(:), allocatable :: symmetry
 logical, dimension(:,,:), allocatable :: div_is_invariant
 end type vamp_equivalences_t

71d <Constants in vamp_equivalences 71d>≡ (71a)
 integer, parameter, public :: &
 VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3

71e <Implementation of vamp_equivalences procedures 71e>≡ (71a) 72b>
 subroutine vamp_equivalence_init (eq, n_dim)
 type(vamp_equivalence_t), intent(inout) :: eq
 integer, intent(in) :: n_dim
 allocate (eq%permutation(n_dim), eq%mode(n_dim))
 end subroutine vamp_equivalence_init

```



72a  $\langle$ Declaration of vamp\_equivalences procedures 72a $\rangle \equiv$  (71a) 72d $\rangle$   
public :: vamp\_equivalences\_init

72b  $\langle$ Implementation of vamp\_equivalences procedures 71e $\rangle + \equiv$  (71a)  $\langle$ 71e 72c $\rangle$   
subroutine vamp\_equivalences\_init (eq, n\_eq, n\_ch, n\_dim)  
type(vamp\_equivalences\_t), intent(inout) :: eq  
integer, intent(in) :: n\_eq, n\_ch, n\_dim  
integer :: i  
eq%n\_eq = n\_eq  
eq%n\_ch = n\_ch  
allocate (eq%eq(n\_eq))  
allocate (eq%pointer(n\_ch+1))  
do i=1, n\_eq  
call vamp\_equivalence\_init (eq%eq(i), n\_dim)  
end do  
allocate (eq%independent(n\_ch), eq%equivalent\_to\_ch(n\_ch))  
allocate (eq%multiplicity(n\_ch), eq%symmetry(n\_ch))  
allocate (eq%div\_is\_invariant(n\_ch, n\_dim))  
eq%independent = .true.  
eq%equivalent\_to\_ch = 0  
eq%multiplicity = 0  
eq%symmetry = 0  
eq%div\_is\_invariant = .false.  
end subroutine vamp\_equivalences\_init

72c  $\langle$ Implementation of vamp\_equivalences procedures 71e $\rangle + \equiv$  (71a)  $\langle$ 72b 72e $\rangle$   
subroutine vamp\_equivalence\_final (eq)  
type(vamp\_equivalence\_t), intent(inout) :: eq  
deallocate (eq%permutation, eq%mode)  
end subroutine vamp\_equivalence\_final

72d  $\langle$ Declaration of vamp\_equivalences procedures 72a $\rangle + \equiv$  (71a)  $\langle$ 72a 73b $\rangle$   
public :: vamp\_equivalences\_final

72e  $\langle$ Implementation of vamp\_equivalences procedures 71e $\rangle + \equiv$  (71a)  $\langle$ 72c 73a $\rangle$   
subroutine vamp\_equivalences\_final (eq)  
type(vamp\_equivalences\_t), intent(inout) :: eq  
! integer :: i  
! do i=1, eq%n\_eq  
! call vamp\_equivalence\_final (eq%eq(i))  
! end do  
if (allocated (eq%eq)) deallocate (eq%eq)  
if (allocated (eq%pointer)) deallocate (eq%pointer)  
if (allocated (eq%multiplicity)) deallocate (eq%multiplicity)  
if (allocated (eq%symmetry)) deallocate (eq%symmetry)  
if (allocated (eq%independent)) deallocate (eq%independent)

```

 if (allocated (eq%equivalent_to_ch)) deallocate (eq%equivalent_to_ch)
 if (allocated (eq%div_is_invariant)) deallocate (eq%div_is_invariant)
 eq%n_eq = 0
 eq%n_ch = 0
 end subroutine vamp_equivalences_final
73a <Implementation of vamp_equivalences procedures 71e>+≡ (71a) <72e 73c>
 subroutine vamp_equivalence_write (eq, unit)
 integer, intent(in), optional :: unit
 integer :: u
 type(vamp_equivalence_t), intent(in) :: eq
 u = 6; if (present (unit)) u = unit
 write (u, "(3x,A,2(1x,I0))") "Equivalent channels:", eq%left, eq%right
 write (u, "(5x,A,99(1x,I0))") "Permutation:", eq%permutation
 write (u, "(5x,A,99(1x,I0))") "Mode: ", eq%mode
 end subroutine vamp_equivalence_write
73b <Declaration of vamp_equivalences procedures 72a>+≡ (71a) <72d 74a>
 public :: vamp_equivalences_write
73c <Implementation of vamp_equivalences procedures 71e>+≡ (71a) <73a 74b>
 subroutine vamp_equivalences_write (eq, unit)
 type(vamp_equivalences_t), intent(in) :: eq
 integer, intent(in), optional :: unit
 integer :: u
 integer :: ch, i
 u = 6; if (present (unit)) u = unit
 write (u, "(1x,A)") "Inequivalent channels:"
 if (allocated (eq%independent)) then
 do ch=1, eq%n_ch
 if (eq%independent(ch)) then
 write (u, "(3x,A,1x,I0,A,4x,A,I0,4x,A,I0,4x,A,999(L1))") &
 "Channel", ch, ":", &
 "Mult. = ", eq%multiplicity(ch), &
 "Symm. = ", eq%symmetry(ch), &
 "Invar.: ", eq%div_is_invariant(ch,:)
 end if
 end do
 else
 write (u, "(3x,A)") "[not allocated]"
 end if
 write (u, "(1x,A)") "Equivalence list:"
 if (allocated (eq%eq)) then
 do i=1, size (eq%eq)
 call vamp_equivalence_write (eq%eq(i), u)
 end do
 end if
 end subroutine vamp_equivalences_write

```

```

 end do
 else
 write (u, "(3x,A)") "[not allocated]"
 end if
end subroutine vamp_equivalences_write

74a <Declaration of vamp_equivalences procedures 72a>+≡ (71a) <73b 74c>
 public :: vamp_equivalence_set

74b <Implementation of vamp_equivalences procedures 71e>+≡ (71a) <73c 74d>
 subroutine vamp_equivalence_set (eq, i, left, right, perm, mode)
 type(vamp_equivalences_t), intent(inout) :: eq
 integer, intent(in) :: i
 integer, intent(in) :: left, right
 integer, dimension(:), intent(in) :: perm, mode
 eq%eq(i)%left = left
 eq%eq(i)%right = right
 eq%eq(i)%permutation = perm
 eq%eq(i)%mode = mode
 end subroutine vamp_equivalence_set

74c <Declaration of vamp_equivalences procedures 72a>+≡ (71a) <74a>
 public :: vamp_equivalences_complete

74d <Implementation of vamp_equivalences procedures 71e>+≡ (71a) <74b>
 subroutine vamp_equivalences_complete (eq)
 type(vamp_equivalences_t), intent(inout) :: eq
 integer :: i, ch
 ch = 0
 do i=1, eq%n_eq
 if (ch /= eq%eq(i)%left) then
 ch = eq%eq(i)%left
 eq%pointer(ch) = i
 end if
 end do
 eq%pointer(ch+1) = eq%n_eq + 1
 do ch=1, eq%n_ch
 call set_multiplicities (eq%eq(eq%pointer(ch):eq%pointer(ch+1)-1))
 end do
 ! call write (6, eq)
contains
 subroutine set_multiplicities (eq_ch)
 type(vamp_equivalence_t), dimension(:), intent(in) :: eq_ch
 integer :: i
 if (.not. all(eq_ch%left == ch) .or. eq_ch(1)%right > ch) then
 do i = 1, size (eq_ch)

```

```

 call vamp_equivalence_write (eq_ch(i))
 end do
 stop "VAMP: Equivalences: Something's wrong with equivalence ordering"
end if
eq%symmetry(ch) = count (eq_ch%right == ch)
if (mod (size(eq_ch), eq%symmetry(ch)) /= 0) then
 do i = 1, size (eq_ch)
 call vamp_equivalence_write (eq_ch(i))
 end do
 stop "VAMP: Equivalences: Something's wrong with permutation count"
end if
eq%multiplicity(ch) = size (eq_ch) / eq%symmetry(ch)
eq%independent(ch) = all (eq_ch%right >= ch)
eq%equivalent_to_ch(ch) = eq_ch(1)%right
eq%div_is_invariant(ch,:) = eq_ch(1)%mode == VEQ_INVARIANT
end subroutine set_multiplicities
end subroutine vamp_equivalences_complete
75a <vamp.f90 70b>+≡ <71a 75b>
module vamp_rest
 use kinds
 use utils
 use exceptions
 use divisions
 use tao_random_numbers
 use vamp_stat
 use linalg
 use iso_fortran_env
 use vamp_grid_type !NODEP!
 use vamp_equivalences !NODEP!
 implicit none
 private
 <Declaration of vamp procedures 76b>
 <Interfaces of vamp procedures 95c>
 <Constants in vamp 152>
 <Declaration of vamp types 77a>
 <Variables in vamp 78a>
contains
 <Implementation of vamp procedures 77d>
end module vamp_rest
75b <vamp.f90 70b>+≡ <75a>
module vamp
 use vamp_grid_type !NODEP!
 use vamp_rest !NODEP!

```

```

 use vamp_equivalences !NODEP!
 public
end module vamp

```

N.B.: In Fortran95 we will be able to give default initializations to components of the type. In particular, we can use the `null ()` intrinsic to initialize the pointers to a disassociated state. Until then, the user *must* call the initializer `vamp_create_grid` himself of herself, because we can't check for the allocation status of the pointers in Fortran90 or F.

⚡ Augment this datatype by `real(kind=default), dimension(2) :: mu_plus, mu_minus` to record positive and negative weight separately, so that we can estimate the efficiency for reweighting from indefinite weights to  $\{+1, -1\}$ . [WK 2015/11/06: done. Those values are recorded but not used inside `vamp`. They can be retrieved by the caller.]

⚡ WK 2015/11/06: `f_min` and `f_max` work with the absolute value of the matrix element, so they record the minimum and maximum absolute value.

76a  $\langle$ Declaration of `vamp_grid_type` types 76a $\rangle \equiv$  (70c)

```

type, public :: vamp_grid
! private ! forced by use association in interface
type(division_t), dimension(:), pointer :: div => null ()
real(kind=default), dimension(:, :), pointer :: map => null ()
real(kind=default), dimension(:), pointer :: mu_x => null ()
real(kind=default), dimension(:), pointer :: sum_mu_x => null ()
real(kind=default), dimension(:, :), pointer :: mu_xx => null ()
real(kind=default), dimension(:, :), pointer :: sum_mu_xx => null ()
real(kind=default), dimension(2) :: mu
real(kind=default), dimension(2) :: mu_plus, mu_minus
real(kind=default) :: sum_integral, sum_weights, sum_chi2
real(kind=default) :: calls, dv2g, jacobi
real(kind=default) :: f_min, f_max
real(kind=default) :: mu_gi, sum_mu_gi
integer, dimension(:), pointer :: num_div => null ()
integer :: num_calls, calls_per_cell
logical :: stratified = .true.
logical :: all_stratified = .true.
logical :: quadrupole = .false.
logical :: independent
integer :: equivalent_to_ch, multiplicity
end type vamp_grid

```

76b  $\langle$ Declaration of `vamp` procedures 76b $\rangle \equiv$  (75a) 77c $\triangleright$

```

public :: vamp_copy_grid, vamp_delete_grid

```

### 5.2.1 Container for application data



By WK for WHIZARD. We define an empty data type that the application can extend according to its needs. The purpose is to hold all sorts of data that are predefined and accessed during the call of the sampling function.

The actual interface for the sampling function is PURE. Nevertheless, we can implement side effects via pointer components of a `vamp_data_t` extension.

```
77a <Declaration of vamp types 77a>≡ (75a) 77b>
 type, public :: vamp_data_t
end type vamp_data_t
```

This is the object to be passed if we want nothing else:

```
77b <Declaration of vamp types 77a>+≡ (75a) <77a 106a>
 type(vamp_data_t), parameter, public :: NO_DATA = vamp_data_t ()
```

### 5.2.2 Initialization

```
77c <Declaration of vamp procedures 76b>+≡ (75a) <76b 78b>
 public :: vamp_create_grid, vamp_create_empty_grid
```

Create a fresh grid for the integration domain

$$\mathcal{D} = [D_{1,1}, D_{2,1}] \times [D_{1,2}, D_{2,2}] \times \dots \times [D_{1,n}, D_{2,n}] \quad (5.9)$$

dropping all accumulated results. This function *must not* be called twice on the first argument, without an intervening `vamp_delete_grid`. If the second variable is given, it will be the number of sampling points for the call to `vamp_sample_grid`.

```
77d <Implementation of vamp procedures 77d>≡ (75a) 79a>
 pure subroutine vamp_create_grid &
 (g, domain, num_calls, num_div, &
 stratified, quadrupole, covariance, map, exc)
 type(vamp_grid), intent(inout) :: g
 real(kind=default), dimension(:, :), intent(in) :: domain
 integer, intent(in) :: num_calls
 integer, dimension(:), intent(in), optional :: num_div
 logical, intent(in), optional :: stratified, quadrupole, covariance
 real(kind=default), dimension(:, :), intent(in), optional :: map
 type(exception), intent(inout), optional :: exc
```

```

character(len=*), parameter :: FN = "vamp_create_grid"
real(kind=default), dimension(size(domain,dim=2)) :: &
 x_min, x_max, x_min_true, x_max_true
integer :: ndim
ndim = size (domain, dim=2)
allocate (g%div(ndim), g%num_div(ndim))
x_min = domain(1,:)
x_max = domain(2,:)
if (present (map)) then
 allocate (g%map(ndim,ndim))
 g%map = map
 x_min_true = x_min
 x_max_true = x_max
 call map_domain (g%map, x_min_true, x_max_true, x_min, x_max)
 call create_division (g%div, x_min, x_max, x_min_true, x_max_true)
else
 nullify (g%map)
 call create_division (g%div, x_min, x_max)
end if
g%num_calls = num_calls
if (present (num_div)) then
 g%num_div = num_div
else
 g%num_div = NUM_DIV_DEFAULT
end if
g%stratified = .true.
g%quadrupole = .false.
g%independent = .true.
g%equivalent_to_ch = 0
g%multiplicity = 1
nullify (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
call vamp_discard_integral &
 (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
end subroutine vamp_create_grid

```

Below, we assume that  $\text{NUM\_DIV\_DEFAULT} \geq 6$ , but we will never go that low anyway.

78a  $\langle \text{Variables in vamp 78a} \rangle \equiv$  (75a) 94b  $\triangleright$   
 integer, private, parameter :: NUM\_DIV\_DEFAULT = 20

Given a linear map  $M$ , find a domain  $\mathcal{D}_0$  such that

$$\mathcal{D} \subset M\mathcal{D}_0 \quad (5.10)$$

78b  $\langle \text{Declaration of vamp procedures 76b} \rangle + \equiv$  (75a)  $\langle 77c \ 79c \rangle$   
 private :: map\_domain

If we can assume that  $M$  is orthogonal  $M^{-1} = M^T$ , then we just have to rotate  $\mathcal{D}$  and determine the maximal and minimal extension of the corners:

$$\mathcal{D}_0^T = \overline{\mathcal{D}^T M} \quad (5.11)$$

The corners are just the powerset of the maximal and minimal extension in each coordinate. It is determined most easily with binary counting:

- 79a *<Implementation of vamp procedures 77d>+≡* (75a) *<77d 79b>*  

```

pure subroutine map_domain (map, true_xmin, true_xmax, xmin, xmax)
 real(kind=default), dimension(:,:), intent(in) :: map
 real(kind=default), dimension(:), intent(in) :: true_xmin, true_xmax
 real(kind=default), dimension(:), intent(out) :: xmin, xmax
 real(kind=default), dimension(2**size(xmin),size(xmin)) :: corners
 integer, dimension(size(xmin)) :: zero_to_n
 integer :: j, ndim, perm
 ndim = size (xmin)
 zero_to_n = (/ (j, j=0,ndim-1) /)
 do perm = 1, 2**ndim
 corners (perm,:) = &
 merge (true_xmin, true_xmax, btest (perm-1, zero_to_n))
 end do
 corners = matmul (corners, map)
 xmin = minval (corners, dim=1)
 xmax = maxval (corners, dim=1)
end subroutine map_domain

```

79b *<Implementation of vamp procedures 77d>+≡* (75a) *<79a 79d>*  

```

elemental subroutine vamp_create_empty_grid (g)
 type(vamp_grid), intent(inout) :: g
 nullify (g%div, g%num_div, g%map, g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
end subroutine vamp_create_empty_grid

```

79c *<Declaration of vamp procedures 76b>+≡* (75a) *<78b 80a>*  

```

public :: vamp_discard_integral

```

Keep the current optimized grid, but drop the accumulated results for the integral (value and errors). Iff the second variable is given, it will be the new number of sampling points for the next call to **vamp\_sample\_grid**.

79d *<Implementation of vamp procedures 77d>+≡* (75a) *<79b 80b>*  

```

pure subroutine vamp_discard_integral &
 (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
 & independent, equivalent_to_ch, multiplicity)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in), optional :: num_calls
 integer, dimension(:), intent(in), optional :: num_div

```



```

logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
character(len=*), parameter :: FN = "vamp_discard_integral"
g%mu = 0.0
g%mu_plus = 0.0
g%mu_minus = 0.0
g%mu_gi = 0.0
g%sum_integral = 0.0
g%sum_weights = 0.0
g%sum_chi2 = 0.0
g%sum_mu_gi = 0.0
if (associated (g%sum_mu_x)) then
 g%sum_mu_x = 0.0
 g%sum_mu_xx = 0.0
end if
call set_grid_options (g, num_calls, num_div, stratified, quadrupole, &
 independent, equivalent_to_ch, multiplicity)
if ((present (num_calls)) &
 .or. (present (num_div)) &
 .or. (present (stratified)) &
 .or. (present (quadrupole)) &
 .or. (present (covariance))) then
 call vamp_reshape_grid &
 (g, g%num_calls, g%num_div, &
 g%stratified, g%quadrupole, covariance, exc)
end if
end subroutine vamp_discard_integral

```

80a  $\langle$ Declaration of vamp procedures 76b $\rangle + \equiv$  (75a)  $\triangleleft$ 79c 82a $\triangleright$

private :: set\_grid\_options

80b  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\triangleleft$ 79d 81 $\triangleright$

```

pure subroutine set_grid_options &
 (g, num_calls, num_div, stratified, quadrupole, &
 independent, equivalent_to_ch, multiplicity)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
if (present (num_calls)) then
 g%num_calls = num_calls

```

```

end if
if (present (num_div)) then
 g%num_div = num_div
end if
if (present (stratified)) then
 g%stratified = stratified
end if
if (present (quadrupole)) then
 g%quadrupole = quadrupole
end if
if (present (independent)) then
 g%independent = independent
end if
if (present (equivalent_to_ch)) then
 g%equivalent_to_ch = equivalent_to_ch
end if
if (present (multiplicity)) then
 g%multiplicity = multiplicity
end if
end subroutine set_grid_options

```

### *Setting Up the Initial Grid*

Keep the current optimized grid and the accumulated results for the integral (value and errors). The second variable will be the new number of sampling points for the next call to `vamp_sample_grid`.

81 *<Implementation of vamp procedures 77d>+≡* (75a) <80b 82b>

```

pure subroutine vamp_reshape_grid_internal &
 (g, num_calls, num_div, &
 stratified, quadrupole, covariance, exc, use_variance, &
 independent, equivalent_to_ch, multiplicity)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
logical, intent(in), optional :: use_variance
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
integer :: ndim, num_cells
integer, dimension(size(g%div)) :: ng
character(len=*), parameter :: FN = "vamp_reshape_grid_internal"
ndim = size (g%div)

```

```

call set_grid_options &
 (g, num_calls, num_div, stratified, quadrupole, &
 & independent, equivalent_to_ch, multiplicity)
<Adjust grid and other state for new num_calls 83>
g%all_stratified = all (stratified_division (g%div))
if (present (covariance)) then
 ndim = size (g%div)
 if (covariance .and. (.not. associated (g%mu_x))) then
 allocate (g%mu_x(ndim), g%mu_xx(ndim,ndim))
 allocate (g%sum_mu_x(ndim), g%sum_mu_xx(ndim,ndim))
 g%sum_mu_x = 0.0
 g%sum_mu_xx = 0.0
 else if ((.not. covariance) .and. (associated (g%mu_x))) then
 deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
 end if
end if
end subroutine vamp_reshape_grid_internal

```

The `use_variance` argument is too dangerous for careless users, because the variance in the divisions will contain garbage before sampling and after reshaping. Build a fence with another routine.

- 82a <Declaration of `vamp` procedures 76b>+≡ (75a) <80a 84c>
- ```

private :: vamp_reshape_grid_internal
public :: vamp_reshape_grid

```
- 82b <Implementation of `vamp` procedures 77d>+≡ (75a) <81 84d>
- ```

pure subroutine vamp_reshape_grid &
 (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
 independent, equivalent_to_ch, multiplicity)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
call vamp_reshape_grid_internal &
 (g, num_calls, num_div, stratified, quadrupole, covariance, &
 exc, use_variance = .false., &
 independent=independent, equivalent_to_ch=equivalent_to_ch, &
 multiplicity=multiplicity)
end subroutine vamp_reshape_grid

```

`vegas` operates in three different modes, which are chosen according to explicit user requests and to the relation of the requested number of sampling

points to the dimensionality of the integration domain.

The simplest case is when the user has overwritten the default of stratified sampling with the optional argument **stratified** in the call to **vamp\_create\_grid**. Then sample points will be chosen randomly with equal probability in each cell of the adaptive grid, as displayed in figure 5.1.

The implementation is actually shared with the stratified case described below, by pretending that there is just a single stratification cell. The number of divisions for the adaptive grid is set to a compile time maximum value.

If the user has agreed on stratified sampling then there are two cases, depending on the dimensionality of the integration region and the number of sample points. First we determine the number of divisions  $n_g$  (i. e. **ng**) of the rigid grid such that there will be two sampling points per cell.

$$N_{\text{calls}} = 2 \cdot (n_g)^{n_{\text{dim}}} \quad (5.12)$$

The additional optional argument  $\hat{n}_g$  specifies an anisotropy in the shape

$$n_{g,j} = \frac{\hat{n}_{g,j}}{\left(\prod_j \hat{n}_{g,j}\right)^{1/n_{\text{dim}}}} \left(\frac{N}{2}\right)^{1/n_{\text{dim}}} \quad (5.13)$$

NB:

$$\prod_j n_{g,j} = \frac{N}{2} \quad (5.14)$$

83 *Adjust grid and other state for new num\_calls 83* (81) 84a

```

if (g%stratified) then
 ng = (g%num_calls / 2.0 + 0.25)**(1.0/ndim)
 ! ng = ng * real (g%num_div, kind=default) &
 ! / (product (real (g%num_div, kind=default)))** (1.0/ndim)
else
 ng = 1
end if
call reshape_division (g%div, g%num_div, ng, use_variance)
call clear_integral_and_variance (g%div)
num_cells = product (rigid_division (g%div))
g%calls_per_cell = max (g%num_calls / num_cells, 2)
g%calls = real (g%calls_per_cell) * real (num_cells)
jacobi = J = Volume / N_calls

```

(5.15)

and

$$\text{dv2g} = \frac{N_{\text{calls}}^2 ((\Delta x)^{n_{\text{dim}}})^2}{N_{\text{calls/cell}}^2 (N_{\text{calls/cell}} - 1)} = \frac{\left(\frac{N_{\text{calls}}}{N_{\text{cells}}}\right)^2}{N_{\text{calls/cell}}^2 (N_{\text{calls/cell}} - 1)} \quad (5.16)$$

84a *<Adjust grid and other state for new num\_calls 83>+≡ (81) <83 84b>*  
`g%jacobi = product (volume_division (g%div)) / g%calls  
g%dv2g = (g%calls / num_cells)**2 &  
/ g%calls_per_cell / g%calls_per_cell / (g%calls_per_cell - 1.0)`

84b *<Adjust grid and other state for new num\_calls 83>+≡ (81) <84a*  
`call vamp_nullify_f_limits (g)`

When the grid is refined or reshaped, the recorded minimum and maximum of the sampling function should be nullified:

84c *<Declaration of vamp procedures 76b>+≡ (75a) <82a 84e>*  
`public :: vamp_nullify_f_limits`

84d *<Implementation of vamp procedures 77d>+≡ (75a) <82b 84f>*  
`elemental subroutine vamp_nullify_f_limits (g)  
type(vamp_grid), intent(inout) :: g  
g%f_min = 1.0  
g%f_max = 0.0  
end subroutine vamp_nullify_f_limits`

84e *<Declaration of vamp procedures 76b>+≡ (75a) <84c 85d>*  
`public :: vamp_rigid_divisions  
public :: vamp_get_covariance, vamp_nullify_covariance  
public :: vamp_get_variance, vamp_nullify_variance`

84f *<Implementation of vamp procedures 77d>+≡ (75a) <84d 84g>*  
`pure function vamp_rigid_divisions (g) result (ng)  
type(vamp_grid), intent(in) :: g  
integer, dimension(size(g%div)) :: ng  
ng = rigid_division (g%div)  
end function vamp_rigid_divisions`

84g *<Implementation of vamp procedures 77d>+≡ (75a) <84f 85a>*  
`pure function vamp_get_covariance (g) result (cov)  
type(vamp_grid), intent(in) :: g  
real(kind=default), dimension(size(g%div),size(g%div)) :: cov  
if (associated (g%mu_x)) then  
if (abs (g%sum_weights) <= tiny (cov(1,1))) then  
where (g%sum_mu_xx == 0.0_default)  
cov = 0.0  
elsewhere  
cov = huge (cov(1,1))  
endwhere  
else  
cov = g%sum_mu_xx / g%sum_weights &  
- outer_product (g%sum_mu_x, g%sum_mu_x) / g%sum_weights**2  
end if`

```

 else
 cov = 0.0
 end if
 end function vamp_get_covariance
85a <Implementation of vamp procedures 77d>+≡ (75a) <84g 85b>
 elemental subroutine vamp_nullify_covariance (g)
 type(vamp_grid), intent(inout) :: g
 if (associated (g%mu_x)) then
 g%sum_mu_x = 0
 g%sum_mu_xx = 0
 end if
 end subroutine vamp_nullify_covariance
85b <Implementation of vamp procedures 77d>+≡ (75a) <85a 85c>
 elemental function vamp_get_variance (g) result (v)
 type(vamp_grid), intent(in) :: g
 real(kind=default) :: v
 if (abs (g%sum_weights) <= tiny (v)) then
 if (g%sum_mu_gi == 0.0_default) then
 v = 0.0
 else
 v = huge (v)
 end if
 else
 v = g%sum_mu_gi / g%sum_weights
 end if
 end function vamp_get_variance
85c <Implementation of vamp procedures 77d>+≡ (75a) <85b 86a>
 elemental subroutine vamp_nullify_variance (g)
 type(vamp_grid), intent(inout) :: g
 g%sum_mu_gi = 0
 end subroutine vamp_nullify_variance

```

### 5.2.3 Sampling

```

85d <Declaration of vamp procedures 76b>+≡ (75a) <84e 91b>
 public :: vamp_sample_grid
 public :: vamp_sample_grid0
 public :: vamp_refine_grid
 public :: vamp_refine_grids

```

*Simple Non-Adaptive Sampling:  $S_0$*

86a *⟨Implementation of vamp procedures 77d⟩*+≡ (75a) <85c 92a>

```

subroutine vamp_sample_grid0 &
 (rng, g, func, data, channel, weights, grids, exc, &
 negative_weights)
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid), intent(inout) :: g
 class(vamp_data_t), intent(in) :: data
 integer, intent(in), optional :: channel
 real(kind=default), dimension(:), intent(in), optional :: weights
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 type(exception), intent(inout), optional :: exc
 ⟨Interface declaration for func 22⟩
 character(len=*), parameter :: FN = "vamp_sample_grid0"
 logical, intent(in), optional :: negative_weights
 ⟨Local variables in vamp_sample_grid0 87b⟩
 integer :: ndim
 logical :: neg_w
 ndim = size (g%div)
 neg_w = .false.
 if (present (negative_weights)) neg_w = negative_weights
 ⟨Check optional arguments in vamp_sample_grid0 91a⟩
 ⟨Reset counters in vamp_sample_grid0 87a⟩
 loop_over_cells: do
 ⟨Sample calls_per_cell points in the current cell 87d⟩
 ⟨Collect integration and grid optimization data for current cell 89b⟩
 ⟨Count up cell, exit if done 86b⟩
 end do loop_over_cells
 ⟨Collect results of vamp_sample_grid0 90a⟩
end subroutine vamp_sample_grid0

```

Count cells like a  $n_g$ -ary number—i.e.  $(1, \dots, 1, 1), (1, \dots, 1, 2), \dots, (1, \dots, 1, n_g), (1, \dots, 2, 1), \dots, (n_g, \dots, n_g, n_g - 1), (n_g, \dots, n_g, n_g)$ —and terminate when all (`cell == 1`) again.

86b *⟨Count up cell, exit if done 86b⟩*≡ (86a)

```

do j = ndim, 1, -1
 cell(j) = modulo (cell(j), rigid_division (g%div(j))) + 1
 if (cell(j) /= 1) then
 cycle loop_over_cells
 end if
end do
exit loop_over_cells

```

```

87a <Reset counters in vamp_sample_grid0 87a>≡ (86a)
 g%mu = 0.0
 g%mu_plus = 0.0
 g%mu_minus = 0.0
 cell = 1
 call clear_integral_and_variance (g%div)
 if (associated (g%mu_x)) then
 g%mu_x = 0.0
 g%mu_xx = 0.0
 end if
 if (present (channel)) then
 g%mu_gi = 0.0
 end if

87b <Local variables in vamp_sample_grid0 87b>≡ (86a) 87c>
 real(kind=default), parameter :: &
 eps = tiny (1._default) / epsilon (1._default)
 character(len=6) :: buffer

87c <Local variables in vamp_sample_grid0 87b>+≡ (86a) <87b 89a>
 integer :: j, k
 integer, dimension(size(g%div)) :: cell

87d <Sample calls_per_cell points in the current cell 87d>≡ (86a)
 sum_f = 0.0
 sum_f_plus = 0.0
 sum_f_minus = 0.0
 sum_f2 = 0.0
 sum_f2_plus = 0.0
 sum_f2_minus = 0.0
 do k = 1, g%calls_per_cell
 <Get x in the current cell 87e>
 <f = wgt * func (x, weights, channel), iff x inside true_domain 88a>
 <Collect integration and grid optimization data for x from f 88b>
 end do

```

We are using the generic procedure `tao_random_number` from the `tao_random_numbers` module for generating an array of uniform deviates. A better alternative would be to pass the random number generator as an argument to `vamp_sample_grid`. Unfortunately, it is not possible to pass *generic* procedures in Fortran90, Fortran95, or F. While we could export a specific procedure from `tao_random_numbers`, a more serious problem is that we have to pass the state `rng` of the random number generator as a `tao_random_state` anyway and we have to hardcode the random number generator anyway.

```

87e <Get x in the current cell 87e>≡ (87d)

```



```

call tao_random_number (rng, r)
call inject_division (g%div, real (r, kind=default), &
 cell, x, x_mid, ia, wgts)
wgt = g%jacobi * product (wgts)
if (associated (g%map)) then
 x = matmul (g%map, x)
end if

```

This somewhat contorted nested if constructs allow to minimize the number of calls to `func`. This is useful, since `func` is the most expensive part of real world applications. Also `func` might be singular outside of `true_domain`.

The original `vegas` used to call `f = wgt * func (x, wgt)` below to allow `func` to use `wgt` (i.e.  $1/p(x)$ ) for integrating another function at the same time. This form of “parallelism” relies on side effects and is therefore impossible with pure functions. Consequently, it is not supported in the current implementation.

```

88a <f = wgt * func (x, weights, channel), iff x inside true_domain 88a>≡ (87d 135d)
 if (associated (g%map)) then
 if (all (inside_division (g%div, x))) then
 f = wgt * func (x, data, weights, channel, grids)
 else
 f = 0.0
 end if
 else
 f = wgt * func (x, data, weights, channel, grids)
 end if

88b <Collect integration and grid optimization data for x from f 88b>≡ (87d) 88c▷
 if (g%f_min > g%f_max) then
 g%f_min = abs (f) * g%calls
 g%f_max = abs (f) * g%calls
 else if (abs (f) * g%calls < g%f_min) then
 g%f_min = abs (f) * g%calls
 else if (abs (f) * g%calls > g%f_max) then
 g%f_max = abs (f) * g%calls
 end if

88c <Collect integration and grid optimization data for x from f 88b>+≡ (87d) <88b
 f2 = f * f
 sum_f = sum_f + f
 sum_f2 = sum_f2 + f2
 if (f > 0) then
 sum_f_plus = sum_f_plus + f
 sum_f2_plus = sum_f2_plus + f * f
 else if (f < 0) then

```

```

 sum_f_minus = sum_f_minus + f
 sum_f2_minus = sum_f2_minus + f * f
end if
call record_integral (g%div, ia, f)
! call record_efficiency (g%div, ia, f/g%f_max)
if ((associated (g%mu_x)) .and. (.not. g%all_stratified)) then
 g%mu_x = g%mu_x + x * f
 g%mu_xx = g%mu_xx + outer_product (x, x) * f
end if
if (present (channel)) then
 g%mu_gi = g%mu_gi + f2
end if

```

89a  $\langle$ Local variables in vamp\_sample\_grid0 87b $\rangle \equiv$  (86a)  $\triangleleft$  87c

```

real(kind=default) :: wgt, f, f2
real(kind=default) :: sum_f, sum_f2, var_f
real(kind=default) :: sum_f_plus, sum_f2_plus, var_f_plus
real(kind=default) :: sum_f_minus, sum_f2_minus, var_f_minus
real(kind=default), dimension(size(g%div)):: x, x_mid, wgts
real(kind=default), dimension(size(g%div)):: r
integer, dimension(size(g%div)) :: ia

```

$$\sigma^2 \cdot N_{\text{calls/cell}}^2 (N_{\text{calls/cell}} - 1) = \text{var}(f) = N^2 \sigma^2 \left( \left\langle \frac{f^2}{p} \right\rangle - \langle f \rangle^2 \right) \quad (5.17)$$

89b  $\langle$ Collect integration and grid optimization data for current cell 89b $\rangle \equiv$  (86a)

```

var_f = sum_f2 * g%calls_per_cell - sum_f**2
var_f_plus = sum_f2_plus * g%calls_per_cell - sum_f_plus**2
var_f_minus = sum_f2_minus * g%calls_per_cell - sum_f_minus**2
if (var_f <= 0.0) then
 var_f = tiny (1.0_default)
end if
if (sum_f_plus /= 0 .and. var_f_plus <= 0) then
 var_f_plus = tiny (1.0_default)
end if
if (sum_f_minus /= 0 .and. var_f_minus <= 0) then
 var_f_minus = tiny (1.0_default)
end if
g%mu = g%mu + (/ sum_f, var_f /)
g%mu_plus = g%mu_plus + (/ sum_f_plus, var_f_plus /)
g%mu_minus = g%mu_minus + (/ sum_f_minus, var_f_minus /)
call record_variance (g%div, ia, var_f)
if ((associated (g%mu_x)) .and. g%all_stratified) then
 if (associated (g%map)) then

```

```

 x_mid = matmul (g%map, x_mid)
end if
g%mu_x = g%mu_x + x_mid * var_f
g%mu_xx = g%mu_xx + outer_product (x_mid, x_mid) * var_f
end if

```

$$\sigma^2 = \frac{\left(\frac{N_{\text{calls}}}{N_{\text{cells}}}\right)^2}{N_{\text{calls/cell}}^2(N_{\text{calls/cell}} - 1)} \sum_{\text{cells}} \sigma_{\text{cell}}^2 \cdot N_{\text{calls/cell}}^2 (N_{\text{calls/cell}} - 1) \quad (5.18)$$

where the  $N_{\text{calls}}^2$  cancels the corresponding factor in the Jacobian and the  $N_{\text{cells}}^{-2}$  is the result of stratification. In order to avoid numerical noise for some OS when using 80bit precision, we wrap the numerical resetting into a negative weights-only if-clause.

```

90a <Collect results of vamp_sample_grid0 90a>≡ (86a) 90b>
 g%mu(2) = g%mu(2) * g%dv2g
 if (g%mu(2) < eps * max (g%mu(1)**2, 1._default)) then
 g%mu(2) = eps * max (g%mu(1)**2, 1._default)
 end if
 if (neg_w) then
 g%mu_plus(2) = g%mu_plus(2) * g%dv2g
 if (g%mu_plus(2) < eps * max (g%mu_plus(1)**2, 1._default)) then
 g%mu_plus(2) = eps * max (g%mu_plus(1)**2, 1._default)
 end if
 g%mu_minus(2) = g%mu_minus(2) * g%dv2g
 if (g%mu_minus(2) < eps * max (g%mu_minus(1)**2, 1._default)) then
 g%mu_minus(2) = eps * max (g%mu_minus(1)**2, 1._default)
 end if
 end if
end if

90b <Collect results of vamp_sample_grid0 90a>+≡ (86a) <90a
 if (g%mu(1)>0) then
 g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
 g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
 g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
 if (associated (g%mu_x)) then
 if (g%all_stratified) then
 g%mu_x = g%mu_x / g%mu(2)
 g%mu_xx = g%mu_xx / g%mu(2)
 else
 g%mu_x = g%mu_x / g%mu(1)
 g%mu_xx = g%mu_xx / g%mu(1)
 end if
 g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
 g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
 end if
 end if

```

```

end if
if (present (channel)) then
 g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
end if
else if (neg_w) then
 g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
 g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
 g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
 if (associated (g%mu_x)) then
 if (g%all_stratified) then
 g%mu_x = g%mu_x / g%mu(2)
 g%mu_xx = g%mu_xx / g%mu(2)
 else
 g%mu_x = g%mu_x / g%mu(1)
 g%mu_xx = g%mu_xx / g%mu(1)
 end if
 g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
 g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
 end if
 if (present (channel)) then
 g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
 end if
else
 if (present(channel) .and. g%mu(1)==0) then
 write (buffer, "(I6)" channel
 call raise_exception (exc, EXC_WARN, "! vamp", &
 "Function identically zero in channel " // buffer)
 else if (present(channel) .and. g%mu(1)<0) then
 write (buffer, "(I6)" channel
 call raise_exception (exc, EXC_ERROR, "! vamp", &
 "Negative integral in channel " // buffer)
 end if
 g%sum_integral = 0
 g%sum_chi2 = 0
 g%sum_weights = 0
end if
91a <Check optional arguments in vamp_sample_grid0 91a>≡ (86a)
 if (present (channel) .neqv. present (weights)) then
 call raise_exception (exc, EXC_FATAL, FN, &
 "channel and weights required together")
 return
 end if
91b <Declaration of vamp procedures 76b>+≡ (75a) <85d 95b>

```

```
public :: vamp_probability
```

92a *<Implementation of vamp procedures 77d>+≡* (75a) <86a 92b>

```
pure function vamp_probability (g, x) result (p)
 type(vamp_grid), intent(in) :: g
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default) :: p
 p = product (probability (g%div, x))
end function vamp_probability
```



%variance should be private to division

92b *<Implementation of vamp procedures 77d>+≡* (75a) <92a 93>

```
subroutine vamp_apply_equivalences (g, eq)
 type(vamp_grids), intent(inout) :: g
 type(vamp_equivalences_t), intent(in) :: eq
 integer :: n_ch, n_dim, nb, i, ch, ch_src, dim, dim_src
 integer, dimension(:,:), allocatable :: n_bin
 real(kind=default), dimension(:,:,:), allocatable :: var_tmp
 n_ch = size (g%grids)
 if (n_ch == 0) return
 n_dim = size (g%grids(1)%div)
 allocate (n_bin(n_ch, n_dim))
 do ch = 1, n_ch
 do dim = 1, n_dim
 n_bin(ch, dim) = size (g%grids(ch)%div(dim)%variance)
 end do
 end do
 allocate (var_tmp (maxval(n_bin), n_dim, n_ch))
 var_tmp = 0
 do i=1, eq%n_eq
 ch = eq%eq(i)%left
 ch_src = eq%eq(i)%right
 do dim=1, n_dim
 nb = n_bin(ch_src, dim)
 dim_src = eq%eq(i)%permutation(dim)
 select case (eq%eq(i)%mode(dim))
 case (VEQ_IDENTITY)
 var_tmp(:,nb,dim,ch) = var_tmp(:,nb,dim,ch) &
 & + g%grids(ch_src)%div(dim_src)%variance
 case (VEQ_INVERT)
 var_tmp(:,nb,dim,ch) = var_tmp(:,nb,dim,ch) &
 & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)
 case (VEQ_SYMMETRIC)
```

```

 var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
 & + g%grids(ch_src)%div(dim_src)%variance / 2 &
 & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)/2
 case (VEQ_INVARIANT)
 var_tmp(:nb,dim,ch) = 1
 end select
end do
end do
do ch=1, n_ch
 do dim=1, n_dim
 g%grids(ch)%div(dim)%variance = var_tmp(:n_bin(ch, dim),dim,ch)
 end do
end do
deallocate (var_tmp)
deallocate (n_bin)
end subroutine vamp_apply_equivalences

```

*Grid Refinement:  $r$*

$$n_{\text{div},j} \rightarrow \frac{Q_j n_{\text{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\text{dim}}}} \quad (5.19)$$

where

$$Q_j = \left( \sqrt{\text{Var}(\{m\}_j)} \right)^\alpha \quad (5.20)$$

93 *<Implementation of vamp procedures 77d>+≡* (75a) <92b 94a>

```

pure subroutine vamp_refine_grid (g, exc)
 type(vamp_grid), intent(inout) :: g
 type(exception), intent(inout), optional :: exc
 real(kind=default), dimension(size(g%div)) :: quad
 integer :: ndim
 if (g%quadrupole) then
 ndim = size (g%div)
 quad = (quadrupole_division (g%div))**QUAD_POWER
 call vamp_reshape_grid_internal &
 (g, use_variance = .true., exc = exc, &
 num_div = int (quad / product (quad)**(1.0/ndim) * g%num_div))
 else
 call refine_division (g%div)
 call vamp_nullify_f_limits (g)
 end if
end subroutine vamp_refine_grid

```

94a *<Implementation of vamp procedures 77d>+≡* (75a) <93 94c>

```
subroutine vamp_refine_grids (g)
 type(vamp_grids), intent(inout) :: g
 integer :: ch
 do ch=1, size(g%grids)
 call refine_division (g%grids(ch)%div)
 call vamp_nullify_f_limits (g%grids(ch))
 end do
end subroutine vamp_refine_grids
```

94b *<Variables in vamp 78a>+≡* (75a) <78a 109a>

```
real(kind=default), private, parameter :: QUAD_POWER = 0.5_default
```

$$\text{Adaptive Sampling: } S_n = S_0(rS_0)^n$$

94c *<Implementation of vamp procedures 77d>+≡* (75a) <94a 95a>

```
subroutine vamp_sample_grid &
 (rng, g, func, data, iterations, &
 integral, std_dev, avg_chi2, accuracy, &
 channel, weights, grids, exc, history)
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid), intent(inout) :: g
 class(vamp_data_t), intent(in) :: data
 integer, intent(in) :: iterations
 real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
 real(kind=default), intent(in), optional :: accuracy
 integer, intent(in), optional :: channel
 real(kind=default), dimension(:), intent(in), optional :: weights
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 type(exception), intent(inout), optional :: exc
 type(vamp_history), dimension(:), intent(inout), optional :: history
 <Interface declaration for func 22>
 character(len=*), parameter :: FN = "vamp_sample_grid"
 real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
 integer :: iteration, ndim
 ndim = size (g%div)
 iterate: do iteration = 1, iterations
 call vamp_sample_grid0 &
 (rng, g, func, data, channel, weights, grids, exc)
 call vamp_average_iterations &
 (g, iteration, local_integral, local_std_dev, local_avg_chi2)
 <Trace results of vamp_sample_grid 106b>
 <Exit iterate if accuracy has been reached 96b>
 if (iteration < iterations) call vamp_refine_grid (g)
```

```

end do iterate
 <Copy results of vamp_sample_grid to dummy variables 96a>
end subroutine vamp_sample_grid

```

Assuming that the iterations have been statistically independent, we can combine them with the usual formulae.

$$\bar{I} = \sigma_I^2 \sum_i \frac{I_i}{\sigma_i^2} \quad (5.21a)$$

$$\frac{1}{\sigma_I^2} = \sum_i \frac{1}{\sigma_i^2} \quad (5.21b)$$

$$\chi^2 = \sum_i \frac{(I_i - \bar{I})^2}{\sigma_i^2} = \sum_i \frac{I_i^2}{\sigma_i^2} - \bar{I} \sum_i \frac{I_i}{\sigma_i^2} \quad (5.21c)$$

```

95a <Implementation of vamp procedures 77d>+≡ (75a) <94c 97a>
 elemental subroutine vamp_average_iterations_grid &
 (g, iteration, integral, std_dev, avg_chi2)
 type(vamp_grid), intent(in) :: g
 integer, intent(in) :: iteration
 real(kind=default), intent(out) :: integral, std_dev, avg_chi2
 real(kind=default), parameter :: eps = 1000 * epsilon (1._default)
 if (g%sum_weights>0) then
 integral = g%sum_integral / g%sum_weights
 std_dev = sqrt (1.0 / g%sum_weights)
 avg_chi2 = &
 max ((g%sum_chi2 - g%sum_integral * integral) / (iteration-0.99), &
 0.0_default)
 if (avg_chi2 < eps * g%sum_chi2) avg_chi2 = 0
 else
 integral = 0
 std_dev = 0
 avg_chi2 = 0
 end if
 end subroutine vamp_average_iterations_grid

95b <Declaration of vamp procedures 76b>+≡ (75a) <91b 96c>
 public :: vamp_average_iterations
 private :: vamp_average_iterations_grid

95c <Interfaces of vamp procedures 95c>≡ (75a) 96d>
 interface vamp_average_iterations
 module procedure vamp_average_iterations_grid
 end interface

```



Lepage suggests [1] to reweight the contributions as in the following improved formulae, which we might implement as an option later.

$$\bar{I} = \frac{1}{\left(\sum_i \frac{I_i^2}{\sigma_i^2}\right)^2} \sum_i I_i \frac{I_i^2}{\sigma_i^2} \quad (5.22a)$$

$$\frac{1}{\sigma_I^2} = \frac{1}{(\bar{I})^2} \sum_i \frac{I_i^2}{\sigma_i^2} \quad (5.22b)$$

$$\chi^2 = \sum_i \frac{(I_i - \bar{I})^2}{(\bar{I})^2} \frac{I_i^2}{\sigma_i^2} \quad (5.22c)$$

Iff possible, copy the result to the caller's variables:

```

96a <Copy results of vamp_sample_grid to dummy variables 96a>≡ (94c 103b 120b)
 if (present (integral)) then
 integral = local_integral
 end if
 if (present (std_dev)) then
 std_dev = local_std_dev
 end if
 if (present (avg_chi2)) then
 avg_chi2 = local_avg_chi2
 end if

96b <Exit iterate if accuracy has been reached 96b>≡ (94c 103b 120b)
 if (present (accuracy)) then
 if (local_std_dev <= accuracy * local_integral) then
 call raise_exception (exc, EXC_INFO, FN, &
 "requested accuracy reached")
 exit iterate
 end if
 end if

```

#### 5.2.4 Forking and Joining

```

96c <Declaration of vamp procedures 76b>+≡ (75a) <95b 102a>
 public :: vamp_fork_grid
 private :: vamp_fork_grid_single, vamp_fork_grid_multi
 public :: vamp_join_grid
 private :: vamp_join_grid_single, vamp_join_grid_multi

96d <Interfaces of vamp procedures 95c>+≡ (75a) <95c 106d>
 interface vamp_fork_grid
 module procedure vamp_fork_grid_single, vamp_fork_grid_multi

```

```

end interface
interface vamp_join_grid
 module procedure vamp_join_grid_single, vamp_join_grid_multi
end interface

```

Caveat emptor: splitting divisions can lead to `num_div < 3` an the application must not try to refine such grids before merging them again! `d == 0` is special.

97a *<Implementation of vamp procedures 77d>+≡* (75a) <95a 99d>

```

pure subroutine vamp_fork_grid_single (g, gs, d, exc)
 type(vamp_grid), intent(in) :: g
 type(vamp_grid), dimension(:), intent(inout) :: gs
 integer, intent(in) :: d
 type(exception), intent(inout), optional :: exc
 character(len=*), parameter :: FN = "vamp_fork_grid_single"
 type(division_t), dimension(:), allocatable :: d_tmp
 integer :: i, j, num_grids, num_div, ndim, num_cells
 num_grids = size (gs)
 ndim = size (g%div)
 <Allocate or resize the divisions 99c>
 do j = 1, ndim
 if (j == d) then
 <call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 98d>
 else
 <call copy_division (gs%div(j), g%div(j)) 99b>
 end if
 end do
 if (d == 0) then
 <Handle g%calls_per_cell for d == 0 97b>
 end if
 <Copy the rest of g to the gs 97c>
end subroutine vamp_fork_grid_single

```

Divide the sampling points among identical grids

97b *<Handle g%calls\_per\_cell for d == 0 97b>≡* (97a)

```

if (any (stratified_division (g%div))) then
 call raise_exception (exc, EXC_FATAL, FN, &
 "d == 0 incompatible w/ stratification")
else
 gs(2:)%calls_per_cell = ceiling (real (g%calls_per_cell) / num_grids)
 gs(1)%calls_per_cell = g%calls_per_cell - sum (gs(2:)%calls_per_cell)
end if

```

97c *<Copy the rest of g to the gs 97c>≡* (97a) 98a>

```

do i = 1, num_grids

```

```

call copy_array_pointer (gs(i)%num_div, g%num_div)
if (associated (g%map)) then
 call copy_array_pointer (gs(i)%map, g%map)
end if
if (associated (g%mu_x)) then
 call create_array_pointer (gs(i)%mu_x, ndim)
 call create_array_pointer (gs(i)%sum_mu_x, ndim)
 call create_array_pointer (gs(i)%mu_xx, (/ ndim, ndim /))
 call create_array_pointer (gs(i)%sum_mu_xx, (/ ndim, ndim /))
end if
end do

```

Reset results

98a  $\langle$ Copy the rest of g to the gs 97c $\rangle + \equiv$

(97a)  $\langle$ 97c 98b $\rangle$

```

gs%mu(1) = 0.0
gs%mu(2) = 0.0
gs%mu_plus(1) = 0.0
gs%mu_plus(2) = 0.0
gs%mu_minus(1) = 0.0
gs%mu_minus(2) = 0.0
gs%sum_integral = 0.0
gs%sum_weights = 0.0
gs%sum_chi2 = 0.0
gs%mu_gi = 0.0
gs%sum_mu_gi = 0.0

```

98b  $\langle$ Copy the rest of g to the gs 97c $\rangle + \equiv$

(97a)  $\langle$ 98a 98c $\rangle$

```

gs%stratified = g%stratified
gs%all_stratified = g%all_stratified
gs%quadrupole = g%quadrupole

```

98c  $\langle$ Copy the rest of g to the gs 97c $\rangle + \equiv$

(97a)  $\langle$ 98b

```

do i = 1, num_grids
 num_cells = product (rigid_division (gs(i)%div))
 gs(i)%calls = gs(i)%calls_per_cell * num_cells
 gs(i)%num_calls = gs(i)%calls
 gs(i)%jacobi = product (volume_division (gs(i)%div)) / gs(i)%calls
 gs(i)%dv2g = (gs(i)%calls / num_cells)**2 &
 / gs(i)%calls_per_cell / gs(i)%calls_per_cell / (gs(i)%calls_per_cell - 1.0)
end do
gs%f_min = g%f_min * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)
gs%f_max = g%f_max * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)

```

This could be self-explaining, if the standard would allow ... Note that we can get away with copying just the pointers, because `fork_division` does the dirty work for the memory management.

```

98d <call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 98d>≡ (97a)
 allocate (d_tmp(num_grids))
 do i = 1, num_grids
 d_tmp(i) = gs(i)%div(j)
 end do
 call fork_division (g%div(j), d_tmp, g%calls_per_cell, gs%calls_per_cell, exc)
 do i = 1, num_grids
 gs(i)%div(j) = d_tmp(i)
 end do
 deallocate (d_tmp)
 <Bail out if exception exc raised 99a>
99a <Bail out if exception exc raised 99a>≡ (98d 100a 103b 140c 142b)
 if (present (exc)) then
 if (exc%level > EXC_WARN) then
 return
 end if
 end if
 We have to do a deep copy (gs(i)%div(j) = g%div(j) does not suffice),
 because copy_division handles the memory management.
99b <call copy_division (gs%div(j), g%div(j)) 99b>≡ (97a)
 do i = 1, num_grids
 call copy_division (gs(i)%div(j), g%div(j))
 end do
99c <Allocate or resize the divisions 99c>≡ (97a)
 num_div = size (g%div)
 do i = 1, size (gs)
 if (associated (gs(i)%div)) then
 if (size (gs(i)%div) /= num_div) then
 allocate (gs(i)%div(num_div))
 call create_empty_division (gs(i)%div)
 end if
 else
 allocate (gs(i)%div(num_div))
 call create_empty_division (gs(i)%div)
 end if
 end do
99d <Implementation of vamp procedures 77d>+≡ (75a) <97a 101b>
 pure subroutine vamp_join_grid_single (g, gs, d, exc)
 type(vamp_grid), intent(inout) :: g
 type(vamp_grid), dimension(:), intent(inout) :: gs
 integer, intent(in) :: d
 type(exception), intent(inout), optional :: exc

```

```

type(division_t), dimension(:), allocatable :: d_tmp
integer :: i, j, num_grids
num_grids = size (gs)
do j = 1, size (g%div)
 if (j == d) then
 <call join_division (g%div(j), gs%div(j)) 100a>
 else
 <call sum_division (g%div(j), gs%div(j)) 100b>
 end if
end do
<Combine the rest of gs onto g 100c>
end subroutine vamp_join_grid_single
100a <call join_division (g%div(j), gs%div(j)) 100a>≡ (99d)
 allocate (d_tmp(num_grids))
 do i = 1, num_grids
 d_tmp(i) = gs(i)%div(j)
 end do
 call join_division (g%div(j), d_tmp, exc)
 deallocate (d_tmp)
 <Bail out if exception exc raised 99a>
100b <call sum_division (g%div(j), gs%div(j)) 100b>≡ (99d)
 allocate (d_tmp(num_grids))
 do i = 1, num_grids
 d_tmp(i) = gs(i)%div(j)
 end do
 call sum_division (g%div(j), d_tmp)
 deallocate (d_tmp)
100c <Combine the rest of gs onto g 100c>≡ (99d)
 g%f_min = minval (gs%f_min * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
 g%f_max = maxval (gs%f_max * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
 g%mu(1) = sum (gs%mu(1))
 g%mu(2) = sum (gs%mu(2))
 g%mu_plus(1) = sum (gs%mu_plus(1))
 g%mu_plus(2) = sum (gs%mu_plus(2))
 g%mu_minus(1) = sum (gs%mu_minus(1))
 g%mu_minus(2) = sum (gs%mu_minus(2))
 g%mu_gi = sum (gs%mu_gi)
 g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
 g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
 g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
 g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
 if (associated (g%mu_x)) then

```

```

do i = 1, num_grids
 g%mu_x = g%mu_x + gs(i)%mu_x
 g%mu_xx = g%mu_xx + gs(i)%mu_xx
end do
g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
end if

```

The following is made a little bit hairy by the fact that `vamp_fork_grid` can't join grids onto a non-existing grid<sup>2</sup> therefore we have to keep a tree of joints. Maybe it would be the right thing to handle this tree of joints as a tree with pointers, but since we need the leaves flattened anyway (as food for multiple `vamp_sample_grid`) we use a similar storage layout for the joints.

101a *<Idioms 101a>*≡ 249c>

```

type(vamp_grid), dimension(:), allocatable :: gx
integer, dimension(:,:), allocatable :: dim
...
allocate (gx(vamp_fork_grid_joints (dim)))
call vamp_fork_grid (g, gs, gx, dim, exc)
...
call vamp_join_grid (g, gs, gx, dim, exc)

```

101b *<Implementation of vamp procedures 77d>*+≡ (75a) <99d 102b>

```

pure recursive subroutine vamp_fork_grid_multi (g, gs, gx, d, exc)
 type(vamp_grid), intent(in) :: g
 type(vamp_grid), dimension(:), intent(inout) :: gs, gx
 integer, dimension(:,:), intent(in) :: d
 type(exception), intent(inout), optional :: exc
 character(len=*), parameter :: FN = "vamp_fork_grid_multi"
 integer :: i, offset, stride, joints_offset, joints_stride
 select case (size (d, dim=2))
 case (0)
 return
 case (1)
 call vamp_fork_grid_single (g, gs, d(1,1), exc)
 case default
 offset = 1
 stride = product (d(2,2:))
 joints_offset = 1 + d(2,1)
 joints_stride = vamp_fork_grid_joints (d(:,2:))
 call vamp_create_empty_grid (gx(1:d(2,1)))
 call vamp_fork_grid_single (g, gx(1:d(2,1)), d(1,1), exc)
 end select
end subroutine vamp_fork_grid_multi

```

---

<sup>2</sup>It would be possible to make it possible by changing many things under the hood, but it doesn't really make sense, anyway.

```

do i = 1, d(2,1)
 call vamp_fork_grid_multi &
 (gx(i), gs(offset:offset+stride-1), &
 gx(joints_offset:joints_offset+joints_stride-1), &
 d(:,2:), exc)
 offset = offset + stride
 joints_offset = joints_offset + joints_stride
end do
end select
end subroutine vamp_fork_grid_multi

```

102a  $\langle$ Declaration of vamp procedures 76b $\rangle + \equiv$  (75a)  $\langle$ 96c 103a $\rangle$

```

public :: vamp_fork_grid_joints

```

$$\sum_{n=1}^{N-1} \prod_{i_n=1}^n d_{i_n} = d_1(1 + d_2(1 + d_3(1 + \dots(1 + d_{N-1})\dots))) \quad (5.23)$$

102b  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 101b 102c $\rangle$

```

pure function vamp_fork_grid_joints (d) result (s)
 integer, dimension(:,:), intent(in) :: d
 integer :: s
 integer :: i
 s = 0
 do i = size (d, dim=2) - 1, 1, -1
 s = (s + 1) * d(2,i)
 end do
end function vamp_fork_grid_joints

```

102c  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 102b 103b $\rangle$

```

pure recursive subroutine vamp_join_grid_multi (g, gs, gx, d, exc)
 type(vamp_grid), intent(inout) :: g
 type(vamp_grid), dimension(:), intent(inout) :: gs, gx
 integer, dimension(:,:), intent(in) :: d
 type(exception), intent(inout), optional :: exc
 character(len=*), parameter :: FN = "vamp_join_grid_multi"
 integer :: i, offset, stride, joints_offset, joints_stride
 select case (size (d, dim=2))
 case (0)
 return
 case (1)
 call vamp_join_grid_single (g, gs, d(1,1), exc)
 case default
 offset = 1
 stride = product (d(2,2:))
 joints_offset = 1 + d(2,1)

```

```

joints_stride = vamp_fork_grid_joints (d(:,2:))
do i = 1, d(2,1)
 call vamp_join_grid_multi &
 (gx(i), gs(offset:offset+stride-1), &
 gx(joints_offset:joints_offset+joints_stride-1), &
 d(:,2:), exc)
 offset = offset + stride
 joints_offset = joints_offset + joints_stride
end do
call vamp_join_grid_single (g, gx(1:d(2,1)), d(1,1), exc)
call vamp_delete_grid (gx(1:d(2,1)))
end select
end subroutine vamp_join_grid_multi

```

### 5.2.5 Parallel Execution

103a *<Declaration of vamp procedures 76b>+≡* (75a) <102a 106c>  
 public :: vamp\_sample\_grid\_parallel  
 public :: vamp\_distribute\_work

HPF [10, 11, 15]:

103b *<Implementation of vamp procedures 77d>+≡* (75a) <102c 105a>  
 subroutine vamp\_sample\_grid\_parallel &  
 (rng, g, func, data, iterations, &  
 integral, std\_dev, avg\_chi2, accuracy, &  
 channel, weights, grids, exc, history)  
 type(tao\_random\_state), dimension(:), intent(inout) :: rng  
 type(vamp\_grid), intent(inout) :: g  
 class(vamp\_data\_t), intent(in) :: data  
 integer, intent(in) :: iterations  
 real(kind=default), intent(out), optional :: integral, std\_dev, avg\_chi2  
 real(kind=default), intent(in), optional :: accuracy  
 integer, intent(in), optional :: channel  
 real(kind=default), dimension(:), intent(in), optional :: weights  
 type(vamp\_grid), dimension(:), intent(in), optional :: grids  
 type(exception), intent(inout), optional :: exc  
 type(vamp\_history), dimension(:), intent(inout), optional :: history  
*<Interface declaration for func 22>*  
 character(len=\*), parameter :: FN = "vamp\_sample\_grid\_parallel"  
 real(kind=default) :: local\_integral, local\_std\_dev, local\_avg\_chi2  
 type(exception), dimension(size(rng)) :: excs  
 type(vamp\_grid), dimension(:), allocatable :: gs, gx  
 !hpf\$ processors p(number\_of\_processors())



```

!hpf$ distribute gs(cyclic(1)) onto p
integer, dimension(:,:), pointer :: d
integer :: iteration, i
integer :: num_workers
nullify (d)
call clear_exception (excs)
iterate: do iteration = 1, iterations
 call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
 num_workers = max (1, product (d(2,:)))
 if (num_workers > 1) then
 allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
 call vamp_create_empty_grid (gs)
 ! vamp_fork_grid is certainly not local. Speed freaks might
 ! want to tune it to the processor topology, but the gain will be small.
 call vamp_fork_grid (g, gs, gx, d, exc)
 !hpf$ independent
 do i = 1, num_workers
 call vamp_sample_grid0 &
 (rng(i), gs(i), func, data, &
 channel, weights, grids, exc)
 end do
 <Gather exceptions in vamp_sample_grid_parallel 104>
 call vamp_join_grid (g, gs, gx, d, exc)
 call vamp_delete_grid (gs)
 deallocate (gs, gx)
 else
 call vamp_sample_grid0 &
 (rng(1), g, func, data, channel, weights, grids, exc)
 end if
 <Bail out if exception exc raised 99a>
 call vamp_average_iterations &
 (g, iteration, local_integral, local_std_dev, local_avg_chi2)
 <Trace results of vamp_sample_grid 106b>
 <Exit iterate if accuracy has been reached 96b>
 if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
deallocate (d)
<Copy results of vamp_sample_grid to dummy variables 96a>
end subroutine vamp_sample_grid_parallel
104 <Gather exceptions in vamp_sample_grid_parallel 104>≡ (103b)
 if ((present (exc)) .and. (any (excs(1:num_workers)%level > 0))) then
 call gather_exceptions (exc, excs(1:num_workers))
 end if

```

We could sort  $d$  such that (5.23) is minimized

$$d_1 \leq d_2 \leq \dots \leq d_N \quad (5.24)$$

but the gain will be negligible.

```

105a <Implementation of vamp procedures 77d>+≡ (75a) <103b 106e>
 pure subroutine vamp_distribute_work (num_workers, ng, d)
 integer, intent(in) :: num_workers
 integer, dimension(:), intent(in) :: ng
 integer, dimension(:, :), pointer :: d
 integer, dimension(32) :: factors
 integer :: n, num_factors, i, j
 integer, dimension(size(ng)) :: num_forks
 integer :: nfork
 try: do n = num_workers, 1, -1
 call factorize (n, factors, num_factors)
 num_forks = 1
 do i = num_factors, 1, -1
 j = sum (maxloc (ng / num_forks))
 nfork = num_forks(j) * factors(i)
 if (nfork <= ng(j)) then
 num_forks(j) = nfork
 else
 cycle try
 end if
 end do
 <Accept distribution among n workers 105b>
 end do try
 end subroutine vamp_distribute_work

105b <Accept distribution among n workers 105b>≡ (105a) 105c>
 j = count (num_forks > 1)
 if (associated (d)) then
 if (size (d, dim = 2) /= j) then
 deallocate (d)
 allocate (d(2, j))
 end if
 else
 allocate (d(2, j))
 end if

105c <Accept distribution among n workers 105b>+≡ (105a) <105b
 j = 1
 do i = 1, size (ng)
 if (num_forks(i) > 1) then

```

```

 d(:,j) = (/ i, num_forks(i) /)
 j = j + 1
 end if
end do
return

```

## 5.2.6 Diagnostics

- 106a *<Declaration of vamp types 77a>+≡* (75a) *<77b 112>*
- ```

type, public :: vamp_history
  private
  real(kind=default) :: &
    integral, std_dev, avg_integral, avg_std_dev, avg_chi2, f_min, f_max
  integer :: calls
  logical :: stratified
  logical :: verbose
  type(div_history), dimension(:), pointer :: div => null ()
end type vamp_history

```
- 106b *<Trace results of vamp_sample_grid 106b>≡* (94c 103b)
- ```

if (present (history)) then
 if (iteration <= size (history)) then
 call vamp_get_history &
 (history(iteration), g, local_integral, local_std_dev, &
 local_avg_chi2)
 else
 call raise_exception (exc, EXC_WARN, FN, "history too short")
 end if
 call vamp_terminate_history (history(iteration+1:))
end if

```
- 106c *<Declaration of vamp procedures 76b>+≡* (75a) *<103a 108a>*
- ```

public :: vamp_create_history, vamp_copy_history, vamp_delete_history
public :: vamp_terminate_history
public :: vamp_get_history, vamp_get_history_single

```
- 106d *<Interfaces of vamp procedures 95c>+≡* (75a) *<96d 108b>*
- ```

interface vamp_get_history
 module procedure vamp_get_history_single
end interface

```
- 106e *<Implementation of vamp procedures 77d>+≡* (75a) *<105a 107a>*
- ```

elemental subroutine vamp_create_history (h, ndim, verbose)
  type(vamp_history), intent(out) :: h
  integer, intent(in), optional :: ndim

```

```

logical, intent(in), optional :: verbose
if (present (verbose)) then
    h%verbose = verbose
else
    h%verbose = .false.
end if
h%calls = 0.0
if (h%verbose .and. (present (ndim))) then
    if (associated (h%div)) then
        deallocate (h%div)
    end if
    allocate (h%div(ndim))
end if
end subroutine vamp_create_history
107a <Implementation of vamp procedures 77d>+≡ (75a) <106e 107b>
    elemental subroutine vamp_terminate_history (h)
        type(vamp_history), intent(inout) :: h
        h%calls = 0.0
    end subroutine vamp_terminate_history
107b <Implementation of vamp procedures 77d>+≡ (75a) <107a 108c>
    pure subroutine vamp_get_history_single (h, g, integral, std_dev, avg_chi2)
        type(vamp_history), intent(inout) :: h
        type(vamp_grid), intent(in) :: g
        real(kind=default), intent(in) :: integral, std_dev, avg_chi2
        h%calls = g%calls
        h%stratified = g%all_stratified
        h%integral = g%mu(1)
        h%std_dev = sqrt (g%mu(2))
        h%avg_integral = integral
        h%avg_std_dev = std_dev
        h%avg_chi2 = avg_chi2
        h%f_min = g%f_min
        h%f_max = g%f_max
        if (h%verbose) then
            <Adjust h%div iff necessary 107c>
            call copy_history (h%div, summarize_division (g%div))
        end if
    end subroutine vamp_get_history_single
107c <Adjust h%div iff necessary 107c>≡ (107b)
    if (associated (h%div)) then
        if (size (h%div) /= size (g%div)) then
            deallocate (h%div)

```

```

        allocate (h%div(size(g%div)))
    end if
else
    allocate (h%div(size(g%div)))
end if

108a <Declaration of vamp procedures 76b>+≡ (75a) <106c 113a>
    public :: vamp_print_history, vamp_write_history
    private :: vamp_print_one_history, vamp_print_histories
    ! private :: vamp_write_one_history, vamp_write_histories

108b <Interfaces of vamp procedures 95c>+≡ (75a) <106d 124b>
    interface vamp_print_history
        module procedure vamp_print_one_history, vamp_print_histories
    end interface
    interface vamp_write_history
        module procedure vamp_write_one_history_unit, vamp_write_histories_unit
    end interface

108c <Implementation of vamp procedures 77d>+≡ (75a) <107b 109b>
    subroutine vamp_print_one_history (h, tag)
        type(vamp_history), dimension(:), intent(in) :: h
        character(len=*), intent(in), optional :: tag
        type(div_history), dimension(:), allocatable :: h_tmp
        character(len=BUFFER_SIZE) :: pfx
        character(len=1) :: s
        integer :: i, imax, j
        if (present (tag)) then
            pfx = tag
        else
            pfx = "[vamp]"
        end if
        print "(1X,A78)", repeat("-", 78)
        print "(1X,A8,1X,A2,A9,A1,1X,A11,1X,8X,1X," &
            // "1X,A13,1X,8X,1X,A5,1X,A5)", &
            pfx, "it", "#calls", "", "integral", "average", "chi2", "eff."
        imax = size (h)
        iterations: do i = 1, imax
            if (h(i)%calls <= 0) then
                imax = i - 1
                exit iterations
            end if
            ! *JR: Skip zero channel
            if (h(i)%f_max==0) cycle
            if (h(i)%stratified) then

```

```

        s = "*"
    else
        s = ""
    end if
    print "(1X,A8,1X,I2,I9,A1,1X,E11.4,A1,E8.2,A1," &
        // "1X,E13.6,A1,E8.2,A1,F5.1,1X,F5.3)", pfx, &
        i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
        h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &
        h(i)%integral / h(i)%f_max
end do iterations
print "(1X,A78)", repeat("-", 78)
if (all (h%verbose) .and. (imax >= 1)) then
    if (associated (h(1)%div)) then
        allocate (h_tmp(imax))
        dimensions: do j = 1, size (h(1)%div)
            do i = 1, imax
                call copy_history (h_tmp(i), h(i)%div(j))
            end do
            if (present (tag)) then
                write (unit = pfx, fmt = "(A,A1,I2.2)") &
                    trim (tag(1:min(len_trim(tag),8))), "#", j
            else
                write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
            end if
            call print_history (h_tmp, tag = pfx)
            print "(1X,A78)", repeat("-", 78)
        end do dimensions
        deallocate (h_tmp)
    end if
end if
flush (output_unit)
end subroutine vamp_print_one_history

```

109a *<Variables in vamp 78a>+≡* (75a) <94b 146a>
integer, private, parameter :: BUFFER_SIZE = 50

109b *<Implementation of vamp procedures 77d>+≡* (75a) <108c 110>
subroutine vamp_print_histories (h, tag)
type(vamp_history), dimension(:,,:), intent(in) :: h
character(len=*), intent(in), optional :: tag
character(len=BUFFER_SIZE) :: pfx
integer :: i
print "(1X,A78)", repeat("=", 78)
channels: do i = 1, size (h, dim=2)
 if (present (tag)) then

```

        write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
    else
        write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
    end if
    call vamp_print_one_history (h(:,i), pfx)
end do channels
print "(1X,A78)", repeat ("=", 78)
flush (output_unit)
end subroutine vamp_print_histories

```

 WK

110 *<Implementation of vamp procedures 77d>+≡ (75a) <109b 113b>*

```

subroutine vamp_write_one_history_unit (u, h, tag)
    integer, intent(in) :: u
    type(vamp_history), dimension(:), intent(in) :: h
    character(len=*), intent(in), optional :: tag
    type(div_history), dimension(:), allocatable :: h_tmp
    character(len=BUFFER_SIZE) :: pfx
    character(len=1) :: s
    integer :: i, imax, j
    if (present (tag)) then
        pfx = tag
    else
        pfx = "[vamp]"
    end if
    write (u, "(1X,A78)") repeat ("-", 78)
    write (u, "(1X,A8,1X,A2,A9,A1,1X,A11,1X,8X,1X," &
        // "1X,A13,1X,8X,1X,A5,1X,A5)") &
        pfx, "it", "#calls", "", "integral", "average", "chi2", "eff."
    imax = size (h)
    iterations: do i = 1, imax
        if (h(i)%calls <= 0) then
            imax = i - 1
            exit iterations
        end if
        ! *WK: Skip zero channel
        if (h(i)%f_max==0) cycle
        if (h(i)%stratified) then
            s = "*"
        else
            s = ""
        end if
        write (u, "(1X,A8,1X,I2,I9,A1,1X,ES11.4,A1,ES8.2,A1," &

```

```

// "1X,ES13.6,A1,ES8.2,A1,F5.1,1X,F5.3)") pfx, &
i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &
h(i)%integral / h(i)%f_max
end do iterations
write (u, "(1X,A78)") repeat ("-", 78)
if (all (h%verbose) .and. (imax >= 1)) then
  if (associated (h(1)%div)) then
    allocate (h_tmp(imax))
    dimensions: do j = 1, size (h(1)%div)
      do i = 1, imax
        call copy_history (h_tmp(i), h(i)%div(j))
      end do
      if (present (tag)) then
        write (unit = pfx, fmt = "(A,A1,I2.2)") &
          trim (tag(1:min(len_trim(tag),8))), "#", j
      else
        write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
      end if
      call write_history (u, h_tmp, tag = pfx)
      print "(1X,A78)", repeat ("-", 78)
    end do dimensions
    deallocate (h_tmp)
  end if
end if
flush (u)
end subroutine vamp_write_one_history_unit
subroutine vamp_write_histories_unit (u, h, tag)
  integer, intent(in) :: u
  type(vamp_history), dimension(:, :), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  character(len=BUFFER_SIZE) :: pfx
  integer :: i
  write (u, "(1X,A78)") repeat ("=", 78)
  channels: do i = 1, size (h, dim=2)
    if (present (tag)) then
      write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
    else
      write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
    end if
    call vamp_write_one_history_unit (u, h(:,i), pfx)
  end do channels
  write (u, "(1X,A78)") repeat ("=", 78)

```



```
flush (u)
end subroutine vamp_write_histories_unit
```

5.2.7 Multi Channel

[23]

$$g(x) = \sum_i \alpha_i g_i(x) \quad (5.25a)$$

$$w(x) = \frac{f(x)}{g(x)} \quad (5.25b)$$

We want to minimize the variance $W(\alpha)$ with the subsidiary condition $\sum_i \alpha_i = 1$. We introduce a Lagrange multiplier λ :

$$\tilde{W}(\alpha) = W(\alpha) + \lambda \left(\sum_i \alpha_i - 1 \right) \quad (5.26)$$

Therefore...

$$W_i(\alpha) = -\frac{\partial}{\partial \alpha_i} W(\alpha) = \int dx g_i(x) (w(x))^2 \approx \left\langle \frac{g_i(x)}{g(x)} (w(x))^2 \right\rangle \quad (5.27)$$



Here it *really* hurts that **Fortran** has no *first-class* functions. The following can be expressed much more elegantly in a functional programming language with *first-class* functions, currying and closures. **Fortran** makes it extra painful since not even procedure pointers are supported. This puts extra burden on the users of this library.

Note that the components of **vamp_grids** are not protected. However, this is not a license for application programs to access it. Only Other libraries (e.g. for parallel processing, like **vampi**) should do so.

```
112 <Declaration of vamp types 77a>+≡ (75a) <106a
    type, public :: vamp_grids
        !!! private ! used by vampi
        real(kind=default), dimension(:), pointer :: weights => null ()
        type(vamp_grid), dimension(:), pointer :: grids => null ()
        integer, dimension(:), pointer :: num_calls => null ()
        real(kind=default) :: sum_chi2, sum_integral, sum_weights
    end type vamp_grids
```

$$g \circ \phi_i = \left| \frac{\partial \phi_i}{\partial x} \right|^{-1} \left(\alpha_i g_i + \sum_{\substack{j=1 \\ j \neq i}}^{N_c} \alpha_j (g_j \circ \pi_{ij}) \left| \frac{\partial \pi_{ij}}{\partial x} \right| \right). \quad (5.28)$$

113a *<Declaration of vamp procedures 76b>+≡* (75a) *<108a 114a>*
`public :: vamp_multi_channel, vamp_multi_channel0`

113b *<Implementation of vamp procedures 77d>+≡* (75a) *<110 113c>*
`function vamp_multi_channel &`
`(func, data, phi, ihp, jacobian, x, weights, channel, grids) result (w_x)`
`class(vamp_data_t), intent(in) :: data`
`real(kind=default), dimension(:), intent(in) :: x`
`real(kind=default), dimension(:), intent(in) :: weights`
`integer, intent(in) :: channel`
`type(vamp_grid), dimension(:), intent(in) :: grids`
<Interface declaration for func 22>
<Interface declaration for phi 31a>
<Interface declaration for ihp 31b>
<Interface declaration for jacobian 31c>
`real(kind=default) :: w_x`
`integer :: i`
`real(kind=default), dimension(size(x)) :: phi_x`
`real(kind=default), dimension(size(weights)) :: g_phi_x, g_pi_x`
`phi_x = phi (x, channel)`
`do i = 1, size (weights)`
`if (i == channel) then`
`g_pi_x(i) = vamp_probability (grids(i), x)`
`else`
`g_pi_x(i) = vamp_probability (grids(i), ihp (phi_x, i))`
`end if`
`end do`
`do i = 1, size (weights)`
`g_phi_x(i) = g_pi_x(i) / g_pi_x(channel) * jacobian (phi_x, data, i)`
`end do`
`w_x = func (phi_x, data, weights, channel, grids) &`
`/ dot_product (weights, g_phi_x)`
`end function vamp_multi_channel`

113c *<Implementation of vamp procedures 77d>+≡* (75a) *<113b 114b>*
`function vamp_multi_channel0 &`
`(func, data, phi, jacobian, x, weights, channel) result (w_x)`
`class(vamp_data_t), intent(in) :: data`
`real(kind=default), dimension(:), intent(in) :: x`
`real(kind=default), dimension(:), intent(in) :: weights`

```

integer, intent(in) :: channel
<Interface declaration for func 22>
<Interface declaration for phi 31a>
<Interface declaration for jacobian 31c>
real(kind=default) :: w_x
real(kind=default), dimension(size(x)) :: x_prime
real(kind=default), dimension(size(weights)) :: g_phi_x
integer :: i
x_prime = phi (x, channel)
do i = 1, size (weights)
    g_phi_x(i) = jacobian (x_prime, data, i)
end do
w_x = func (x_prime, data) / dot_product (weights, g_phi_x)
end function vamp_multi_channel0

```



WK

114a <Declaration of vamp procedures 76b>+≡ (75a) <113a 117a>
 public :: vamp_jacobian, vamp_check_jacobian

114b <Implementation of vamp procedures 77d>+≡ (75a) <113c 115>
 pure subroutine vamp_jacobian (phi, channel, x, region, jacobian, delta_x)
 integer, intent(in) :: channel
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:, :), intent(in) :: region
 real(kind=default), intent(out) :: jacobian
 real(kind=default), intent(in), optional :: delta_x
 interface
 pure function phi (xi, channel) result (x)
 use kinds
 real(kind=default), dimension(:), intent(in) :: xi
 integer, intent(in) :: channel
 real(kind=default), dimension(size(xi)) :: x
 end function phi
 end interface
 real(kind=default), dimension(size(x)) :: x_min, x_max
 real(kind=default), dimension(size(x)) :: x_plus, x_minus
 real(kind=default), dimension(size(x), size(x)) :: d_phi
 real(kind=default), parameter :: &
 dx_default = 10.0_default**(-precision(jacobian)/3)
 real(kind=default) :: dx
 integer :: j
 if (present (delta_x)) then
 dx = delta_x

```

else
    dx = dx_default
end if
x_min = region(1,:)
x_max = region(2,:)
x_minus = max (x_min, x)
x_plus = min (x_max, x)
do j = 1, size (x)
    x_minus(j) = max (x_min(j), x(j) - dx)
    x_plus(j) = min (x_max(j), x(j) + dx)
    d_phi(:,j) = (phi (x_plus, channel) - phi (x_minus, channel)) &
        / (x_plus(j) - x_minus(j))
    x_minus(j) = max (x_min(j), x(j))
    x_plus(j) = min (x_max(j), x(j))
end do
call determinant (d_phi, jacobian)
jacobian = abs (jacobian)
end subroutine vamp_jacobian

```

$$g(\phi(x)) = \frac{1}{\left| \frac{\partial \phi}{\partial x} \right| (x)} \quad (5.29)$$

115 *<Implementation of vamp procedures 77d>+≡ (75a) <114b 117b>*

```

subroutine vamp_check_jacobian &
    (rng, n, func, data, phi, channel, region, delta, x_delta)
type(tao_random_state), intent(inout) :: rng
integer, intent(in) :: n
class(vamp_data_t), intent(in) :: data
integer, intent(in) :: channel
real(kind=default), dimension(:,,:), intent(in) :: region
real(kind=default), intent(out) :: delta
real(kind=default), dimension(:), intent(out), optional :: x_delta
<Interface declaration for func 22>
<Interface declaration for phi 31a>
real(kind=default), dimension(size(region,dim=2)) :: x, r
real(kind=default) :: jac, d
real(kind=default), dimension(0) :: wgts
integer :: i
delta = 0.0
do i = 1, max (1, n)
    call tao_random_number (rng, r)
    x = region(1,:) + (region(2,:) - region(1,:)) * r
    call vamp_jacobian (phi, channel, x, region, jac)
    d = func (phi (x, channel), data, wgts, channel) * jac &
        - 1.0_default

```

```

    if (abs (d) >= abs (delta)) then
        delta = d
        if (present (x_delta)) then
            x_delta = x
        end if
    end if
end do
end subroutine vamp_check_jacobian

```

This is a subroutine to comply with F's rules, otherwise, we would code it as a function.

116a *<Declaration of vamp procedures (removed from WHIZARD) 116a>≡*

```
private :: numeric_jacobian
```

116b *<Implementation of vamp procedures (removed from WHIZARD) 116b>≡*

```

pure subroutine numeric_jacobian (phi, channel, x, region, jacobian, delta_x)
    integer, intent(in) :: channel
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:, :), intent(in) :: region
    real(kind=default), intent(out) :: jacobian
    real(kind=default), intent(in), optional :: delta_x
    <Interface declaration for phi 31a>
    real(kind=default), dimension(size(x)) :: x_min, x_max
    real(kind=default), dimension(size(x)) :: x_plus, x_minus
    real(kind=default), dimension(size(x), size(x)) :: d_phi
    real(kind=default), parameter :: &
        dx_default = 10.0_default**(-precision(jacobian)/3)
    real(kind=default) :: dx
    integer :: j
    if (present (delta_x)) then
        dx = delta_x
    else
        dx = dx_default
    end if
    x_min = region(1, :)
    x_max = region(2, :)
    x_minus = max (x_min, x)
    x_plus = min (x_max, x)
    do j = 1, size (x)
        x_minus(j) = max (x_min(j), x(j) - dx)
        x_plus(j) = min (x_max(j), x(j) + dx)
        d_phi(:, j) = (phi (x_plus, channel) - phi (x_minus, channel)) &
            / (x_plus(j) - x_minus(j))
        x_minus(j) = max (x_min(j), x(j))
    end do

```

```

        x_plus(j) = min (x_max(j), x(j))
    end do
    call determinant (d_phi, jacobian)
    jacobian = abs (jacobian)
end subroutine numeric_jacobian

```

117a *<Declaration of vamp procedures 76b>+≡* (75a) *<114a 118b>*

```

    public :: vamp_create_grids, vamp_create_empty_grids
    public :: vamp_copy_grids, vamp_delete_grids

```

The rules for optional arguments forces us to handle special cases, because we can't just pass a array section of an optional array as an actual argument (cf. 12.4.1.5(4) in [9]) even if the dummy argument is optional itself.

117b *<Implementation of vamp procedures 77d>+≡* (75a) *<115 118a>*

```

pure subroutine vamp_create_grids &
    (g, domain, num_calls, weights, maps, num_div, &
     stratified, quadrupole, exc)
type(vamp_grids), intent(inout) :: g
real(kind=default), dimension(:,,:), intent(in) :: domain
integer, intent(in) :: num_calls
real(kind=default), dimension(:), intent(in) :: weights
real(kind=default), dimension(:,:,:), intent(in), optional :: maps
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
character(len=*), parameter :: FN = "vamp_create_grids"
integer :: ch, nch
nch = size (weights)
allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
g%weights = weights / sum (weights)
g%num_calls = g%weights * num_calls
do ch = 1, size (g%grids)
    if (present (maps)) then
        call vamp_create_grid &
            (g%grids(ch), domain, g%num_calls(ch), num_div, &
             stratified, quadrupole, map = maps(:, :, ch), exc = exc)
    else
        call vamp_create_grid &
            (g%grids(ch), domain, g%num_calls(ch), num_div, &
             stratified, quadrupole, exc = exc)
    end if
end do
g%sum_integral = 0.0
g%sum_chi2 = 0.0

```

```

    g%sum_weights = 0.0
end subroutine vamp_create_grids
118a <Implementation of vamp procedures 77d>+≡ (75a) <117b 118c>
    pure subroutine vamp_create_empty_grids (g)
        type(vamp_grids), intent(inout) :: g
        nullify (g%grids, g%weights, g%num_calls)
    end subroutine vamp_create_empty_grids
118b <Declaration of vamp procedures 76b>+≡ (75a) <117a 118d>
    public :: vamp_discard_integrals
118c <Implementation of vamp procedures 77d>+≡ (75a) <118a 118e>
    pure subroutine vamp_discard_integrals &
        (g, num_calls, num_div, stratified, quadrupole, exc, eq)
        type(vamp_grids), intent(inout) :: g
        integer, intent(in), optional :: num_calls
        integer, dimension(:), intent(in), optional :: num_div
        logical, intent(in), optional :: stratified, quadrupole
        type(exception), intent(inout), optional :: exc
        type(vamp_equivalences_t), intent(in), optional :: eq
        integer :: ch
        character(len=*), parameter :: FN = "vamp_discard_integrals"
        g%sum_integral = 0.0
        g%sum_weights = 0.0
        g%sum_chi2 = 0.0
        do ch = 1, size (g%grids)
            call vamp_discard_integral (g%grids(ch))
        end do
        if (present (num_calls)) then
            call vamp_reshape_grids &
                (g, num_calls, num_div, stratified, quadrupole, exc, eq)
        end if
    end subroutine vamp_discard_integrals
118d <Declaration of vamp procedures 76b>+≡ (75a) <118b 119a>
    public :: vamp_update_weights
    We must discard the accumulated integrals, because the weight function  $w = f / \sum_i \alpha_i g_i$  changes:
118e <Implementation of vamp procedures 77d>+≡ (75a) <118c 119b>
    pure subroutine vamp_update_weights &
        (g, weights, num_calls, num_div, stratified, quadrupole, exc)
        type(vamp_grids), intent(inout) :: g
        real(kind=default), dimension(:), intent(in) :: weights
        integer, intent(in), optional :: num_calls

```

```

integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
character(len=*), parameter :: FN = "vamp_update_weights"
if (sum (weights) > 0) then
    g%weights = weights / sum (weights)
else
    g%weights = 1._default / size(g%weights)
end if
if (present (num_calls)) then
    call vamp_discard_integrals (g, num_calls, num_div, &
                                stratified, quadrupole, exc)
else
    call vamp_discard_integrals (g, sum (g%num_calls), num_div, &
                                stratified, quadrupole, exc)
end if
end subroutine vamp_update_weights
119a  <Declaration of vamp procedures 76b>+≡ (75a) <118d 120a>
      public :: vamp_reshape_grids
119b  <Implementation of vamp procedures 77d>+≡ (75a) <118e 120b>
      pure subroutine vamp_reshape_grids &
          (g, num_calls, num_div, stratified, quadrupole, exc, eq)
      type(vamp_grids), intent(inout) :: g
      integer, intent(in) :: num_calls
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole
      type(exception), intent(inout), optional :: exc
      type(vamp_equivalences_t), intent(in), optional :: eq
      integer, dimension(size(g%grids(1)%num_div)) :: num_div_new
      integer :: ch
      character(len=*), parameter :: FN = "vamp_reshape_grids"
      g%num_calls = g%weights * num_calls
      do ch = 1, size (g%grids)
          if (g%num_calls(ch) >= 2) then
              if (present (eq)) then
                  if (present (num_div)) then
                      num_div_new = num_div
                  else
                      num_div_new = g%grids(ch)%num_div
                  end if
                  where (eq%div_is_invariant(ch,:))
                      num_div_new = 1
                  end where
              end if
          end if
      end do

```



```

        call vamp_reshape_grid (g%grids(ch), g%num_calls(ch), &
                                num_div_new, stratified, quadrupole, exc = exc, &
                                independent = eq%independent(ch), &
                                equivalent_to_ch = eq%equivalent_to_ch(ch), &
                                multiplicity = eq%multiplicity(ch))
    else
        call vamp_reshape_grid (g%grids(ch), g%num_calls(ch), &
                                num_div, stratified, quadrupole, exc = exc)
    end if
else
    g%num_calls(ch) = 0
end if
end do
end subroutine vamp_reshape_grids

```

120a *<Declaration of vamp procedures 76b>+≡* (75a) <119a 122b>
 public :: vamp_sample_grids

Even if `g%num_calls` is derived from `g%weights`, we must *not* use the latter, allow for integer arithmetic in `g%num_calls`.

120b *<Implementation of vamp procedures 77d>+≡* (75a) <119b 122c>
 subroutine vamp_sample_grids &
 (rng, g, func, data, iterations, integral, std_dev, avg_chi2, &
 accuracy, history, histories, exc, eq, warn_error, negative_weights)
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grids), intent(inout) :: g
 class(vamp_data_t), intent(in) :: data
 integer, intent(in) :: iterations
 real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
 real(kind=default), intent(in), optional :: accuracy
 type(vamp_history), dimension(:), intent(inout), optional :: history
 type(vamp_history), dimension(:, :), intent(inout), optional :: histories
 type(exception), intent(inout), optional :: exc
 type(vamp_equivalences_t), intent(in), optional :: eq
 logical, intent(in), optional :: warn_error, negative_weights
<Interface declaration for func 22>
 integer :: ch, iteration
 logical :: neg_w
 type(exception), dimension(size(g%grids)) :: excs
 logical, dimension(size(g%grids)) :: active
 real(kind=default), dimension(size(g%grids)) :: weights, integrals, std_devs
 real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
 character(len=*), parameter :: FN = "vamp_sample_grids"
 integrals = 0

```

std_devs = 0
neg_w = .false.
if (present (negative_weights)) neg_w = negative_weights
active = (g%num_calls >= 2)
where (active)
  weights = g%num_calls
elsewhere
  weights = 0.0
endwhere
if (sum (weights) /= 0) weights = weights / sum (weights)
call clear_exception (excs)
iterate: do iteration = 1, iterations
  do ch = 1, size (g%grids)
    if (active(ch)) then
      call vamp_discard_integral (g%grids(ch))
      <Sample the grid g%grids(ch) 122a>
    else
      call vamp_nullify_variance (g%grids(ch))
      call vamp_nullify_covariance (g%grids(ch))
    end if
  end do
  if (present(eq)) call vamp_apply_equivalences (g, eq)
  if (iteration < iterations) then
    do ch = 1, size (g%grids)
      active(ch) = (integrals(ch) /= 0)
      if (active(ch)) then
        call vamp_refine_grid (g%grids(ch))
      end if
    end do
  end if
  if (present (exc) .and. (any (excs%level > 0))) then
    call gather_exceptions (exc, excs)
!    return
  end if
  call vamp_reduce_channels (g, integrals, std_devs, active)
  call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
  <Trace results of vamp_sample_grids 124d>
  <Exit iterate if accuracy has been reached 96b>
end do iterate
<Copy results of vamp_sample_grid to dummy variables 96a>
end subroutine vamp_sample_grids

```

We must refine the grids after *all* grids have been sampled, therefore we use `vamp_sample_grid0` instead of `vamp_sample_grid`:

```

122a <Sample the grid g%grids(ch) 122a>≡ (120b)
    call vamp_sample_grid0 &
        (rng, g%grids(ch), func, data, &
         ch, weights, g%grids, excs(ch), neg_w)
    if (present (exc) .and. present (warn_error)) then
        if (warn_error) call handle_exception (excs(ch))
    end if
    call vamp_average_iterations &
        (g%grids(ch), iteration, integrals(ch), std_devs(ch), local_avg_chi2)
    if (present (histories)) then
        if (iteration <= ubound (histories, dim=1)) then
            call vamp_get_history &
                (histories(iteration,ch), g%grids(ch), &
                 integrals(ch), std_devs(ch), local_avg_chi2)
        else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
        end if
        call vamp_terminate_history (histories(iteration+1:,ch))
    end if

122b <Declaration of vamp procedures 76b>+≡ (75a) <120a 123a>
    public :: vamp_reduce_channels

```

$$I = \frac{1}{N} \sum_c N_c I_c \quad (5.30a)$$

$$\sigma^2 = \frac{1}{N^2} \sum_c N_c^2 \sigma_c^2 \quad (5.30b)$$

$$N = \sum_c N_c \quad (5.30c)$$

where (5.30b) is actually

$$\sigma^2 = \frac{1}{N} (\mu_2 - \mu_1^1) = \frac{1}{N} \left(\frac{1}{N} \sum_c N_c \mu_{2,c} - I^2 \right) = \frac{1}{N} \left(\frac{1}{N} \sum_c (N_c^2 \sigma_c^2 + N_c I_c^2) - I^2 \right)$$

but the latter form suffers from numerical instability and (5.30b) is thus preferred.

```

122c <Implementation of vamp procedures 77d>+≡ (75a) <120b 123b>
    pure subroutine vamp_reduce_channels (g, integrals, std_devs, active)

```

```

type(vamp_grids), intent(inout) :: g
real(kind=default), dimension(:), intent(in) :: integrals, std_devs
logical, dimension(:), intent(in) :: active
real(kind=default) :: this_integral, this_weight, total_calls
real(kind=default) :: total_variance
if (.not.any(active)) return
total_calls = sum (g%num_calls, mask=active)
if (total_calls > 0) then
    this_integral = sum (g%num_calls * integrals, mask=active) / total_calls
else
    this_integral = 0
end if
total_variance = sum ((g%num_calls*std_devs)**2, mask=active)
if (total_variance > 0) then
    this_weight = total_calls**2 / total_variance
else
    this_weight = 0
end if
g%sum_weights = g%sum_weights + this_weight
g%sum_integral = g%sum_integral + this_weight * this_integral
g%sum_chi2 = g%sum_chi2 + this_weight * this_integral**2
end subroutine vamp_reduce_channels

```

123a *<Declaration of vamp procedures 76b>+≡* (75a) <122b 124a>
 public :: vamp_refine_weights

123b *<Implementation of vamp procedures 77d>+≡* (75a) <122c 124c>
 elemental subroutine vamp_average_iterations_grids &
 (g, iteration, integral, std_dev, avg_chi2)
 type(vamp_grids), intent(in) :: g
 integer, intent(in) :: iteration
 real(kind=default), intent(out) :: integral, std_dev, avg_chi2
 real(kind=default), parameter :: eps = 1000 * epsilon (1._default)
 if (g%sum_weights>0) then
 integral = g%sum_integral / g%sum_weights
 std_dev = sqrt (1.0 / g%sum_weights)
 avg_chi2 = &
 max ((g%sum_chi2 - g%sum_integral * integral) / (iteration-0.99), &
 0.0_default)
 if (avg_chi2 < eps * g%sum_chi2) avg_chi2 = 0
 else
 integral = 0
 std_dev = 0
 avg_chi2 = 0
 end if

```

        end subroutine vamp_average_iterations_grids
124a  <Declaration of vamp procedures 76b>+≡ (75a) <123a 124e>
        private :: vamp_average_iterations_grids
124b  <Interfaces of vamp procedures 95c>+≡ (75a) <108b 124f>
        interface vamp_average_iterations
            module procedure vamp_average_iterations_grids
        end interface


$$\alpha_i \rightarrow \alpha_i \sqrt{V_i} \quad (5.31)$$

124c  <Implementation of vamp procedures 77d>+≡ (75a) <123b 125a>
        pure subroutine vamp_refine_weights (g, power)
            type(vamp_grids), intent(inout) :: g
            real(kind=default), intent(in), optional :: power
            real(kind=default) :: local_power
            real(kind=default), parameter :: DEFAULT_POWER = 0.5_default
            if (present (power)) then
                local_power = power
            else
                local_power = DEFAULT_POWER
            end if
            call vamp_update_weights &
                (g, g%weights * vamp_get_variance (g%grids) ** local_power)
        end subroutine vamp_refine_weights
124d  <Trace results of vamp_sample_grids 124d>≡ (120b)
        if (present (history)) then
            if (iteration <= size (history)) then
                call vamp_get_history &
                    (history(iteration), g, local_integral, local_std_dev, &
                     local_avg_chi2)
            else
                call raise_exception (exc, EXC_WARN, FN, "history too short")
            end if
            call vamp_terminate_history (history(iteration+1:))
        end if
124e  <Declaration of vamp procedures 76b>+≡ (75a) <124a 125b>
        private :: vamp_get_history_multi
124f  <Interfaces of vamp procedures 95c>+≡ (75a) <124b 130c>
        interface vamp_get_history
            module procedure vamp_get_history_multi
        end interface

```

125a *Implementation of vamp procedures 77d*+≡ (75a) <124c 125c>

```

pure subroutine vamp_get_history_multi (h, g, integral, std_dev, avg_chi2)
  type(vamp_history), intent(inout) :: h
  type(vamp_grids), intent(in) :: g
  real(kind=default), intent(in) :: integral, std_dev, avg_chi2
  h%calls = sum (g%grids%calls)
  h%stratified = all (g%grids%all_stratified)
  h%integral = 0.0
  h%std_dev = 0.0
  h%avg_integral = integral
  h%avg_std_dev = std_dev
  h%avg_chi2 = avg_chi2
  h%f_min = 0.0
  h%f_max = huge (h%f_max)
  if (h%verbose) then
    h%verbose = .false.
    if (associated (h%div)) then
      deallocate (h%div)
    end if
  end if
end subroutine vamp_get_history_multi

```



125b *Declaration of vamp procedures 76b*+≡ (75a) <124e 126>

```

public :: vamp_sum_channels

```

125c *Implementation of vamp procedures 77d*+≡ (75a) <125a 127b>

```

function vamp_sum_channels (x, weights, func, data, grids) result (g)
  real(kind=default), dimension(:), intent(in) :: x, weights
  class(vamp_data_t), intent(in) :: data
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  interface
    function func (xi, data, weights, channel, grids) result (f)
      use kinds
      use vamp_grid_type !NODEP!
      import vamp_data_t
      real(kind=default), dimension(:), intent(in) :: xi
      class(vamp_data_t), intent(in) :: data
      real(kind=default), dimension(:), intent(in), optional :: weights
      integer, intent(in), optional :: channel
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: f
    end function func
  end interface


```

```

end interface
real(kind=default) :: g
integer :: ch
g = 0.0
do ch = 1, size (weights)
    g = g + weights(ch) * func (x, data, weights, ch, grids)
end do
end function vamp_sum_channels

```

5.2.8 Mapping

 This section is still under construction. The basic algorithm is in place, but the heuristics have not been developed yet.

The most naive approach is to use the rotation matrix R that diagonalizes the covariance C :

$$R_{ij} = (v_j)_i \quad (5.32)$$

where

$$Cv_j = \lambda_j v_j \quad (5.33)$$

with the eigenvalues $\{\lambda_j\}$ and eigenvectors $\{v_j\}$. Then

$$R^T C R = \text{diag}(\lambda_1, \dots) \quad (5.34)$$

After call `diagonalize_real_symmetric (cov, evals, evects)`, we have `evals(j) = λ_j` and `evects(:,j) = v_j` . This is equivalent with `evects(i,j) = R_{ij}` .

This approach will not work in high dimensions, however. In general, R will *not* leave most of the axes invariant, even if the covariance matrix is almost isotropic in these directions. In this case the benefit from the rotation is rather small and offset by the negative effects from the misalignment of the integration region.

A better strategy is to find the axis of the original coordinate system around which a rotation is most beneficial. There are two extreme cases:

- “pancake”: one eigenvalue much smaller than the others
- “cigar”: one eigenvalue much larger than the others

Actually, instead of rotating around a specific axis, we can as well diagonalize in a subspace. Empirically, rotation around an axis is better than diagonalizing in a two-dimensional subspace, but diagonalizing in a three-dimensional subspace can be even better.

```

126  <Declaration of vamp procedures 76b>+≡ (75a) <125b 128a>
      public :: select_rotation_axis
      public :: select_rotation_subspace

127a  <Set iv to the index of the optimal eigenvector 127a>≡ (129a 130a)
      if (num_pancake > 0) then
        print *, "FORCED PANCAKE: ", num_pancake
        iv = sum (minloc (evals))
      else if (num_cigar > 0) then
        print *, "FORCED CIGAR: ", num_cigar
        iv = sum (maxloc (evals))
      else
        call more_pancake_than_cigar (evals, like_pancake)
        if (like_pancake) then
          iv = sum (minloc (evals))
        else
          iv = sum (maxloc (evals))
        end if
      end if

127b  <Implementation of vamp procedures 77d>+≡ (75a) <125c 129a>
      subroutine more_pancake_than_cigar (eval, yes_or_no)
        real(kind=default), dimension(:), intent(in) :: eval
        logical, intent(out) :: yes_or_no
        integer, parameter :: N_CL = 2
        real(kind=default), dimension(size(eval)) :: evals
        real(kind=default), dimension(N_CL) :: cluster_pos
        integer, dimension(N_CL,2) :: clusters
        evals = eval
        call sort (evals)
        call condense (evals, cluster_pos, clusters)
        print *, clusters(1,2) - clusters(1,1) + 1, "small EVs: ", &
          evals(clusters(1,1):clusters(1,2))
        print *, clusters(2,2) - clusters(2,1) + 1, "large EVs: ", &
          evals(clusters(2,1):clusters(2,2))
        if ((clusters(1,2) - clusters(1,1)) &
          < (clusters(2,2) - clusters(2,1))) then
          print *, " => PANCAKE!"
          yes_or_no = .true.
        else
          print *, " => CIGAR!"
          yes_or_no = .false.
        end if
      end subroutine more_pancake_than_cigar

```


128a \langle Declaration of `vamp` procedures 76b $\rangle + \equiv$ (75a) \triangleleft 126 130d \triangleright
`private :: more_pancake_than_cigar`

In both cases, we can rotate in the plane P_{ij} closest to eigenvector corresponding to the the singled out eigenvalue. This plane is given by

$$\max_{i \neq i'} \sqrt{(v_j)_i^2 + (v_j)_{i'}^2} \quad (5.35)$$

which is simply found by looking for the two largest $|(v_j)_i|$:³

128b \langle Set `i(1)`, `i(2)` to the axes of the optimal plane 128b $\rangle \equiv$ (129a) 128d \triangleright
`abs_evec = abs (evecs(:,iv))`
`i(1) = sum (maxloc (abs_evec))`
`abs_evec(i(1)) = -1.0`
`i(2) = sum (maxloc (abs_evec))`

The following is cute, but unfortunately broken, since it fails for degenerate eigenvalues:

128c \langle Set `i(1)`, `i(2)` to the axes of the optimal plane (broken!) 128c $\rangle \equiv$
`abs_evec = abs (evecs(:,iv))`
`i(1) = sum (maxloc (abs_evec))`
`i(2) = sum (maxloc (abs_evec, mask = abs_evec < abs_evec(i(1))))`

128d \langle Set `i(1)`, `i(2)` to the axes of the optimal plane 128b $\rangle + \equiv$ (129a) \triangleleft 128b \triangleright
`print *, iv, evals(iv), " => ", evecs(:,iv)`
`print *, i(1), abs_evec(i(1)), ", ", i(2), abs_evec(i(2))`
`print *, i(1), evecs(i(1),iv), ", ", i(2), evecs(i(2),iv)`

128e \langle Get $\cos \theta$ and $\sin \theta$ from `evecs` 128e $\rangle \equiv$ (129a)
`cos_theta = evecs(i(1),iv)`
`sin_theta = evecs(i(2),iv)`
`norm = 1.0 / sqrt (cos_theta**2 + sin_theta**2)`
`cos_theta = cos_theta * norm`
`sin_theta = sin_theta * norm`

$$\hat{R}(\theta; i, j) = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & \cos \theta & \cdots & -\sin \theta \\ & & \vdots & 1 & \vdots \\ & & \sin \theta & \cdots & \cos \theta & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \quad (5.36)$$

³The `sum` intrinsic is a convenient Fortran90 trick for turning the rank-one array with one element returned by `maxloc` into its value. It has no semantic significance.

```

128f   $\langle \text{Construct } \hat{R}(\theta; i, j) \text{ 128f} \rangle \equiv$  (129a)
      call unit (r)
      r(i(1),i) = (/ cos_theta, - sin_theta /)
      r(i(2),i) = (/ sin_theta, cos_theta /)

129a   $\langle \text{Implementation of vamp procedures 77d} \rangle + \equiv$  (75a)  $\langle 127b \text{ 129c} \rangle$ 
      subroutine select_rotation_axis (cov, r, pancake, cigar)
        real(kind=default), dimension(:, :), intent(in) :: cov
        real(kind=default), dimension(:, :), intent(out) :: r
        integer, intent(in), optional :: pancake, cigar
        integer :: num_pancake, num_cigar
        logical :: like_pancake
        real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evecs
        real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
        integer :: iv
        integer, dimension(2) :: i
        real(kind=default) :: cos_theta, sin_theta, norm
         $\langle \text{Handle optional pancake and cigar 129b} \rangle$ 
        call diagonalize_real_symmetric (cov, evals, evecs)
         $\langle \text{Set iv to the index of the optimal eigenvector 127a} \rangle$ 
         $\langle \text{Set i(1), i(2) to the axes of the optimal plane 128b} \rangle$ 
         $\langle \text{Get cos } \theta \text{ and sin } \theta \text{ from evecs 128e} \rangle$ 
         $\langle \text{Construct } \hat{R}(\theta; i, j) \text{ 128f} \rangle$ 
      end subroutine select_rotation_axis

129b   $\langle \text{Handle optional pancake and cigar 129b} \rangle \equiv$  (129a 130a)
      if (present (pancake)) then
        num_pancake = pancake
      else
        num_pancake = -1
      endif
      if (present (cigar)) then
        num_cigar = cigar
      else
        num_cigar = -1
      endif

```

Here's a less efficient version that can be easily generalized to more than two dimension, however:

```

129c   $\langle \text{Implementation of vamp procedures 77d} \rangle + \equiv$  (75a)  $\langle 129a \text{ 130a} \rangle$ 
      subroutine select_subspace_explicit (cov, r, subspace)
        real(kind=default), dimension(:, :), intent(in) :: cov
        real(kind=default), dimension(:, :), intent(out) :: r
        integer, dimension(:), intent(in) :: subspace
        real(kind=default), dimension(size(subspace)) :: eval_sub

```

```

    real(kind=default), dimension(size(subspace),size(subspace)) :: &
        cov_sub, evec_sub
    cov_sub = cov(subspace,subspace)
    call diagonalize_real_symmetric (cov_sub, eval_sub, evec_sub)
    call unit (r)
    r(subspace,subspace) = evec_sub
end subroutine select_subspace_explicit
130a <Implementation of vamp procedures 77d>+≡ (75a) <129c 131a>
    subroutine select_subspace_guess (cov, r, ndim, pancake, cigar)
    real(kind=default), dimension(:,,:), intent(in) :: cov
    real(kind=default), dimension(:,,:), intent(out) :: r
    integer, intent(in) :: ndim
    integer, intent(in), optional :: pancake, cigar
    integer :: num_pancake, num_cigar
    logical :: like_pancake
    real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evecs
    real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
    integer :: iv, i
    integer, dimension(ndim) :: subspace
    <Handle optional pancake and cigar 129b>
    call diagonalize_real_symmetric (cov, evals, evecs)
    <Set iv to the index of the optimal eigenvector 127a>
    <Set subspace to the axes of the optimal plane 130b>
    call select_subspace_explicit (cov, r, subspace)
end subroutine select_subspace_guess
130b <Set subspace to the axes of the optimal plane 130b>≡ (130a)
    abs_evec = abs (evecs(:,iv))
    subspace(1) = sum (maxloc (abs_evec))
    do i = 2, ndim
        abs_evec(subspace(i-1)) = -1.0
        subspace(i) = sum (maxloc (abs_evec))
    end do
130c <Interfaces of vamp procedures 95c>+≡ (75a) <124f 135a>
    interface select_rotation_subspace
    module procedure select_subspace_explicit, select_subspace_guess
    end interface
130d <Declaration of vamp procedures 76b>+≡ (75a) <128a 130e>
    private :: select_subspace_explicit
    private :: select_subspace_guess
130e <Declaration of vamp procedures 76b>+≡ (75a) <130d 131b>
    public :: vamp_print_covariance

```

131a \langle Implementation of vamp procedures 77d $\rangle + \equiv$ (75a) \langle 130a 133b \rangle

```

subroutine vamp_print_covariance (cov)
  real(kind=default), dimension(:, :), intent(in) :: cov
  real(kind=default), dimension(size(cov,dim=1)) :: &
    evals, abs_evals, tmp
  real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: &
    evecs, abs_evecs
  integer, dimension(size(cov,dim=1)) :: idx
  integer :: i, i_max, j
  i_max = size (evals)
  call diagonalize_real_symmetric (cov, evals, evecs)
  call sort (evals, evecs)
  abs_evals = abs (evals)
  abs_evecs = abs (evecs)
  print "(1X,A78)", repeat ("-", 78)
  print "(1X,A)", "Eigenvalues and eigenvectors:"
  print "(1X,A78)", repeat ("-", 78)
  do i = 1, i_max
    print "(1X,I2,A1,1X,E11.4,1X,A1,10(1X,F5.2)/,18X))", &
      i, ":", evals(i), "|", evecs(:,i)
  end do
  print "(1X,A78)", repeat ("-", 78)
  print "(1X,A)", "Approximate subspaces:"
  print "(1X,A78)", repeat ("-", 78)
  do i = 1, i_max
    idx = (/ (j, j=1,i_max) /)
    tmp = abs_evecs(:,i)
    call sort (tmp, idx, reverse = .true.)
    print "(1X,I2,A1,1X,E11.4,1X,A1,10(1X,I5))", &
      i, ":", evals(i), "|", idx(1:min(10,size(idx)))
    print "(17X,A1,10(1X,F5.2))", &
      "|", evecs(idx(1:min(10,size(idx))),i)
  end do
  print "(1X,A78)", repeat ("-", 78)
end subroutine vamp_print_covariance

```

Condensing Eigenvalues

In order to decide whether we have a “pancake” or a “cigar”, we have to classify the eigenvalues of the covariance matrix. We do this by condensing the n_{dim} eigenvalues into $n_{\text{cl}} \ll n_{\text{dim}}$ clusters.

131b \langle Declaration of vamp procedures 76b $\rangle + \equiv$ (75a) \langle 130e 133c \rangle

```

! private :: condense

```

```
public :: condense
```

The rough description is as follows: in each step, combine the nearest neighbours (according to an appropriate metric) to form a smaller set. This is an extremely simplified, discretized modeling of molecules condensing under the influence of some potential.

⚡ If there's not a clean separation, this algorithm is certainly chaotic and we need to apply some form of damping!

```
132a <Initialize clusters 132a>≡ (133b)
      cl_pos = x
      cl_num = size (cl_pos)
      cl = spread ((/ (i, i=1,cl_num) /), dim = 2, ncopies = 2)
```

It appears that the logarithmic metric

$$d_0(x, y) = \left| \log \left(\frac{x}{y} \right) \right| \quad (5.37a)$$

performs better than the linear metric

$$d_1(x, y) = |x - y| \quad (5.37b)$$

since the latter won't separate very small eigenvalues from the bulk. Another option is

$$d_\alpha(x, y) = |x^\alpha - y^\alpha| \quad (5.37c)$$

with $\alpha \neq 1$, in particular $\alpha \approx -1$. I haven't studied it yet, though.

⚡ but I should perform more empirical studies to determine whether the logarithmic or the linear metric is more appropriate in realistic cases.

```
132b <Join closest clusters 132b>≡ (133b) 133a>
      if (linear_metric) then
        gap = sum (minloc (cl_pos(2:cl_num) - cl_pos(1:cl_num-1)))
      else
        gap = sum (minloc (cl_pos(2:cl_num) / cl_pos(1:cl_num-1)))
      end if
      wgt0 = cl(gap,2) - cl(gap,1) + 1
      wgt1 = cl(gap+1,2) - cl(gap+1,1) + 1
      cl_pos(gap) = (wgt0 * cl_pos(gap) + wgt1 * cl_pos(gap+1)) / (wgt0 + wgt1)
      cl(gap,2) = cl(gap+1,2)
```

133a *Join closest clusters 132b*)+≡ (133b) <132b

```
cl_pos(gap+1:cl_num-1) = cl_pos(gap+2:cl_num)
cl(gap+1:cl_num-1,:) = cl(gap+2:cl_num,:)
```

133b *Implementation of vamp procedures 77d*)+≡ (75a) <131a 133d>

```
subroutine condense (x, cluster_pos, clusters, linear)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(out) :: cluster_pos
  integer, dimension(:,:), intent(out) :: clusters
  logical, intent(in), optional :: linear
  logical :: linear_metric
  real(kind=default), dimension(size(x)) :: cl_pos
  real(kind=default) :: wgt0, wgt1
  integer :: cl_num
  integer, dimension(size(x),2) :: cl
  integer :: i, gap
  linear_metric = .false.
  if (present (linear)) then
    linear_metric = linear
  end if
  Initialize clusters 132a
  do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
    Join closest clusters 132b
    print *, cl_num, ": action = ", condense_action (x, cl)
  end do
  cluster_pos = cl_pos(1:cl_num)
  clusters = cl(1:cl_num,:)
end subroutine condense
```

133c *Declaration of vamp procedures 76b*)+≡ (75a) <131b 134b>

```
! private :: condense_action
public :: condense_action
```

$$S = \sum_{c \in \text{clusters}} \text{var}^{\frac{\alpha}{2}}(c) \quad (5.38)$$

133d *Implementation of vamp procedures 77d*)+≡ (75a) <133b 135c>

```
function condense_action (positions, clusters) result (s)
  real(kind=default), dimension(:), intent(in) :: positions
  integer, dimension(:,:), intent(in) :: clusters
  real(kind=default) :: s
  integer :: i
  integer, parameter :: POWER = 2
  s = 0
  do i = 1, size (clusters, dim = 1)
    s = s + standard_deviation (positions(clusters(i,1) &
```

```

                                                    :clusters(i,2))) ** POWER
        end do
    end function condense_action
134a <ctest.f90 134a>≡
    program ctest
        use kinds
        use utils
        use vamp_stat
        use tao_random_numbers
        use vamp
        implicit none
        integer, parameter :: N = 16, NC = 2
        real(kind=default), dimension(N) :: eval
        real(kind=default), dimension(NC) :: cluster_pos
        integer, dimension(NC,2) :: clusters
        integer :: i
        call tao_random_number (eval)
        call sort (eval)
        print *, eval
        eval(1:N/2) = 0.95*eval(1:N/2)
        eval(N/2+1:N) = 1.0 - 0.95*(1.0 - eval(N/2+1:N))
        print *, eval
        call condense (eval, cluster_pos, clusters, linear=.true.)
        do i = 1, NC
            print "(I2,A,F5.2,A,I2,A,I2,A,A,F5.2,A,F5.2,A,32F5.2)", &
                i, ":", cluster_pos(i), &
                " [", clusters(i,1), "-", clusters(i,2), "]", &
                " [", eval(clusters(i,1)), " - ", eval(clusters(i,2)), "]", &
                eval(clusters(i,1)+1:clusters(i,2)) &
                - eval(clusters(i,1):clusters(i,2)-1)
            print *, average (eval(clusters(i,1):clusters(i,2))), "+/-", &
                standard_deviation (eval(clusters(i,1):clusters(i,2)))
        end do
    end program ctest

```

5.2.9 Event Generation

Automagically adaptive tools are not always appropriate for unweighted event generation, but we can give it a try.

```

134b <Declaration of vamp procedures 76b>+≡ (75a) <133c 135b>
    public :: vamp_next_event

```

135a *<Interfaces of vamp procedures 95c>+≡* (75a) <130c 140b>

```
interface vamp_next_event
  module procedure vamp_next_event_single, vamp_next_event_multi
end interface
```

135b *<Declaration of vamp procedures 76b>+≡* (75a) <134b 138d>

```
private :: vamp_next_event_single, vamp_next_event_multi
```

Both event generation routines operate in two modes, depending on whether the optional argument `weight` is present.

135c *<Implementation of vamp procedures 77d>+≡* (75a) <133d 136c>

```
subroutine vamp_next_event_single &
  (x, rng, g, func, data, &
   weight, channel, weights, grids, exc)
  real(kind=default), dimension(:), intent(out) :: x
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  real(kind=default), intent(out), optional :: weight
  class(vamp_data_t), intent(in) :: data
  integer, intent(in), optional :: channel
  real(kind=default), dimension(:), intent(in), optional :: weights
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  type(exception), intent(inout), optional :: exc
  <Interface declaration for func 22>
  character(len=*), parameter :: FN = "vamp_next_event_single"
  real(kind=default), dimension(size(g%div)):: wgts
  real(kind=default), dimension(size(g%div)):: r
  integer, dimension(size(g%div)):: ia
  real(kind=default) :: f, wgt
  real(kind=default) :: r0
  rejection: do
    <Choose a x and calculate f(x) 135d>
    if (present (weight)) then
      <Unconditionally accept weighted event 136a>
    else
      <Maybe accept unweighted event 136b>
    end if
  end do rejection
end subroutine vamp_next_event_single
```

135d *<Choose a x and calculate f(x) 135d>≡* (135c)

```
call tao_random_number (rng, r)
call inject_division_short (g%div, real(r, kind=default), x, ia, wgts)
wgt = g%jacobi * product (wgts)
wgt = g%calls * wgt ! the calling procedure will divide by #calls
```



```

    if (associated (g%map)) then
        x = matmul (g%map, x)
    end if
    <f = wgt * func (x, weights, channel), iff x inside true_domain 88a>
    ! call record_efficiency (g%div, ia, f/g%f_max)
136a <Unconditionally accept weighted event 136a>≡ (135c)
    weight = f
    exit rejection
136b <Maybe accept unweighted event 136b>≡ (135c)
    if (f > g%f_max) then
        g%f_max = f
        call raise_exception (exc, EXC_WARN, FN, "weight > 1")
        exit rejection
    end if
    call tao_random_number (rng, r0)
    if (r0 * g%f_max <= f) then
        exit rejection
    end if

```

We know that `g%weights` are normalized: `sum (g%weights) == 1.0`. The basic formula for multi channel sampling is

$$f(x) = \sum_i \alpha_i g_i(x) w(x) \quad (5.39)$$

with $w(x) = f(x)/g(x) = f(x)/\sum_i \alpha_i g_i(x)$ and $\sum_i \alpha_i = 1$. The non-trivial problem is that the adaptive grid is different in each channel, so we can't just reject on $w(x)$.

```

136c <Implementation of vamp procedures 77d>+≡ (75a) <135c 139a>
    subroutine vamp_next_event_multi &
        (x, rng, g, func, data, phi, weight, excess, positive, exc)
    real(kind=default), dimension(:), intent(out) :: x
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids), intent(inout) :: g
    class(vamp_data_t), intent(in) :: data
    real(kind=default), intent(out), optional :: weight
    real(kind=default), intent(out), optional :: excess
    logical, intent(out), optional :: positive
    type(exception), intent(inout), optional :: exc
    <Interface declaration for func 22>
    <Interface declaration for phi 31a>
    character(len=*), parameter :: FN = "vamp_next_event_multi"
    real(kind=default), dimension(size(x)) :: xi

```

```

real(kind=default) :: r, wgt
real(kind=default), dimension(size(g%weights)) :: weights
integer :: channel
⟨weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  137a⟩
rejection: do
  ⟨Select channel from weights 137b⟩
  call vamp_next_event_single &
    (xi, rng, g%grids(channel), func, data, wgt, &
     channel, g%weights, g%grids, exc)
  if (present (weight)) then
    ⟨Unconditionally accept weighted multi channel event 138a⟩
  else
    ⟨Maybe accept unweighted multi channel event 138b⟩
  end if
end do rejection
x = phi (xi, channel)
end subroutine vamp_next_event_multi

```

We can either reject with the weights

$$\frac{w_i(x)}{\max_i \max_x w_i(x)} \quad (5.40)$$

after using the apriori weights α_i to select a channel i or we can reject with the weights

$$\frac{w_i(x)}{\max_x w_i(x)} \quad (5.41)$$

after using the apriori weights $\alpha_i(\max_x w_i(x))/(\max_i \max_x w_i(x))$. The latter method is more efficient if the $\max_x w_i(x)$ have a wide spread.

137a ⟨weights: $\alpha_i \rightarrow w_{\max,i}\alpha_i$ 137a⟩≡ (136c 138c)

```

if (any (g%grids%f_max > 0)) then
  weights = g%weights * g%grids%f_max
else
  weights = g%weights
end if
weights = weights / sum (weights)

```

137b ⟨Select channel from weights 137b⟩≡ (136c)

```

call tao_random_number (rng, r)
select_channel: do channel = 1, size (g%weights)
  r = r - weights(channel)
  if (r <= 0.0) then
    exit select_channel
  end if
end do

```

```

end do select_channel
channel = min (channel, size (g%weights)) ! for  $r = 1$  and rounding errors
138a  $\langle$ Unconditionally accept weighted multi channel event 138a $\rangle \equiv$  (136c)
weight = wgt * g%weights(channel) / weights(channel)
exit rejection
138b  $\langle$ Maybe accept unweighted multi channel event 138b $\rangle \equiv$  (136c)
if (abs (wgt) > g%grids(channel)%f_max) then
  if (present(excess)) then
    excess = abs (wgt) / g%grids(channel)%f_max - 1
  else
    call raise_exception (exc, EXC_WARN, FN, "weight > 1")
!    print *, "weight > 1 (", wgt/g%grids(channel)%f_max, &
!    & ") in channel ", channel

    end if
! exit rejection
else
  if (present(excess)) excess = 0
end if
call tao_random_number (rng, r)
if (r * g%grids(channel)%f_max <= abs (wgt)) then
  if (present (positive)) positive = wgt >= 0
  exit rejection
end if
138c  $\langle$ Maybe accept unweighted multi channel event (old version) 138c $\rangle \equiv$ 
if (wgt > g%grids(channel)%f_max) then
  g%grids(channel)%f_max = wgt
   $\langle$ weights:  $\alpha_i \rightarrow w_{\max,i} \alpha_i$  137a $\rangle$ 
  call raise_exception (exc, EXC_WARN, FN, "weight > 1")
  exit rejection
end if
call tao_random_number (rng, r)
if (r * g%grids(channel)%f_max <= wgt) then
  exit rejection
end if

```

Using `vamp_sample_grid` (`g`, ...) to warm up the grid `g` has a somewhat subtle problem: the minimum and maximum weights `g%f_min` and `g%f_max` refer to the grid *before* the final refinement. One could require an additional `vamp_sample_grid0` (`g`, ...), but users are likely to forget such technical details. A better solution is a wrapper `vamp_warmup_grid` (`g`, ...) that drops the final refinement transparently.

138d *<Declaration of vamp procedures 76b>+≡* (75a) <135b 140a>

```
public :: vamp_warmup_grid, vamp_warmup_grids
```

139a *<Implementation of vamp procedures 77d>+≡* (75a) <136c 139b>

```
subroutine vamp_warmup_grid &
  (rng, g, func, data, iterations, exc, history)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  class(vamp_data_t), intent(in) :: data
  integer, intent(in) :: iterations
  type(exception), intent(inout), optional :: exc
  type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
  call vamp_sample_grid &
    (rng, g, func, data, &
      iterations - 1, exc = exc, history = history)
  call vamp_sample_grid0 (rng, g, func, data, exc = exc)
end subroutine vamp_warmup_grid
```



WHERE ... END WHERE alert!

139b *<Implementation of vamp procedures 77d>+≡* (75a) <139a 140c>

```
subroutine vamp_warmup_grids &
  (rng, g, func, data, iterations, history, histories, exc)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grids), intent(inout) :: g
  class(vamp_data_t), intent(in) :: data
  integer, intent(in) :: iterations
  type(vamp_history), dimension(:), intent(inout), optional :: history
  type(vamp_history), dimension(:, :), intent(inout), optional :: histories
  type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>
  integer :: ch
  logical, dimension(size(g%grids)) :: active
  real(kind=default), dimension(size(g%grids)) :: weights
  active = (g%num_calls >= 2)
  where (active)
    weights = g%num_calls
  elsewhere
    weights = 0.0
  end where
  weights = weights / sum (weights)
  call vamp_sample_grids (rng, g, func, data, iterations - 1, &
    exc = exc, history = history, histories = histories)
```

```

do ch = 1, size (g%grids)
  if (g%grids(ch)%num_calls >= 2) then
    call vamp_sample_grid0 &
      (rng, g%grids(ch), func, data, &
       ch, weights, g%grids, exc = exc)
  end if
end do
end subroutine vamp_warmup_grids

```

5.2.10 Convenience Routines

- 140a *<Declaration of vamp procedures 76b>+≡* (75a) <138d 141b>

```

public :: vamp_integrate
private :: vamp_integrate_grid, vamp_integrate_region

```
- 140b *<Interfaces of vamp procedures 95c>+≡* (75a) <135a 142a>

```

interface vamp_integrate
  module procedure vamp_integrate_grid, vamp_integrate_region
end interface

```
- 140c *<Implementation of vamp procedures 77d>+≡* (75a) <139b 141a>

```

subroutine vamp_integrate_grid &
  (rng, g, func, data, calls, integral, std_dev, avg_chi2, num_div, &
   stratified, quadrupole, accuracy, exc, history)
type(tao_random_state), intent(inout) :: rng
type(vamp_grid), intent(inout) :: g
class(vamp_data_t), intent(in) :: data
integer, dimension(:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_integrate_grid"
integer :: step, last_step, it
last_step = size (calls, dim = 2)
it = 1
do step = 1, last_step - 1
  call vamp_discard_integral (g, calls(2,step), num_div, &
                             stratified, quadrupole, exc = exc)
  call vamp_sample_grid (rng, g, func, data, calls(1,step), &
                        exc = exc, history = history(it:))

```

```

        <Bail out if exception exc raised 99a>
        it = it + calls(1,step)
    end do
    call vamp_discard_integral (g, calls(2,last_step), exc = exc)
    call vamp_sample_grid (rng, g, func, data, calls(1,last_step), &
        integral, std_dev, avg_chi2, accuracy, exc = exc, &
        history = history(it:))
end subroutine vamp_integrate_grid
141a <Implementation of vamp procedures 77d>+≡ (75a) <140c 142b>
subroutine vamp_integrate_region &
    (rng, region, func, data, calls, &
    integral, std_dev, avg_chi2, num_div, &
    stratified, quadrupole, accuracy, map, covariance, exc, history)
type(tao_random_state), intent(inout) :: rng
real(kind=default), dimension(:,:), intent(in) :: region
class(vamp_data_t), intent(in) :: data
integer, dimension(:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
real(kind=default), dimension(:,:), intent(in), optional :: map
real(kind=default), dimension(:,:), intent(out), optional :: covariance
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_integrate_region"
type(vamp_grid) :: g
call vamp_create_grid &
    (g, region, calls(2,1), num_div, &
    stratified, quadrupole, present (covariance), map, exc)
call vamp_integrate_grid &
    (rng, g, func, data, calls, &
    integral, std_dev, avg_chi2, num_div, &
    accuracy = accuracy, exc = exc, history = history)
if (present (covariance)) then
    covariance = vamp_get_covariance (g)
end if
call vamp_delete_grid (g)
end subroutine vamp_integrate_region
141b <Declaration of vamp procedures 76b>+≡ (75a) <140a 143a>
public :: vamp_integratex
private :: vamp_integratex_region

```

142a *<Interfaces of vamp procedures 95c>+≡* (75a) <140b 143c>
 interface vamp_integratex
 module procedure vamp_integratex_region
 end interface

142b *<Implementation of vamp procedures 77d>+≡* (75a) <141a 144b>
 subroutine vamp_integratex_region &
 (rng, region, func, data, calls, integral, std_dev, avg_chi2, &
 num_div, stratified, quadrupole, accuracy, pancake, cigar, &
 exc, history)
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), dimension(:,:), intent(in) :: region
 class(vamp_data_t), intent(in) :: data
 integer, dimension(:,:,:), intent(in) :: calls
 real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
 integer, dimension(:), intent(in), optional :: num_div
 logical, intent(in), optional :: stratified, quadrupole
 real(kind=default), intent(in), optional :: accuracy
 integer, intent(in), optional :: pancake, cigar
 type(exception), intent(inout), optional :: exc
 type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
 real(kind=default), dimension(size(region,dim=2)) :: eval
 real(kind=default), dimension(size(region,dim=2),size(region,dim=2)) :: evec
 type(vamp_grid) :: g
 integer :: step, last_step, it
 it = 1
 call vamp_create_grid &
 (g, region, calls(2,1,1), num_div, &
 stratified, quadrupole, covariance = .true., exc = exc)
 call vamp_integrate_grid &
 (rng, g, func, data, calls(:, :, 1), num_div = num_div, &
 exc = exc, history = history(it:))
<Bail out if exception exc raised 99a>
 it = it + sum (calls(1, :, 1))
 last_step = size (calls, dim = 3)
 do step = 2, last_step - 1
 call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
 call sort (eval, evec)
 call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
 call vamp_delete_grid (g)
 call vamp_create_grid &
 (g, region, calls(2,1,step), num_div, stratified, quadrupole, &
 covariance = .true., map = evec, exc = exc)

```

call vamp_integrate_grid &
  (rng, g, func, data, calls(:, :, step), num_div = num_div, &
   exc = exc, history = history(it:))
  <Bail out if exception exc raised 99a>
  it = it + sum (calls(1, :, step))
end do
call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
call sort (eval, evec)
call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
call vamp_delete_grid (g)
call vamp_create_grid &
  (g, region, calls(2, 1, last_step), num_div, stratified, quadrupole, &
   covariance = .true., map = evec, exc = exc)
call vamp_integrate_grid &
  (rng, g, func, data, calls(:, :, last_step), &
   integral, std_dev, avg_chi2, &
   num_div = num_div, exc = exc, history = history(it:))
call vamp_delete_grid (g)
end subroutine vamp_integratex_region

```

5.2.11 I/O

- 143a <Declaration of vamp procedures 76b>+≡ (75a) <141b 143b>
- ```

public :: vamp_write_grid
private :: write_grid_unit, write_grid_name
public :: vamp_read_grid
private :: read_grid_unit, read_grid_name
public :: vamp_write_grids
private :: write_grids_unit, write_grids_name
public :: vamp_read_grids
private :: read_grids_unit, read_grids_name

```
- 143b <Declaration of vamp procedures 76b>+≡ (75a) <143a 157c>
- ```

public :: vamp_read_grids_raw
private :: read_grids_raw_unit, read_grids_raw_name
public :: vamp_read_grid_raw
private :: read_grid_raw_unit, read_grid_raw_name
public :: vamp_write_grids_raw
private :: write_grids_raw_unit, write_grids_raw_name
public :: vamp_write_grid_raw
private :: write_grid_raw_unit, write_grid_raw_name

```
- 143c <Interfaces of vamp procedures 95c>+≡ (75a) <142a 144a>
- ```

interface vamp_write_grid

```



```

 module procedure write_grid_unit, write_grid_name
end interface
interface vamp_read_grid
 module procedure read_grid_unit, read_grid_name
end interface
interface vamp_write_grids
 module procedure write_grids_unit, write_grids_name
end interface
interface vamp_read_grids
 module procedure read_grids_unit, read_grids_name
end interface
144a <Interfaces of vamp procedures 95c>+≡ (75a) <143c
interface vamp_write_grid_raw
 module procedure write_grid_raw_unit, write_grid_raw_name
end interface
interface vamp_read_grid_raw
 module procedure read_grid_raw_unit, read_grid_raw_name
end interface
interface vamp_write_grids_raw
 module procedure write_grids_raw_unit, write_grids_raw_name
end interface
interface vamp_read_grids_raw
 module procedure read_grids_raw_unit, read_grids_raw_name
end interface
144b <Implementation of vamp procedures 77d>+≡ (75a) <142b 146b>
subroutine write_grid_unit (g, unit, write_integrals)
 type(vamp_grid), intent(in) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: write_integrals
 integer :: i, j
 write (unit = unit, fmt = descr_fmt) "begin type(vamp_grid) :: g"
 write (unit = unit, fmt = integer_fmt) "size (g%div) = ", size (g%div)
 write (unit = unit, fmt = integer_fmt) "num_calls = ", g%num_calls
 write (unit = unit, fmt = integer_fmt) "calls_per_cell = ", g%calls_per_cell
 write (unit = unit, fmt = logical_fmt) "stratified = ", g%stratified
 write (unit = unit, fmt = logical_fmt) "all_stratified = ", g%all_stratified
 write (unit = unit, fmt = logical_fmt) "quadrupole = ", g%quadrupole
 write (unit = unit, fmt = double_fmt) "mu(1) = ", g%mu(1)
 write (unit = unit, fmt = double_fmt) "mu(2) = ", g%mu(2)
 write (unit = unit, fmt = double_fmt) "mu_plus(1) = ", g%mu_plus(1)
 write (unit = unit, fmt = double_fmt) "mu_plus(2) = ", g%mu_plus(2)
 write (unit = unit, fmt = double_fmt) "mu_minus(1) = ", g%mu_minus(1)
 write (unit = unit, fmt = double_fmt) "mu_minus(2) = ", g%mu_minus(2)

```

```

write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
write (unit = unit, fmt = double_fmt) "calls = ", g%calls
write (unit = unit, fmt = double_fmt) "dv2g = ", g%dv2g
write (unit = unit, fmt = double_fmt) "jacobi = ", g%jacobi
write (unit = unit, fmt = double_fmt) "f_min = ", g%f_min
write (unit = unit, fmt = double_fmt) "f_max = ", g%f_max
write (unit = unit, fmt = double_fmt) "mu_gi = ", g%mu_gi
write (unit = unit, fmt = double_fmt) "sum_mu_gi = ", g%sum_mu_gi
write (unit = unit, fmt = descr_fmt) "begin g%num_div"
do i = 1, size (g%div)
 write (unit = unit, fmt = integer_array_fmt) i, g%num_div(i)
end do
write (unit = unit, fmt = descr_fmt) "end g%num_div"
write (unit = unit, fmt = descr_fmt) "begin g%div"
do i = 1, size (g%div)
 call write_division (g%div(i), unit, write_integrals)
end do
write (unit = unit, fmt = descr_fmt) "end g%div"
if (associated (g%map)) then
 write (unit = unit, fmt = descr_fmt) "begin g%map"
 do i = 1, size (g%div)
 do j = 1, size (g%div)
 write (unit = unit, fmt = double_array2_fmt) i, j, g%map(i,j)
 end do
 end do
 write (unit = unit, fmt = descr_fmt) "end g%map"
else
 write (unit = unit, fmt = descr_fmt) "empty g%map"
end if
if (associated (g%mu_x)) then
 write (unit = unit, fmt = descr_fmt) "begin g%mu_x"
 do i = 1, size (g%div)
 write (unit = unit, fmt = double_array_fmt) i, g%mu_x(i)
 write (unit = unit, fmt = double_array_fmt) i, g%sum_mu_x(i)
 do j = 1, size (g%div)
 write (unit = unit, fmt = double_array2_fmt) i, j, g%mu_xx(i,j)
 write (unit = unit, fmt = double_array2_fmt) i, j, g%sum_mu_xx(i,j)
 end do
 end do
 write (unit = unit, fmt = descr_fmt) "end g%mu_x"
else

```

```

 write (unit = unit, fmt = descr_fmt) "empty g%mu_x"
 end if
 write (unit = unit, fmt = descr_fmt) "end type(vamp_grid)"
end subroutine write_grid_unit

146a <Variables in vamp 78a>+≡ (75a) <109a
character(len=*), parameter, private :: &
 descr_fmt = "(1x,a)", &
 integer_fmt = "(1x,a17,1x,i15)", &
 integer_array_fmt = "(1x,i17,1x,i15)", &
 logical_fmt = "(1x,a17,1x,l1)", &
 double_fmt = "(1x,a17,1x,e30.22e4)", &
 double_array_fmt = "(1x,i17,1x,e30.22e4)", &
 double_array2_fmt = "(2(1x,i8),1x,e30.22e4)"

146b <Implementation of vamp procedures 77d>+≡ (75a) <144b 148d>
subroutine read_grid_unit (g, unit, read_integrals)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: read_integrals
 character(len=*), parameter :: FN = "vamp_read_grid"
 character(len=80) :: chdum
 integer :: ndim, i, j, idum, jdum
 read (unit = unit, fmt = descr_fmt) chdum
 read (unit = unit, fmt = integer_fmt) chdum, ndim
 <Insure that size (g%div) == ndim 148a>
 call create_array_pointer (g%num_div, ndim)
 read (unit = unit, fmt = integer_fmt) chdum, g%num_calls
 read (unit = unit, fmt = integer_fmt) chdum, g%calls_per_cell
 read (unit = unit, fmt = logical_fmt) chdum, g%stratified
 read (unit = unit, fmt = logical_fmt) chdum, g%all_stratified
 read (unit = unit, fmt = logical_fmt) chdum, g%quadrupole
 read (unit = unit, fmt = double_fmt) chdum, g%mu(1)
 read (unit = unit, fmt = double_fmt) chdum, g%mu(2)
 read (unit = unit, fmt = double_fmt) chdum, g%mu_plus(1)
 read (unit = unit, fmt = double_fmt) chdum, g%mu_plus(2)
 read (unit = unit, fmt = double_fmt) chdum, g%mu_minus(1)
 read (unit = unit, fmt = double_fmt) chdum, g%mu_minus(2)
 read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
 read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
 read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
 read (unit = unit, fmt = double_fmt) chdum, g%calls
 read (unit = unit, fmt = double_fmt) chdum, g%dv2g
 read (unit = unit, fmt = double_fmt) chdum, g%jacobi
 read (unit = unit, fmt = double_fmt) chdum, g%f_min

```

```

read (unit = unit, fmt = double_fmt) chdum, g%f_max
read (unit = unit, fmt = double_fmt) chdum, g%mu_gi
read (unit = unit, fmt = double_fmt) chdum, g%sum_mu_gi
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
 read (unit = unit, fmt = integer_array_fmt) idum, g%num_div(i)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
 call read_division (g%div(i), unit, read_integrals)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
if (chdum == "begin g%map") then
 call create_array_pointer (g%map, (/ ndim, ndim /))
 do i = 1, size (g%div)
 do j = 1, size (g%div)
 read (unit = unit, fmt = double_array2_fmt) idum, jdum, g%map(i,j)
 end do
 end do
 read (unit = unit, fmt = descr_fmt) chdum
else
 <Insure that associated (g%map) == .false. 148b>
end if
read (unit = unit, fmt = descr_fmt) chdum
if (chdum == "begin g%mu_x") then
 call create_array_pointer (g%mu_x, ndim)
 call create_array_pointer (g%sum_mu_x, ndim)
 call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
 call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
 do i = 1, size (g%div)
 read (unit = unit, fmt = double_array_fmt) idum, jdum, g%mu_x(i)
 read (unit = unit, fmt = double_array_fmt) idum, jdum, g%sum_mu_x(i)
 do j = 1, size (g%div)
 read (unit = unit, fmt = double_array2_fmt) &
 idum, jdum, g%mu_xx(i,j)
 read (unit = unit, fmt = double_array2_fmt) &
 idum, jdum, g%sum_mu_xx(i,j)
 end do
 end do
 read (unit = unit, fmt = descr_fmt) chdum
else

```

```

 <Insure that associated (g%mu_x) == .false. 148c>
 end if
 read (unit = unit, fmt = descr_fmt) chdum
end subroutine read_grid_unit

148a <Insure that size (g%div) == ndim 148a>≡ (146b 153 160)
 if (associated (g%div)) then
 if (size (g%div) /= ndim) then
 call delete_division (g%div)
 deallocate (g%div)
 allocate (g%div(ndim))
 call create_empty_division (g%div)
 end if
 else
 allocate (g%div(ndim))
 call create_empty_division (g%div)
 end if

148b <Insure that associated (g%map) == .false. 148b>≡ (146b 153 160)
 if (associated (g%map)) then
 deallocate (g%map)
 end if

148c <Insure that associated (g%mu_x) == .false. 148c>≡ (146b 153 160)
 if (associated (g%mu_x)) then
 deallocate (g%mu_x)
 end if
 if (associated (g%mu_xx)) then
 deallocate (g%mu_xx)
 end if
 if (associated (g%sum_mu_x)) then
 deallocate (g%sum_mu_x)
 end if
 if (associated (g%sum_mu_xx)) then
 deallocate (g%sum_mu_xx)
 end if

148d <Implementation of vamp procedures 77d>+≡ (75a) <146b 149a>
 subroutine write_grid_name (g, name, write_integrals)
 type(vamp_grid), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: write_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", file = name)
 call write_grid_unit (g, unit, write_integrals)

```

```

 close (unit = unit)
 end subroutine write_grid_name
149a <Implementation of vamp procedures 77d>+≡ (75a) <148d 149b>
 subroutine read_grid_name (g, name, read_integrals)
 type(vamp_grid), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: read_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", file = name)
 call read_grid_unit (g, unit, read_integrals)
 close (unit = unit)
 end subroutine read_grid_name
149b <Implementation of vamp procedures 77d>+≡ (75a) <149a 149c>
 subroutine write_grids_unit (g, unit, write_integrals)
 type(vamp_grids), intent(in) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: write_integrals
 integer :: i
 write (unit = unit, fmt = descr_fmt) "begin type(vamp_grids) :: g"
 write (unit = unit, fmt = integer_fmt) "size (g%grids) = ", size (g%grids)
 write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
 write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
 write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
 write (unit = unit, fmt = descr_fmt) "begin g%weights"
 do i = 1, size (g%grids)
 write (unit = unit, fmt = double_array_fmt) i, g%weights(i)
 end do
 write (unit = unit, fmt = descr_fmt) "end g%weights"
 write (unit = unit, fmt = descr_fmt) "begin g%num_calls"
 do i = 1, size (g%grids)
 write (unit = unit, fmt = integer_array_fmt) i, g%num_calls(i)
 end do
 write (unit = unit, fmt = descr_fmt) "end g%num_calls"
 write (unit = unit, fmt = descr_fmt) "begin g%grids"
 do i = 1, size (g%grids)
 call write_grid_unit (g%grids(i), unit, write_integrals)
 end do
 write (unit = unit, fmt = descr_fmt) "end g%grids"
 write (unit = unit, fmt = descr_fmt) "end type(vamp_grids)"
 end subroutine write_grids_unit
149c <Implementation of vamp procedures 77d>+≡ (75a) <149b 150>

```

```

subroutine read_grids_unit (g, unit, read_integrals)
 type(vamp_grids), intent(inout) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: read_integrals
 character(len=*), parameter :: FN = "vamp_read_grids"
 character(len=80) :: chdum
 integer :: i, nch, idum
 read (unit = unit, fmt = descr_fmt) chdum
 read (unit = unit, fmt = integer_fmt) chdum, nch
 if (associated (g%grids)) then
 if (size (g%grids) /= nch) then
 call vamp_delete_grid (g%grids)
 deallocate (g%grids, g%weights, g%num_calls)
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
 else
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
 read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
 read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
 read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
 read (unit = unit, fmt = descr_fmt) chdum
 do i = 1, nch
 read (unit = unit, fmt = double_array_fmt) idum, g%weights(i)
 end do
 read (unit = unit, fmt = descr_fmt) chdum
 read (unit = unit, fmt = descr_fmt) chdum
 do i = 1, nch
 read (unit = unit, fmt = integer_array_fmt) idum, g%num_calls(i)
 end do
 read (unit = unit, fmt = descr_fmt) chdum
 read (unit = unit, fmt = descr_fmt) chdum
 do i = 1, nch
 call read_grid_unit (g%grids(i), unit, read_integrals)
 end do
 read (unit = unit, fmt = descr_fmt) chdum
 read (unit = unit, fmt = descr_fmt) chdum
end subroutine read_grids_unit

```

150  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 149c 151a $\rangle$

```

subroutine write_grids_name (g, name, write_integrals)
 type(vamp_grids), intent(inout) :: g

```

```

character(len=*), intent(in) :: name
logical, intent(in), optional :: write_integrals
integer :: unit
call find_free_unit (unit)
open (unit = unit, action = "write", status = "replace", file = name)
call write_grids_unit (g, unit, write_integrals)
close (unit = unit)
end subroutine write_grids_name
151a <Implementation of vamp procedures 77d>+≡ (75a) <150 151b>
subroutine read_grids_name (g, name, read_integrals)
type(vamp_grids), intent(inout) :: g
character(len=*), intent(in) :: name
logical, intent(in), optional :: read_integrals
integer :: unit
call find_free_unit (unit)
open (unit = unit, action = "read", status = "old", file = name)
call read_grids_unit (g, unit, read_integrals)
close (unit = unit)
end subroutine read_grids_name
151b <Implementation of vamp procedures 77d>+≡ (75a) <151a 153>
subroutine write_grid_raw_unit (g, unit, write_integrals)
type(vamp_grid), intent(in) :: g
integer, intent(in) :: unit
logical, intent(in), optional :: write_integrals
integer :: i, j
write (unit = unit) MAGIC_GRID_BEGIN
write (unit = unit) size (g%div)
write (unit = unit) g%num_calls
write (unit = unit) g%calls_per_cell
write (unit = unit) g%stratified
write (unit = unit) g%all_stratified
write (unit = unit) g%quadrupole
write (unit = unit) g%mu(1)
write (unit = unit) g%mu(2)
write (unit = unit) g%mu_plus(1)
write (unit = unit) g%mu_plus(2)
write (unit = unit) g%mu_minus(1)
write (unit = unit) g%mu_minus(2)
write (unit = unit) g%sum_integral
write (unit = unit) g%sum_weights
write (unit = unit) g%sum_chi2
write (unit = unit) g%calls
write (unit = unit) g%dv2g

```



```

write (unit = unit) g%jacobi
write (unit = unit) g%f_min
write (unit = unit) g%f_max
write (unit = unit) g%mu_gi
write (unit = unit) g%sum_mu_gi
do i = 1, size (g%div)
 write (unit = unit) g%num_div(i)
end do
do i = 1, size (g%div)
 call write_division_raw (g%div(i), unit, write_integrals)
end do
if (associated (g%map)) then
 write (unit = unit) MAGIC_GRID_MAP
 do i = 1, size (g%div)
 do j = 1, size (g%div)
 write (unit = unit) g%map(i,j)
 end do
 end do
else
 write (unit = unit) MAGIC_GRID_EMPTY
end if
if (associated (g%mu_x)) then
 write (unit = unit) MAGIC_GRID_MU_X
 do i = 1, size (g%div)
 write (unit = unit) g%mu_x(i)
 write (unit = unit) g%sum_mu_x(i)
 do j = 1, size (g%div)
 write (unit = unit) g%mu_xx(i,j)
 write (unit = unit) g%sum_mu_xx(i,j)
 end do
 end do
else
 write (unit = unit) MAGIC_GRID_EMPTY
end if
write (unit = unit) MAGIC_GRID_END
end subroutine write_grid_raw_unit

```

152    *<Constants in vamp 152>*≡ (75a) 156a▷

```

integer, parameter, private :: MAGIC_GRID = 22222222
integer, parameter, private :: MAGIC_GRID_BEGIN = MAGIC_GRID + 1
integer, parameter, private :: MAGIC_GRID_END = MAGIC_GRID + 2
integer, parameter, private :: MAGIC_GRID_EMPTY = MAGIC_GRID + 3
integer, parameter, private :: MAGIC_GRID_MAP = MAGIC_GRID + 4
integer, parameter, private :: MAGIC_GRID_MU_X = MAGIC_GRID + 5

```

```

153 <Implementation of vamp procedures 77d>+≡ (75a) <151b 154>
 subroutine read_grid_raw_unit (g, unit, read_integrals)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: read_integrals
 character(len=*), parameter :: FN = "vamp_read_raw_grid"
 integer :: ndim, i, j, magic
 read (unit = unit) magic
 if (magic /= MAGIC_GRID_BEGIN) then
 print *, FN, " fatal: expecting magic ", MAGIC_GRID_BEGIN, &
 ", found ", magic
 stop
 end if
 read (unit = unit) ndim
 <Insure that size (g%div) == ndim 148a>
 call create_array_pointer (g%num_div, ndim)
 read (unit = unit) g%num_calls
 read (unit = unit) g%calls_per_cell
 read (unit = unit) g%stratified
 read (unit = unit) g%all_stratified
 read (unit = unit) g%quadrupole
 read (unit = unit) g%mu(1)
 read (unit = unit) g%mu(2)
 read (unit = unit) g%mu_plus(1)
 read (unit = unit) g%mu_plus(2)
 read (unit = unit) g%mu_minus(1)
 read (unit = unit) g%mu_minus(2)
 read (unit = unit) g%sum_integral
 read (unit = unit) g%sum_weights
 read (unit = unit) g%sum_chi2
 read (unit = unit) g%calls
 read (unit = unit) g%dv2g
 read (unit = unit) g%jacobi
 read (unit = unit) g%f_min
 read (unit = unit) g%f_max
 read (unit = unit) g%mu_gi
 read (unit = unit) g%sum_mu_gi
 do i = 1, size (g%div)
 read (unit = unit) g%num_div(i)
 end do
 do i = 1, size (g%div)
 call read_division_raw (g%div(i), unit, read_integrals)
 end do

```

```

read (unit = unit) magic
if (magic == MAGIC_GRID_MAP) then
 call create_array_pointer (g%map, (/ ndim, ndim /))
 do i = 1, size (g%div)
 do j = 1, size (g%div)
 read (unit = unit) g%map(i,j)
 end do
 end do
else if (magic == MAGIC_GRID_EMPTY) then
 <Insure that associated (g%map) == .false. 148b>
else
 print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
 " or ", MAGIC_GRID_MAP, ", found ", magic
 stop
end if
read (unit = unit) magic
if (magic == MAGIC_GRID_MU_X) then
 call create_array_pointer (g%mu_x, ndim)
 call create_array_pointer (g%sum_mu_x, ndim)
 call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
 call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
 do i = 1, size (g%div)
 read (unit = unit) g%mu_x(i)
 read (unit = unit) g%sum_mu_x(i)
 do j = 1, size (g%div)
 read (unit = unit) g%mu_xx(i,j)
 read (unit = unit) g%sum_mu_xx(i,j)
 end do
 end do
else if (magic == MAGIC_GRID_EMPTY) then
 <Insure that associated (g%mu_x) == .false. 148c>
else
 print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
 " or ", MAGIC_GRID_MU_X, ", found ", magic
 stop
end if
read (unit = unit) magic
if (magic /= MAGIC_GRID_END) then
 print *, FN, " fatal: expecting magic ", MAGIC_GRID_END, &
 " found ", magic
 stop
end if
end subroutine read_grid_raw_unit

```

```

154 <Implementation of vamp procedures 77d>+≡ (75a) <153 155a>
 subroutine write_grid_raw_name (g, name, write_integrals)
 type(vamp_grid), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: write_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", &
 form = "unformatted", file = name)
 call write_grid_raw_unit (g, unit, write_integrals)
 close (unit = unit)
 end subroutine write_grid_raw_name

155a <Implementation of vamp procedures 77d>+≡ (75a) <154 155b>
 subroutine read_grid_raw_name (g, name, read_integrals)
 type(vamp_grid), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: read_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", &
 form = "unformatted", file = name)
 call read_grid_raw_unit (g, unit, read_integrals)
 close (unit = unit)
 end subroutine read_grid_raw_name

155b <Implementation of vamp procedures 77d>+≡ (75a) <155a 156b>
 subroutine write_grids_raw_unit (g, unit, write_integrals)
 type(vamp_grids), intent(in) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: write_integrals
 integer :: i
 write (unit = unit) MAGIC_GRIDS_BEGIN
 write (unit = unit) size (g%grids)
 write (unit = unit) g%sum_integral
 write (unit = unit) g%sum_weights
 write (unit = unit) g%sum_chi2
 do i = 1, size (g%grids)
 write (unit = unit) g%weights(i)
 end do
 do i = 1, size (g%grids)
 write (unit = unit) g%num_calls(i)
 end do
 do i = 1, size (g%grids)
 call write_grid_raw_unit (g%grids(i), unit, write_integrals)
 end do
 end subroutine write_grids_raw_unit

```

```

 end do
 write (unit = unit) MAGIC_GRIDS_END
 end subroutine write_grids_raw_unit
156a <Constants in vamp 152>+≡ (75a) <152
 integer, parameter, private :: MAGIC_GRIDS = 33333333
 integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1
 integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2
156b <Implementation of vamp procedures 77d>+≡ (75a) <155b 157a>
 subroutine read_grids_raw_unit (g, unit, read_integrals)
 type(vamp_grids), intent(inout) :: g
 integer, intent(in) :: unit
 logical, intent(in), optional :: read_integrals
 character(len=*), parameter :: FN = "vamp_read_grids_raw"
 integer :: i, nch, magic
 read (unit = unit) magic
 if (magic /= MAGIC_GRIDS_BEGIN) then
 print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_BEGIN, &
 " found ", magic
 stop
 end if
 read (unit = unit) nch
 if (associated (g%grids)) then
 if (size (g%grids) /= nch) then
 call vamp_delete_grid (g%grids)
 deallocate (g%grids, g%weights, g%num_calls)
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
 else
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
 read (unit = unit) g%sum_integral
 read (unit = unit) g%sum_weights
 read (unit = unit) g%sum_chi2
 do i = 1, nch
 read (unit = unit) g%weights(i)
 end do
 do i = 1, nch
 read (unit = unit) g%num_calls(i)
 end do
 do i = 1, nch
 call read_grid_raw_unit (g%grids(i), unit, read_integrals)

```

```

 end do
 read (unit = unit) magic
 if (magic /= MAGIC_GRIDS_END) then
 print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_END, &
 " found ", magic
 stop
 end if
 end subroutine read_grids_raw_unit
157a <Implementation of vamp procedures 77d>+≡ (75a) <156b 157b>
 subroutine write_grids_raw_name (g, name, write_integrals)
 type(vamp_grids), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: write_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", &
 form = "unformatted", file = name)
 call write_grids_raw_unit (g, unit, write_integrals)
 close (unit = unit)
 end subroutine write_grids_raw_name
157b <Implementation of vamp procedures 77d>+≡ (75a) <157a 157d>
 subroutine read_grids_raw_name (g, name, read_integrals)
 type(vamp_grids), intent(inout) :: g
 character(len=*), intent(in) :: name
 logical, intent(in), optional :: read_integrals
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", &
 form = "unformatted", file = name)
 call read_grids_raw_unit (g, unit, read_integrals)
 close (unit = unit)
 end subroutine read_grids_raw_name

```

### 5.2.12 Marshaling

[WK] Note: mu\_plus and mu\_minus not transferred (hard-coded buffer indices)!

```

157c <Declaration of vamp procedures 76b>+≡ (75a) <143b 161a>
 public :: vamp_marshall_grid_size, vamp_marshall_grid, vamp_unmarshal_grid
157d <Implementation of vamp procedures 77d>+≡ (75a) <157b 159>
 pure subroutine vamp_marshall_grid (g, ibuf, dbuf)

```

```

type(vamp_grid), intent(in) :: g
integer, dimension(:), intent(inout) :: ibuf
real(kind=default), dimension(:), intent(inout) :: dbuf
integer :: i, iwords, dwords, iidx, didx, ndim
ndim = size (g%div)
ibuf(1) = g%num_calls
ibuf(2) = g%calls_per_cell
ibuf(3) = ndim
if (g%stratified) then
 ibuf(4) = 1
else
 ibuf(4) = 0
end if
if (g%all_stratified) then
 ibuf(5) = 1
else
 ibuf(5) = 0
end if
if (g%quadrupole) then
 ibuf(6) = 1
else
 ibuf(6) = 0
end if
dbuf(1:2) = g%mu
dbuf(3) = g%sum_integral
dbuf(4) = g%sum_weights
dbuf(5) = g%sum_chi2
dbuf(6) = g%calls
dbuf(7) = g%dv2g
dbuf(8) = g%jacobi
dbuf(9) = g%f_min
dbuf(10) = g%f_max
dbuf(11) = g%mu_gi
dbuf(12) = g%sum_mu_gi
ibuf(7:6+ndim) = g%num_div
iidx = 7 + ndim
didx = 13
do i = 1, ndim
 call marshal_division_size (g%div(i), iwords, dwords)
 ibuf(iidx) = iwords
 ibuf(iidx+1) = dwords
 iidx = iidx + 2
 call marshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &

```

```

 dbuf(didx:didx-1+dwords))

 iidx = iidx + iwords
 didx = didx + dwords
end do
if (associated (g%map)) then
 ibuf(iidx) = 1
 dbuf(didx:didx-1+ndim**2) = reshape (g%map, (/ ndim**2 /))
 didx = didx + ndim**2
else
 ibuf(iidx) = 0
end if
iidx = iidx + 1
if (associated (g%mu_x)) then
 ibuf(iidx) = 1
 dbuf(didx:didx-1+ndim) = g%mu_x
 didx = didx + ndim
 dbuf(didx:didx-1+ndim) = g%sum_mu_x
 didx = didx + ndim
 dbuf(didx:didx-1+ndim**2) = reshape (g%mu_xx, (/ ndim**2 /))
 didx = didx + ndim**2
 dbuf(didx:didx-1+ndim**2) = reshape (g%sum_mu_xx, (/ ndim**2 /))
 didx = didx + ndim**2
else
 ibuf(iidx) = 0
end if
iidx = iidx + 1
end subroutine vamp_marshall_grid

```

159    *<Implementation of vamp procedures 77d>+≡* (75a) <157d 160>

```

pure subroutine vamp_marshall_grid_size (g, iwords, dwords)
 type(vamp_grid), intent(in) :: g
 integer, intent(out) :: iwords, dwords
 integer :: i, ndim, iw, dw
 ndim = size (g%div)
 iwords = 6 + ndim
 dwords = 12
 do i = 1, ndim
 call marshal_division_size (g%div(i), iw, dw)
 iwords = iwords + 2 + iw
 dwords = dwords + dw
 end do
 iwords = iwords + 1
 if (associated (g%map)) then
 dwords = dwords + ndim**2
 end if
end subroutine

```



```

 end if
 iwords = iwords + 1
 if (associated (g%mu_x)) then
 dwords = dwords + 2 * (ndim + ndim**2)
 end if
end subroutine vamp_marshall_grid_size
160 <Implementation of vamp procedures 77d>+≡ (75a) <159 161b>
pure subroutine vamp_unmarshal_grid (g, ibuf, dbuf)
 type(vamp_grid), intent(inout) :: g
 integer, dimension(:), intent(in) :: ibuf
 real(kind=default), dimension(:), intent(in) :: dbuf
 integer :: i, iwords, dwords, iidx, didx, ndim
 g%num_calls = ibuf(1)
 g%calls_per_cell = ibuf(2)
 ndim = ibuf(3)
 g%stratified = ibuf(4) /= 0
 g%all_stratified = ibuf(5) /= 0
 g%quadrupole = ibuf(6) /= 0
 g%mu = dbuf(1:2)
 g%sum_integral = dbuf(3)
 g%sum_weights = dbuf(4)
 g%sum_chi2 = dbuf(5)
 g%calls = dbuf(6)
 g%dv2g = dbuf(7)
 g%jacobi = dbuf(8)
 g%f_min = dbuf(9)
 g%f_max = dbuf(10)
 g%mu_gi = dbuf(11)
 g%sum_mu_gi = dbuf(12)
 call copy_array_pointer (g%num_div, ibuf(7:6+ndim))
 <Insure that size (g%div) == ndim 148a>
 iidx = 7 + ndim
 didx = 13
 do i = 1, ndim
 iwords = ibuf(iidx)
 dwords = ibuf(iidx+1)
 iidx = iidx + 2
 call unmarshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
 dbuf(didx:didx-1+dwords))

 iidx = iidx + iwords
 didx = didx + dwords
 end do
 if (ibuf(iidx) > 0) then

```

```

 call copy_array_pointer &
 (g%map, reshape (dbuf(didx:didx-1+ibuf(iidx)), (/ ndim, ndim /)))
 didx = didx + ibuf(iidx)
 else
 <Insure that associated (g%map) == .false. 148b>
 end if
 iidx = iidx + 1
 if (ibuf(iidx) > 0) then
 call copy_array_pointer (g%mu_x, dbuf(didx:didx-1+ndim))
 didx = didx + ndim
 call copy_array_pointer (g%sum_mu_x, dbuf(didx:didx-1+ndim))
 didx = didx + ndim
 call copy_array_pointer &
 (g%mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
 didx = didx + ndim**2
 call copy_array_pointer &
 (g%sum_mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
 didx = didx + ndim**2
 else
 <Insure that associated (g%mu_x) == .false. 148c>
 end if
 iidx = iidx + 1
end subroutine vamp_unmarshal_grid

161a <Declaration of vamp procedures 76b>+≡ (75a) <157c
 public :: vamp_marshal_history_size, vamp_marshal_history
 public :: vamp_unmarshal_history

161b <Implementation of vamp procedures 77d>+≡ (75a) <160 162a>
 pure subroutine vamp_marshal_history (h, ibuf, dbuf)
 type(vamp_history), intent(in) :: h
 integer, dimension(:), intent(inout) :: ibuf
 real(kind=default), dimension(:), intent(inout) :: dbuf
 integer :: j, ndim, iidx, didx, iwords, dwords
 if (h%verbose .and. (associated (h%div))) then
 ndim = size (h%div)
 else
 ndim = 0
 end if
 ibuf(1) = ndim
 ibuf(2) = h%calls
 if (h%stratified) then
 ibuf(3) = 1
 else
 ibuf(3) = 0

```

```

end if
dbuf(1) = h%integral
dbuf(2) = h%std_dev
dbuf(3) = h%avg_integral
dbuf(4) = h%avg_std_dev
dbuf(5) = h%avg_chi2
dbuf(6) = h%f_min
dbuf(7) = h%f_max
iidx = 4
didx = 8
do j = 1, ndim
 call marshal_div_history_size (h%div(j), iwords, dwords)
 ibuf(iidx) = iwords
 ibuf(iidx+1) = dwords
 iidx = iidx + 2
 call marshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
 dbuf(didx:didx-1+dwords))

 iidx = iidx + iwords
 didx = didx + dwords
end do
end subroutine vamp_marshal_history

```

162a  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\triangleleft$ 161b 162b $\triangleright$

```

pure subroutine vamp_marshal_history_size (h, iwords, dwords)
 type(vamp_history), intent(in) :: h
 integer, intent(out) :: iwords, dwords
 integer :: i, ndim, iw, dw
 if (h%verbose .and. (associated (h%div))) then
 ndim = size (h%div)
 else
 ndim = 0
 end if
 iwords = 3
 dwords = 7
 do i = 1, ndim
 call marshal_div_history_size (h%div(i), iw, dw)
 iwords = iwords + 2 + iw
 dwords = dwords + dw
 end do
end subroutine vamp_marshal_history_size

```

162b  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\triangleleft$ 162a 163 $\triangleright$

```

pure subroutine vamp_unmarshal_history (h, ibuf, dbuf)
 type(vamp_history), intent(inout) :: h
 integer, dimension(:), intent(in) :: ibuf

```

```

real(kind=default), dimension(:), intent(in) :: dbuf
integer :: j, ndim, iidx, didx, iwords, dwords
ndim = ibuf(1)
h%calls = ibuf(2)
h%stratified = ibuf(3) /= 0
h%integral = dbuf(1)
h%std_dev = dbuf(2)
h%avg_integral = dbuf(3)
h%avg_std_dev = dbuf(4)
h%avg_chi2 = dbuf(5)
h%f_min = dbuf(6)
h%f_max = dbuf(7)
if (ndim > 0) then
 if (associated (h%div)) then
 if (size (h%div) /= ndim) then
 deallocate (h%div)
 allocate (h%div(ndim))
 end if
 else
 allocate (h%div(ndim))
 end if
 iidx = 4
 didx = 8
 do j = 1, ndim
 iwords = ibuf(iidx)
 dwords = ibuf(iidx+1)
 iidx = iidx + 2
 call unmarshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
 dbuf(didx:didx-1+dwords))

 iidx = iidx + iwords
 didx = didx + dwords
 end do
end if
end subroutine vamp_unmarshal_history

```

### 5.2.13 Boring Copying and Deleting of Objects

163  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\triangleleft$ 162b 164 $\triangleright$

```

elemental subroutine vamp_copy_grid (lhs, rhs)
 type(vamp_grid), intent(inout) :: lhs
 type(vamp_grid), intent(in) :: rhs
 integer :: ndim
 ndim = size (rhs%div)

```

```

lhs%mu = rhs%mu
lhs%mu_plus = rhs%mu_plus
lhs%mu_minus = rhs%mu_minus
lhs%sum_integral = rhs%sum_integral
lhs%sum_weights = rhs%sum_weights
lhs%sum_chi2 = rhs%sum_chi2
lhs%calls = rhs%calls
lhs%num_calls = rhs%num_calls
call copy_array_pointer (lhs%num_div, rhs%num_div)
lhs%dv2g = rhs%dv2g
lhs%jacobi = rhs%jacobi
lhs%f_min = rhs%f_min
lhs%f_max = rhs%f_max
lhs%mu_gi = rhs%mu_gi
lhs%sum_mu_gi = rhs%sum_mu_gi
lhs%calls_per_cell = rhs%calls_per_cell
lhs%stratified = rhs%stratified
lhs%all_stratified = rhs%all_stratified
lhs%quadrupole = rhs%quadrupole
if (associated (lhs%div)) then
 if (size (lhs%div) /= ndim) then
 call delete_division (lhs%div)
 deallocate (lhs%div)
 allocate (lhs%div(ndim))
 end if
else
 allocate (lhs%div(ndim))
end if
call copy_division (lhs%div, rhs%div)
if (associated (rhs%map)) then
 call copy_array_pointer (lhs%map, rhs%map)
else if (associated (lhs%map)) then
 deallocate (lhs%map)
end if
if (associated (rhs%mu_x)) then
 call copy_array_pointer (lhs%mu_x, rhs%mu_x)
 call copy_array_pointer (lhs%mu_xx, rhs%mu_xx)
 call copy_array_pointer (lhs%sum_mu_x, rhs%sum_mu_x)
 call copy_array_pointer (lhs%sum_mu_xx, rhs%sum_mu_xx)
else if (associated (lhs%mu_x)) then
 deallocate (lhs%mu_x, lhs%mu_xx, lhs%sum_mu_x, lhs%sum_mu_xx)
end if
end subroutine vamp_copy_grid

```

164  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 163 165a $\rangle$

```

elemental subroutine vamp_delete_grid (g)
 type(vamp_grid), intent(inout) :: g
 if (associated (g%div)) then
 call delete_division (g%div)
 deallocate (g%div, g%num_div)
 end if
 if (associated (g%map)) then
 deallocate (g%map)
 end if
 if (associated (g%mu_x)) then
 deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
 end if
end subroutine vamp_delete_grid

```

165a  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 164 165b $\rangle$

```

elemental subroutine vamp_copy_grids (lhs, rhs)
 type(vamp_grids), intent(inout) :: lhs
 type(vamp_grids), intent(in) :: rhs
 integer :: nch
 nch = size (rhs%grids)
 lhs%sum_integral = rhs%sum_integral
 lhs%sum_chi2 = rhs%sum_chi2
 lhs%sum_weights = rhs%sum_weights
 if (associated (lhs%grids)) then
 if (size (lhs%grids) /= nch) then
 deallocate (lhs%grids)
 allocate (lhs%grids(nch))
 call vamp_create_empty_grid (lhs%grids(nch))
 end if
 else
 allocate (lhs%grids(nch))
 call vamp_create_empty_grid (lhs%grids(nch))
 end if
 call vamp_copy_grid (lhs%grids, rhs%grids)
 call copy_array_pointer (lhs%weights, rhs%weights)
 call copy_array_pointer (lhs%num_calls, rhs%num_calls)
end subroutine vamp_copy_grids

```

165b  $\langle$ Implementation of vamp procedures 77d $\rangle + \equiv$  (75a)  $\langle$ 165a 166a $\rangle$

```

elemental subroutine vamp_delete_grids (g)
 type(vamp_grids), intent(inout) :: g
 if (associated (g%grids)) then
 call vamp_delete_grid (g%grids)
 deallocate (g%weights, g%grids, g%num_calls)
 end if
end subroutine vamp_delete_grids

```

```

 end if
 end subroutine vamp_delete_grids
166a <Implementation of vamp procedures 77d>+≡ (75a) <165b 166b>
 elemental subroutine vamp_copy_history (lhs, rhs)
 type(vamp_history), intent(inout) :: lhs
 type(vamp_history), intent(in) :: rhs
 lhs%calls = rhs%calls
 lhs%stratified = rhs%stratified
 lhs%verbose = rhs%verbose
 lhs%integral = rhs%integral
 lhs%std_dev = rhs%std_dev
 lhs%avg_integral = rhs%avg_integral
 lhs%avg_std_dev = rhs%avg_std_dev
 lhs%avg_chi2 = rhs%avg_chi2
 lhs%f_min = rhs%f_min
 lhs%f_max = rhs%f_max
 if (rhs%verbose) then
 if (associated (lhs%div)) then
 if (size (lhs%div) /= size (rhs%div)) then
 deallocate (lhs%div)
 allocate (lhs%div(size(rhs%div)))
 end if
 else
 allocate (lhs%div(size(rhs%div)))
 end if
 call copy_history (lhs%div, rhs%div)
 end if
 end subroutine vamp_copy_history

166b <Implementation of vamp procedures 77d>+≡ (75a) <166a
 elemental subroutine vamp_delete_history (h)
 type(vamp_history), intent(inout) :: h
 if (associated (h%div)) then
 deallocate (h%div)
 end if
 end subroutine vamp_delete_history

```

### 5.3 Interface to MPI

The module `vamp` makes no specific assumptions about the hardware and software supporting parallel execution. In this section, we present a specific

example of a parallel implementation of multi channel sampling using the message passing paradigm.

The modules `vamp_serial_mpi` and `vamp_parallel_mpi` are not intended to be used directly by application programs. For this purpose, the module `vampi` is provided. `vamp_serial_mpi` is identical to `vamp`, but some types, procedures and variables are renamed so that `vamp_parallel_mpi` can redefine them:

```
167a <vampi.f90 167a>≡ 167b>
! vampi.f90 --
<Coryleft notice 1>
module vamp_serial_mpi
 use vamp, &
 <vamp0_* => vamp.* 168b>
 public
end module vamp_serial_mpi
```

`vamp_parallel_mpi` contains the non trivial MPI code and will be discussed in detail below.

```
167b <vampi.f90 167a>+≡ <167a 167c>
module vamp_parallel_mpi
 use kinds
 use utils
 use tao_random_numbers
 use exceptions
 use mpi90
 use divisions
 use vamp_serial_mpi !NODEP!
 use iso_fortran_env
 implicit none
 private
 <Declaration of vampi procedures 168a>
 <Interfaces of vampi procedures 172d>
 <Parameters in vampi 169a>
 <Declaration of vampi types 173a>
contains
 <Implementation of vampi procedures 168c>
end module vamp_parallel_mpi
```

`vampi` is now a plug-in replacement for `vamp` and *must not* be used together with `vamp`:

```
167c <vampi.f90 167a>+≡ <167b>
module vampi
 use vamp_serial_mpi !NODEP!
 use vamp_parallel_mpi !NODEP!
```



```

public
end module vampi

```

### 5.3.1 Parallel Execution

#### Single Channel

```

168a <Declaration of vampi procedures 168a>≡ (167b) 172b>
public :: vamp_create_grid
public :: vamp_discard_integral
public :: vamp_reshape_grid
public :: vamp_sample_grid
public :: vamp_delete_grid

168b <vamp0.* => vamp.* 168b>≡ (167a) 172c>
vamp0_create_grid => vamp_create_grid, &
vamp0_discard_integral => vamp_discard_integral, &
vamp0_reshape_grid => vamp_reshape_grid, &
vamp0_sample_grid => vamp_sample_grid, &
vamp0_delete_grid => vamp_delete_grid, &

168c <Implementation of vampi procedures 168c>≡ (167b) 169b>
subroutine vamp_create_grid &
 (g, domain, num_calls, num_div, &
 stratified, quadrupole, covariance, map, exc)
type(vamp_grid), intent(inout) :: g
real(kind=default), dimension(:,,:), intent(in) :: domain
integer, intent(in) :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
real(kind=default), dimension(:,,:), intent(in), optional :: map
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
 call vamp0_create_grid &
 (g, domain, num_calls, num_div, &
 stratified, quadrupole, covariance, map, exc)
else
 call vamp_create_empty_grid (g)
end if
end subroutine vamp_create_grid

```

169a  $\langle$ Parameters in vampi 169a $\rangle \equiv$  (167b) 176a $\triangleright$   
integer, public, parameter :: VAMP\_ROOT = 0

169b  $\langle$ Implementation of vampi procedures 168c $\rangle + \equiv$  (167b)  $\triangleleft$ 168c 169c $\triangleright$   
subroutine vamp\_discard\_integral &  
(g, num\_calls, num\_div, stratified, quadrupole, covariance, exc)  
type(vamp\_grid), intent(inout) :: g  
integer, intent(in), optional :: num\_calls  
integer, dimension(:), intent(in), optional :: num\_div  
logical, intent(in), optional :: stratified, quadrupole, covariance  
type(exception), intent(inout), optional :: exc  
integer :: proc\_id  
call mpi90\_rank (proc\_id)  
if (proc\_id == VAMP\_ROOT) then  
call vamp0\_discard\_integral &  
(g, num\_calls, num\_div, stratified, quadrupole, covariance, exc)  
end if  
end subroutine vamp\_discard\_integral

169c  $\langle$ Implementation of vampi procedures 168c $\rangle + \equiv$  (167b)  $\triangleleft$ 169b 169d $\triangleright$   
subroutine vamp\_reshape\_grid &  
(g, num\_calls, num\_div, stratified, quadrupole, covariance, exc)  
type(vamp\_grid), intent(inout) :: g  
integer, intent(in), optional :: num\_calls  
integer, dimension(:), intent(in), optional :: num\_div  
logical, intent(in), optional :: stratified, quadrupole, covariance  
type(exception), intent(inout), optional :: exc  
integer :: proc\_id  
call mpi90\_rank (proc\_id)  
if (proc\_id == VAMP\_ROOT) then  
call vamp0\_reshape\_grid &  
(g, num\_calls, num\_div, stratified, quadrupole, covariance, exc)  
end if  
end subroutine vamp\_reshape\_grid

NB: grids has to have intent(inout) because we will call vamp\_broadcast\_grid on it.

169d  $\langle$ Implementation of vampi procedures 168c $\rangle + \equiv$  (167b)  $\triangleleft$ 169c 172a $\triangleright$   
subroutine vamp\_sample\_grid &  
(rng, g, func, iterations, integral, std\_dev, avg\_chi2, accuracy, &  
channel, weights, grids, exc, history)  
type(tao\_random\_state), intent(inout) :: rng  
type(vamp\_grid), intent(inout) :: g  
integer, intent(in) :: iterations  
real(kind=default), intent(out), optional :: integral, std\_dev, avg\_chi2

```

real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: channel
real(kind=default), dimension(:), intent(in), optional :: weights
type(vamp_grid), dimension(:), intent(inout), optional :: grids
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_sample_grid"
real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
type(vamp_grid), dimension(:), allocatable :: gs, gx
integer, dimension(:,:), pointer :: d
integer :: iteration, i
integer :: num_proc, proc_id, num_workers
nullify (d)
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
iterate: do iteration = 1, iterations
 if (proc_id == VAMP_ROOT) then
 call vamp_distribute_work (num_proc, vamp_rigid_divisions (g), d)
 num_workers = max (1, product (d(2,:)))
 end if
 call mpi90_broadcast (num_workers, VAMP_ROOT)
 if ((present (grids)) .and. (num_workers > 1)) then
 call vamp_broadcast_grid (grids, VAMP_ROOT)
 end if
 if (proc_id == VAMP_ROOT) then
 allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
 call vamp_create_empty_grid (gs)
 call vamp_fork_grid (g, gs, gx, d, exc)
 do i = 2, num_workers
 call vamp_send_grid (gs(i), i-1, 0)
 end do
 else if (proc_id < num_workers) then
 call vamp_receive_grid (g, VAMP_ROOT, 0)
 end if
 if (proc_id == VAMP_ROOT) then
 if (num_workers > 1) then
 call vamp_sample_grid0 &
 (rng, gs(1), func, channel, weights, grids, exc)
 else
 call vamp_sample_grid0 &
 (rng, g, func, channel, weights, grids, exc)
 end if
 end if
end do

```

```

else if (proc_id < num_workers) then
 call vamp_sample_grid0 &
 (rng, g, func, channel, weights, grids, exc)
end if
if (proc_id == VAMP_ROOT) then
 do i = 2, num_workers
 call vamp_receive_grid (gs(i), i-1, 0)
 end do
 call vamp_join_grid (g, gs, gx, d, exc)
 call vamp0_delete_grid (gs)
 deallocate (gs, gx)
 call vamp_refine_grid (g)
 call vamp_average_iterations &
 (g, iteration, local_integral, local_std_dev, local_avg_chi2)
 if (present (history)) then
 if (iteration <= size (history)) then
 call vamp_get_history &
 (history(iteration), g, &
 local_integral, local_std_dev, local_avg_chi2)
 else
 call raise_exception (exc, EXC_WARN, FN, "history too short")
 end if
 call vamp_terminate_history (history(iteration+1:))
 end if
 if (present (accuracy)) then
 if (local_std_dev <= accuracy * local_integral) then
 call raise_exception (exc, EXC_INFO, FN, &
 "requested accuracy reached")
 exit iterate
 end if
 end if
else if (proc_id < num_workers) then
 call vamp_send_grid (g, VAMP_ROOT, 0)
end if
end do iterate
if (proc_id == VAMP_ROOT) then
 deallocate (d)
 if (present (integral)) then
 integral = local_integral
 end if
 if (present (std_dev)) then
 std_dev = local_std_dev
 end if
end if

```

```

 if (present (avg_chi2)) then
 avg_chi2 = local_avg_chi2
 end if
 end if
end subroutine vamp_sample_grid

172a <Implementation of vampi procedures 168c>+≡ (167b) <169d 172e>
 subroutine vamp_delete_grid (g)
 type(vamp_grid), intent(inout) :: g
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_reshape_grid (g)
 end if
 end subroutine vamp_delete_grid

172b <Declaration of vampi procedures 168a>+≡ (167b) <168a 173c>
 public :: vamp_print_history
 private :: vamp_print_one_history, vamp_print_histories

172c <vamp0_* => vamp_* 168b>+≡ (167a) <168b 173b>
 vamp0_print_history => vamp_print_history, &

172d <Interfaces of vampi procedures 172d>≡ (167b) 182a>
 interface vamp_print_history
 module procedure vamp_print_one_history, vamp_print_histories
 end interface

172e <Implementation of vampi procedures 168c>+≡ (167b) <172a 172f>
 subroutine vamp_print_one_history (h, tag)
 type(vamp_history), dimension(:), intent(in) :: h
 character(len=*), intent(in), optional :: tag
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_print_history (h, tag)
 end if
 end subroutine vamp_print_one_history

172f <Implementation of vampi procedures 168c>+≡ (167b) <172e 173e>
 subroutine vamp_print_histories (h, tag)
 type(vamp_history), dimension(:, :), intent(in) :: h
 character(len=*), intent(in), optional :: tag
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_print_history (h, tag)

```

```

end if
end subroutine vamp_print_histories

```

### Multi Channel

173a *<Declaration of vampi types 173a>*≡ (167b)

```

type, public :: vamp_grids
 !!! private
 type(vamp0_grids) :: g0
 logical, dimension(:), pointer :: active
 integer, dimension(:), pointer :: proc
 real(kind=default), dimension(:), pointer :: integrals, std_devs
end type vamp_grids

```

173b *<vamp0\_\* => vamp\_\* 168b>*+≡ (167a) <172c 173d>

```

vamp0_grids => vamp_grids, &

```

Partially duplicate the API of **vamp**:

173c *<Declaration of vampi procedures 168a>*+≡ (167b) <172b 178d>

```

public :: vamp_create_grids
public :: vamp_discard_integrals
public :: vamp_update_weights
public :: vamp_refine_weights
public :: vamp_delete_grids
public :: vamp_sample_grids

```

173d *<vamp0\_\* => vamp\_\* 168b>*+≡ (167a) <173b 181b>

```

vamp0_create_grids => vamp_create_grids, &
vamp0_discard_integrals => vamp_discard_integrals, &
vamp0_update_weights => vamp_update_weights, &
vamp0_refine_weights => vamp_refine_weights, &
vamp0_delete_grids => vamp_delete_grids, &
vamp0_sample_grids => vamp_sample_grids, &

```

Call **vamp\_create\_grids** just like the serial version. It will create the actual grids on the root processor and create stubs on the other processors

173e *<Implementation of vampi procedures 168c>*+≡ (167b) <172f 174a>

```

subroutine vamp_create_grids (g, domain, num_calls, weights, maps, &
 num_div, stratified, quadrupole, exc)
 type(vamp_grids), intent(inout) :: g
 real(kind=default), dimension(:, :), intent(in) :: domain
 integer, intent(in) :: num_calls
 real(kind=default), dimension(:), intent(in) :: weights
 real(kind=default), dimension(:, :, :), intent(in), optional :: maps
 integer, dimension(:), intent(in), optional :: num_div

```

```

logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
integer :: proc_id, nch
call mpi90_rank (proc_id)
nch = size (weights)
allocate (g%active(nch), g%proc(nch), g%integrals(nch), g%std_devs(nch))
if (proc_id == VAMP_ROOT) then
 call vamp0_create_grids (g%g0, domain, num_calls, weights, maps, &
 num_div, stratified, quadrupole, exc)
else
 allocate (g%g0%grids(nch), g%g0%weights(nch), g%g0%num_calls(nch))
 call vamp_create_empty_grid (g%g0%grids)
end if
end subroutine vamp_create_grids
174a <Implementation of vampi procedures 168c>+≡ (167b) <173e 174b>
subroutine vamp_discard_integrals &
 (g, num_calls, num_div, stratified, quadrupole, exc)
type(vamp_grids), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
 call vamp0_discard_integrals &
 (g%g0, num_calls, num_div, stratified, quadrupole, exc)
end if
end subroutine vamp_discard_integrals
174b <Implementation of vampi procedures 168c>+≡ (167b) <174a 175a>
subroutine vamp_update_weights &
 (g, weights, num_calls, num_div, stratified, quadrupole, exc)
type(vamp_grids), intent(inout) :: g
real(kind=default), dimension(:), intent(in) :: weights
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
 call vamp0_update_weights &
 (g%g0, weights, num_calls, num_div, stratified, quadrupole, exc)

```

```

 end if
 end subroutine vamp_update_weights

175a <Implementation of vampi procedures 168c>+≡ (167b) <174b 175b>
 subroutine vamp_refine_weights (g, power)
 type(vamp_grids), intent(inout) :: g
 real(kind=default), intent(in), optional :: power
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_refine_weights (g%g0, power)
 end if
 end subroutine vamp_refine_weights

175b <Implementation of vampi procedures 168c>+≡ (167b) <175a 175c>
 subroutine vamp_delete_grids (g)
 type(vamp_grids), intent(inout) :: g
 character(len=*), parameter :: FN = "vamp_delete_grids"
 deallocate (g%active, g%proc, g%integrals, g%std_devs)
 call vamp0_delete_grids (g%g0)
 end subroutine vamp_delete_grids

 Call vamp_sample_grids just like vamp0_sample_grids.

175c <Implementation of vampi procedures 168c>+≡ (167b) <175b 179a>
 subroutine vamp_sample_grids &
 (rng, g, func, iterations, integral, std_dev, avg_chi2, &
 accuracy, history, histories, exc)
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grids), intent(inout) :: g
 integer, intent(in) :: iterations
 real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
 real(kind=default), intent(in), optional :: accuracy
 type(vamp_history), dimension(:), intent(inout), optional :: history
 type(vamp_history), dimension(:, :), intent(inout), optional :: histories
 type(exception), intent(inout), optional :: exc
 <Interface declaration for func 22>
 character(len=*), parameter :: FN = "vamp_sample_grids"
 integer :: num_proc, proc_id, nch, ch, iteration
 real(kind=default), dimension(size(g%g0%weights)) :: weights
 real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
 real(kind=default) :: current_accuracy, waste
 logical :: distribute_complete_grids
 call mpi90_size (num_proc)
 call mpi90_rank (proc_id)
 nch = size (g%g0%weights)

```



```

if (proc_id == VAMP_ROOT) then
 g%active = (g%g0%num_calls >= 2)
 where (g%active)
 weights = g%g0%num_calls
 elsewhere
 weights = 0.0
 endwhere
 weights = weights / sum (weights)
 call schedule (weights, num_proc, g%proc, waste)
 distribute_complete_grids = (waste <= VAMP_MAX_WASTE)
end if
call mpi90_broadcast (weights, VAMP_ROOT)
call mpi90_broadcast (g%active, VAMP_ROOT)
call mpi90_broadcast (distribute_complete_grids, VAMP_ROOT)
if (distribute_complete_grids) then
 call mpi90_broadcast (g%proc, VAMP_ROOT)
end if
iterate: do iteration = 1, iterations
 if (distribute_complete_grids) then
 call vamp_broadcast_grid (g%g0%grids, VAMP_ROOT)
 <Distribute complete grids among processes 176b>
 else
 <Distribute each grid among processes 180c>
 end if
 <Exit iterate if accuracy has been reached (MPI) 179d>
end do iterate
<Copy results of vamp_sample_grids to dummy variables 179c>
end subroutine vamp_sample_grids

```

Setting **VAMP\_MAX\_WASTE** to 1 disables the splitting of grids, which doesn't work yet.

```

176a <Parameters in vampi 169a>+≡ (167b) <169a 179b>
 real(kind=default), private, parameter :: VAMP_MAX_WASTE = 1.0
 ! real(kind=default), private, parameter :: VAMP_MAX_WASTE = 0.3

176b <Distribute complete grids among processes 176b>≡ (175c) 177a>
 do ch = 1, nch
 if (g%active(ch)) then
 if (proc_id == g%proc(ch)) then
 call vamp0_discard_integral (g%g0%grids(ch))
 <Sample g%g0%grids(ch) 177b>
 end if
 else
 call vamp_nullify_variance (g%g0%grids(ch))
 end if
 end do

```

```

 call vamp_nullify_covariance (g%g0%grids(ch))
 end if
end do
Refine the grids after all grids have been sampled:
177a <Distribute complete grids among processes 176b>+≡ (175c) <176b 177c>
 do ch = 1, nch
 if (g%active(ch) .and. (proc_id == g%proc(ch))) then
 call vamp_refine_grid (g%g0%grids(ch))
 if (proc_id /= VAMP_ROOT) then
 <Ship the result for channel #ch back to the root 178b>
 end if
 end if
 end do
therefore we use vamp_sample_grid0 instead of vamp0_sample_grid:
177b <Sample g%g0%grids(ch) 177b>≡ (176b)
 call vamp_sample_grid0 &
 (rng, g%g0%grids(ch), func, ch, weights, g%g0%grids, exc)
 call vamp_average_iterations &
 (g%g0%grids(ch), iteration, g%integrals(ch), g%std_devs(ch), local_avg_chi2)
 if (present (histories)) then
 if (iteration <= ubound (histories, dim=1)) then
 call vamp_get_history &
 (histories(iteration,ch), g%g0%grids(ch), &
 g%integrals(ch), g%std_devs(ch), local_avg_chi2)
 else
 call raise_exception (exc, EXC_WARN, FN, "history too short")
 end if
 call vamp_terminate_history (histories(iteration+1:,ch))
 end if
177c <Distribute complete grids among processes 176b>+≡ (175c) <177a
 if (proc_id == VAMP_ROOT) then
 do ch = 1, nch
 if (g%active(ch) .and. (g%proc(ch) /= proc_id)) then
 <Receive the result for channel #ch at the root 178c>
 end if
 end do
 call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
 call vamp_average_iterations &
 (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
 if (present (history)) then
 if (iteration <= size (history)) then
 call vamp_get_history &

```

```

 (history(iteration), g%g0, local_integral, local_std_dev, &
 local_avg_chi2)
 else
 call raise_exception (exc, EXC_WARN, FN, "history too short")
 end if
 call vamp_terminate_history (history(iteration+1:))
end if
end if

```

This would be cheaper than `vamp.broadcast_grid`, but we need the latter to support the adaptive multi channel sampling:

- 178a *⟨Ship g%g0%grids from the root to the assigned processor 178a⟩≡*
- ```

do ch = 1, nch
    if (g%active(ch) .and. (g%proc(ch) /= VAMP_ROOT)) then
        if (proc_id == VAMP_ROOT) then
            call vamp_send_grid &
                (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
        else if (proc_id == g%proc(ch)) then
            call vamp_receive_grid &
                (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
        end if
    end if
end if
end do

```
- 178b *⟨Ship the result for channel #ch back to the root 178b⟩≡* (177a)
- ```

call mpi90_send (g%integrals(ch), VAMP_ROOT, object (ch, TAG_INTEGRAL))
call mpi90_send (g%std_devs(ch), VAMP_ROOT, object (ch, TAG_STD_DEV))
call vamp_send_grid (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
if (present (histories)) then
 call vamp_send_history &
 (histories(iteration,ch), VAMP_ROOT, object (ch, TAG_HISTORY))
end if

```
- 178c *⟨Receive the result for channel #ch at the root 178c⟩≡* (177c)
- ```

call mpi90_receive (g%integrals(ch), g%proc(ch), object (ch, TAG_INTEGRAL))
call mpi90_receive (g%std_devs(ch), g%proc(ch), object (ch, TAG_STD_DEV))
call vamp_receive_grid (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
if (present (histories)) then
    call vamp_receive_history &
        (histories(iteration,ch), g%proc(ch), object (ch, TAG_HISTORY))
end if

```
- 178d *⟨Declaration of vampi procedures 168a⟩+≡* (167b) <173c 179e>
- ```

private :: object

```

```

179a <Implementation of vampi procedures 168c>+≡ (167b) <175c 180a>
 pure function object (ch, obj) result (tag)
 integer, intent(in) :: ch, obj
 integer :: tag
 tag = 100 * ch + obj
 end function object

179b <Parameters in vampi 169a>+≡ (167b) <176a
 integer, public, parameter :: &
 TAG_INTEGRAL = 1, &
 TAG_STD_DEV = 2, &
 TAG_GRID = 3, &
 TAG_HISTORY = 6, &
 TAG_NEXT_FREE = 9

179c <Copy results of vamp_sample_grids to dummy variables 179c>≡ (175c)
 if (present (integral)) then
 call mpi90_broadcast (local_integral, VAMP_ROOT)
 integral = local_integral
 end if
 if (present (std_dev)) then
 call mpi90_broadcast (local_std_dev, VAMP_ROOT)
 std_dev = local_std_dev
 end if
 if (present (avg_chi2)) then
 call mpi90_broadcast (local_avg_chi2, VAMP_ROOT)
 avg_chi2 = local_avg_chi2
 end if

179d <Exit iterate if accuracy has been reached (MPI) 179d>≡ (175c)
 if (present (accuracy)) then
 if (proc_id == VAMP_ROOT) then
 current_accuracy = local_std_dev / local_integral
 end if
 call mpi90_broadcast (current_accuracy, VAMP_ROOT)
 if (current_accuracy <= accuracy) then
 call raise_exception (exc, EXC_INFO, FN, &
 "requested accuracy reached")
 exit iterate
 end if
 end if

 A very simple minded scheduler: maximizes processor utilization and, does
 not pay attention to communication costs.

179e <Declaration of vampi procedures 168a>+≡ (167b) <178d 181a>
 private :: schedule

```

We disfavor the root process a little bit (by starting up with a fake filling ratio of 10%) so that it is likely to be ready to answer all communication requests.

180a  $\langle$ Implementation of vampi procedures 168c $\rangle + \equiv$  (167b)  $\langle$ 179a 182b $\rangle$

```

pure subroutine schedule (jobs, num_procs, assign, waste)
 real(kind=default), dimension(:), intent(in) :: jobs
 integer, intent(in) :: num_procs
 integer, dimension(:), intent(out) :: assign
 real(kind=default), intent(out), optional :: waste
 integer, dimension(size(jobs)) :: idx
 real(kind=default), dimension(size(jobs)) :: sjobs
 real(kind=default), dimension(num_procs) :: fill
 integer :: job, proc
 sjobs = jobs / sum (jobs) * num_procs
 idx = (/ (job, job = 1, size(jobs)) /)
 call sort (sjobs, idx, reverse = .true.)
 fill = 0.0
 fill(VAMP_ROOT+1) = 0.1
 do job = 1, size (sjobs)
 proc = sum (minloc (fill))
 fill(proc) = fill(proc) + sjobs(job)
 assign(idx(job)) = proc - 1
 end do
 Estimate waste of processor time 180b
end subroutine schedule

```

Assuming equivalent processors and uniform computation costs, the waste is given by the fraction of the time that it spent by the other processors waiting for the processor with the biggest assignment:

180b  $\langle$ Estimate waste of processor time 180b $\rangle \equiv$  (180a)

```

if (present (waste)) then
 waste = 1.0 - sum (fill) / (num_procs * maxval (fill))
end if

```

Accordingly, if the waste caused by distributing only complete grids, we switch to splitting the grids, just like in single channel sampling. This is *not* the default, because the communication costs are measurably higher for many grids and many processors.

 This version is broken!

180c  $\langle$ Distribute each grid among processes 180c $\rangle \equiv$  (175c)

```

do ch = 1, size (g%g0%grids)
 if (g%active(ch)) then
 call vamp_discard_integral (g%g0%grids(ch))
 end if
end do

```

```

 if (present (histories)) then
 call vamp_sample_grid &
 (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
 channel = ch, weights = weights, grids = g%g0%grids, &
 history = histories(iteration:iteration,ch))
 else
 call vamp_sample_grid &
 (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
 channel = ch, weights = weights, grids = g%g0%grids)
 end if
else
 if (proc_id == VAMP_ROOT) then
 call vamp_nullify_variance (g%g0%grids(ch))
 call vamp_nullify_covariance (g%g0%grids(ch))
 end if
end if
end do
if (proc_id == VAMP_ROOT) then
 call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
 call vamp_average_iterations &
 (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
 if (present (history)) then
 if (iteration <= size (history)) then
 call vamp_get_history &
 (history(iteration), g%g0, local_integral, local_std_dev, &
 local_avg_chi2)
 else
 call raise_exception (exc, EXC_WARN, FN, "history too short")
 end if
 call vamp_terminate_history (history(iteration+1:))
 end if
end if
end if

```

### 5.3.2 Event Generation

This is currently only a syntactical translation ...

|      |                                                                                                                                                                                                                         |                                      |
|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|
| 181a | $\langle$ Declaration of vampi procedures 168a $\rangle + \equiv$<br>public :: vamp_warmup_grid<br>public :: vamp_warmup_grids<br>public :: vamp_next_event<br>private :: vamp_next_event_single, vamp_next_event_multi | (167b) $\langle$ 179e 183c $\rangle$ |
| 181b | $\langle$ vamp0_* $\Rightarrow$ vamp_* 168b $\rangle + \equiv$                                                                                                                                                          | (167a) $\langle$ 173d 183d $\rangle$ |

```
vamp0_warmup_grid => vamp_warmup_grid, &
vamp0_warmup_grids => vamp_warmup_grids, &
vamp0_next_event => vamp_next_event, &
```

182a *<Interfaces of vampi procedures 172d>+≡ (167b) <172d 184a>*

```
interface vamp_next_event
 module procedure vamp_next_event_single, vamp_next_event_multi
end interface
```

182b *<Implementation of vampi procedures 168c>+≡ (167b) <180a 182c>*

```
subroutine vamp_next_event_single &
 (x, rng, g, func, weight, channel, weights, grids, exc)
 real(kind=default), dimension(:), intent(out) :: x
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid), intent(inout) :: g
 real(kind=default), intent(out), optional :: weight
 integer, intent(in), optional :: channel
 real(kind=default), dimension(:), intent(in), optional :: weights
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 type(exception), intent(inout), optional :: exc
 <Interface declaration for func 22>
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_next_event &
 (x, rng, g, func, weight, channel, weights, grids, exc)
 end if
end subroutine vamp_next_event_single
```

182c *<Implementation of vampi procedures 168c>+≡ (167b) <182b 183a>*

```
subroutine vamp_next_event_multi (x, rng, g, func, phi, weight, exc)
 real(kind=default), dimension(:), intent(out) :: x
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grids), intent(inout) :: g
 real(kind=default), intent(out), optional :: weight
 type(exception), intent(inout), optional :: exc
 <Interface declaration for func 22>
 <Interface declaration for phi 31a>
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_next_event (x, rng, g%g0, func, phi, weight, exc)
 end if
end subroutine vamp_next_event_multi
```

183a *<Implementation of vampi procedures 168c>+≡* (167b) <182c 183b>  
`subroutine vamp_warmup_grid (rng, g, func, iterations, exc, history)`  
`type(tao_random_state), intent(inout) :: rng`  
`type(vamp_grid), intent(inout) :: g`  
`integer, intent(in) :: iterations`  
`type(exception), intent(inout), optional :: exc`  
`type(vamp_history), dimension(:), intent(inout), optional :: history`  
`<Interface declaration for func 22>`  
`call vamp_sample_grid &`  
`(rng, g, func, iterations - 1, exc = exc, history = history)`  
`call vamp_sample_grid0 (rng, g, func, exc = exc)`  
`end subroutine vamp_warmup_grid`

183b *<Implementation of vampi procedures 168c>+≡* (167b) <183a 184b>  
`subroutine vamp_warmup_grids &`  
`(rng, g, func, iterations, history, histories, exc)`  
`type(tao_random_state), intent(inout) :: rng`  
`type(vamp_grids), intent(inout) :: g`  
`integer, intent(in) :: iterations`  
`type(vamp_history), dimension(:), intent(inout), optional :: history`  
`type(vamp_history), dimension(:, :), intent(inout), optional :: histories`  
`type(exception), intent(inout), optional :: exc`  
`<Interface declaration for func 22>`  
`integer :: ch`  
`call vamp0_sample_grids (rng, g%g0, func, iterations - 1, exc = exc, &`  
`history = history, histories = histories)`  
`do ch = 1, size (g%g0%grids)`  
`! if (g%g0%grids(ch)%num_calls >= 2) then`  
`call vamp_sample_grid0 (rng, g%g0%grids(ch), func, exc = exc)`  
`! end if`  
`end do`  
`end subroutine vamp_warmup_grids`

### 5.3.3 I/O

183c *<Declaration of vampi procedures 168a>+≡* (167b) <181a 185a>  
`public :: vamp_write_grid, vamp_read_grid`  
`private :: write_grid_unit, write_grid_name`  
`private :: read_grid_unit, read_grid_name`

183d *<vamp0.\* => vamp.\* 168b>+≡* (167a) <181b 185b>  
`vamp0_write_grid => vamp_write_grid, &`  
`vamp0_read_grid => vamp_read_grid, &`



184a *<Interfaces of vampi procedures 172d>+≡* (167b) <182a 185c>  
 interface **vamp\_write\_grid**  
   module procedure **write\_grid\_unit**, **write\_grid\_name**  
end interface  
 interface **vamp\_read\_grid**  
   module procedure **read\_grid\_unit**, **read\_grid\_name**  
end interface

184b *<Implementation of vampi procedures 168c>+≡* (167b) <183b 184c>  
**subroutine write\_grid\_unit** (g, unit)  
 type(**vamp\_grid**), intent(in) :: g  
 integer, intent(in) :: unit  
 integer :: proc\_id  
 call **mpi90\_rank** (proc\_id)  
 if (proc\_id == **VAMP\_ROOT**) then  
   call **vamp0\_write\_grid** (g, unit)  
 end if  
end **subroutine write\_grid\_unit**

184c *<Implementation of vampi procedures 168c>+≡* (167b) <184b 184d>  
**subroutine read\_grid\_unit** (g, unit)  
 type(**vamp\_grid**), intent(inout) :: g  
 integer, intent(in) :: unit  
 integer :: proc\_id  
 call **mpi90\_rank** (proc\_id)  
 if (proc\_id == **VAMP\_ROOT**) then  
   call **vamp0\_read\_grid** (g, unit)  
 end if  
end **subroutine read\_grid\_unit**

184d *<Implementation of vampi procedures 168c>+≡* (167b) <184c 184e>  
**subroutine write\_grid\_name** (g, name)  
 type(**vamp\_grid**), intent(inout) :: g  
 character(len=\*), intent(in) :: name  
 integer :: proc\_id  
 call **mpi90\_rank** (proc\_id)  
 if (proc\_id == **VAMP\_ROOT**) then  
   call **vamp0\_write\_grid** (g, name)  
 end if  
end **subroutine write\_grid\_name**

184e *<Implementation of vampi procedures 168c>+≡* (167b) <184d 185d>  
**subroutine read\_grid\_name** (g, name)  
 type(**vamp\_grid**), intent(inout) :: g  
 character(len=\*), intent(in) :: name  
 integer :: proc\_id

```

 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_read_grid (g, name)
 end if
 end subroutine read_grid_name
185a <Declaration of vampi procedures 168a>+≡ (167b) <183c 186c>
 public :: vamp_write_grids, vamp_read_grids
 private :: write_grids_unit, write_grids_name
 private :: read_grids_unit, read_grids_name
185b <vamp0.* => vamp.* 168b>+≡ (167a) <183d
 vamp0_write_grids => vamp_write_grids, &
 vamp0_read_grids => vamp_read_grids, &
185c <Interfaces of vampi procedures 172d>+≡ (167b) <184a 188b>
 interface vamp_write_grids
 module procedure write_grids_unit, write_grids_name
 end interface
 interface vamp_read_grids
 module procedure read_grids_unit, read_grids_name
 end interface

185d <Implementation of vampi procedures 168c>+≡ (167b) <184e 185e>
 subroutine write_grids_unit (g, unit)
 type(vamp_grids), intent(in) :: g
 integer, intent(in) :: unit
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_write_grids (g%g0, unit)
 end if
 end subroutine write_grids_unit

185e <Implementation of vampi procedures 168c>+≡ (167b) <185d 186a>
 subroutine read_grids_unit (g, unit)
 type(vamp_grids), intent(inout) :: g
 integer, intent(in) :: unit
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_read_grids (g%g0, unit)
 end if
 end subroutine read_grids_unit

```

186a *<Implementation of vampi procedures 168c>+≡* (167b) <185e 186b>

```

subroutine write_grids_name (g, name)
 type(vamp_grids), intent(inout) :: g
 character(len=*), intent(in) :: name
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_write_grids (g%g0, name)
 end if
end subroutine write_grids_name

```

186b *<Implementation of vampi procedures 168c>+≡* (167b) <186a 186d>

```

subroutine read_grids_name (g, name)
 type(vamp_grids), intent(inout) :: g
 character(len=*), intent(in) :: name
 integer :: proc_id
 call mpi90_rank (proc_id)
 if (proc_id == VAMP_ROOT) then
 call vamp0_read_grids (g%g0, name)
 end if
end subroutine read_grids_name

```

### 5.3.4 Communicating Grids

186c *<Declaration of vampi procedures 168a>+≡* (167b) <185a 190a>

```

public :: vamp_send_grid
public :: vamp_receive_grid
public :: vamp_broadcast_grid
public :: vamp_broadcast_grids

```



The next two are still kludged. Nicer implementations with one message less per call below, but MPICH does funny things during `mpi_get_count`, which is called by `mpi90_receive_pointer`.

Caveat: this `vamp_send_grid` uses *three* tags: `tag`, `tag+1` and `tag+2`:

186d *<Implementation of vampi procedures 168c>+≡* (167b) <186b 187a>

```

subroutine vamp_send_grid (g, target, tag, domain, error)
 type(vamp_grid), intent(in) :: g
 integer, intent(in) :: target, tag
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer, dimension(2) :: words

```

```

integer, dimension(:), allocatable :: ibuf
real(kind=default), dimension(:), allocatable :: dbuf
call vamp_marshall_grid_size (g, words(1), words(2))
allocate (ibuf(words(1)), dbuf(words(2)))
call vamp_marshall_grid (g, ibuf, dbuf)
call mpi90_send (words, target, tag, domain, error)
call mpi90_send (ibuf, target, tag+1, domain, error)
call mpi90_send (dbuf, target, tag+2, domain, error)
deallocate (ibuf, dbuf)
end subroutine vamp_send_grid

```

187a *<Implementation of vampi procedures 168c>+≡ (167b) <186d 188c>*

```

subroutine vamp_receive_grid (g, source, tag, domain, status, error)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in) :: source, tag
 integer, intent(in), optional :: domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 integer, dimension(2) :: words
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call mpi90_receive (words, source, tag, domain, status, error)
 allocate (ibuf(words(1)), dbuf(words(2)))
 call mpi90_receive (ibuf, source, tag+1, domain, status, error)
 call mpi90_receive (dbuf, source, tag+2, domain, status, error)
 call vamp_unmarshal_grid (g, ibuf, dbuf)
 deallocate (ibuf, dbuf)
end subroutine vamp_receive_grid

```

Caveat: the real `vamp_send_grid` uses *two* tags: `tag` and `tag+1`:

187b *<Implementation of vampi procedures (doesn't work with MPICH yet) 187b>≡ 188a>*

```

subroutine vamp_send_grid (g, target, tag, domain, error)
 type(vamp_grid), intent(in) :: g
 integer, intent(in) :: target, tag
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer :: iwwords, dwwords
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call vamp_marshall_grid_size (g, iwwords, dwwords)
 allocate (ibuf(iwwords), dbuf(dwwords))
 call vamp_marshall_grid (g, ibuf, dbuf)

```

```

 call mpi90_send (ibuf, target, tag, domain, error)
 call mpi90_send (dbuf, target, tag+1, domain, error)
 deallocate (ibuf, dbuf)
end subroutine vamp_send_grid

```

⚠ There's something wrong with MPICH: if I call `mpi90_receive_pointer` in the opposite order, the low level call to `mpi_get_count` bombs for no apparent reason!

⚠ There are also funky things going on with tag: `mpi90_receive_pointer` should leave it alone, but ...

188a *<Implementation of vampi procedures (doesn't work with MPICH yet) 187b>+≡ <187b*

```

subroutine vamp_receive_grid (g, source, tag, domain, status, error)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in) :: source, tag
 integer, intent(in), optional :: domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 integer, dimension(:), pointer :: ibuf
 real(kind=default), dimension(:), pointer :: dbuf
 nullify (ibuf, dbuf)
 call mpi90_receive_pointer (dbuf, source, tag+1, domain, status, error)
 call mpi90_receive_pointer (ibuf, source, tag, domain, status, error)
 call vamp_unmarshal_grid (g, ibuf, dbuf)
 deallocate (ibuf, dbuf)
end subroutine vamp_receive_grid

```

This is not a good idea, with respect to communication costs. For SMP machines, it appears to be negligible however.

188b *<Interfaces of vampi procedures 172d>+≡ (167b) <185c*

```

interface vamp_broadcast_grid
 module procedure &
 vamp_broadcast_one_grid, vamp_broadcast_many_grids
end interface

```

188c *<Implementation of vampi procedures 168c>+≡ (167b) <187a 189a>*

```

subroutine vamp_broadcast_one_grid (g, root, domain, error)
 type(vamp_grid), intent(inout) :: g
 integer, intent(in) :: root
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer, dimension(:), allocatable :: ibuf

```

```

real(kind=default), dimension(:), allocatable :: dbuf
integer :: iwords, dwords, me
call mpi90_rank (me)
if (me == root) then
 call vamp_marshall_grid_size (g, iwords, dwords)
end if
call mpi90_broadcast (iwords, root, domain, error)
call mpi90_broadcast (dwords, root, domain, error)
allocate (ibuf(iwords), dbuf(dwords))
if (me == root) then
 call vamp_marshall_grid (g, ibuf, dbuf)
end if
call mpi90_broadcast (ibuf, root, domain, error)
call mpi90_broadcast (dbuf, root, domain, error)
if (me /= root) then
 call vamp_unmarshal_grid (g, ibuf, dbuf)
end if
deallocate (ibuf, dbuf)
end subroutine vamp_broadcast_one_grid

```

189a *<Implementation of vampi procedures 168c>+≡ (167b) <188c 189b>*

```

subroutine vamp_broadcast_many_grids (g, root, domain, error)
 type(vamp_grid), dimension(:), intent(inout) :: g
 integer, intent(in) :: root
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer :: i
 do i = 1, size(g)
 call vamp_broadcast_one_grid (g(i), root, domain, error)
 end do
end subroutine vamp_broadcast_many_grids

```

189b *<Implementation of vampi procedures 168c>+≡ (167b) <189a 190b>*

```

subroutine vamp_broadcast_grids (g, root, domain, error)
 type(vamp0_grids), intent(inout) :: g
 integer, intent(in) :: root
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer :: nch, me
 call mpi90_broadcast (g%sum_chi2, root, domain, error)
 call mpi90_broadcast (g%sum_integral, root, domain, error)
 call mpi90_broadcast (g%sum_weights, root, domain, error)
 call mpi90_rank (me)

```

```

if (me == root) then
 nch = size (g%grids)
end if
call mpi90_broadcast (nch, root, domain, error)
if (me /= root) then
 if (associated (g%grids)) then
 if (size (g%grids) /= nch) then
 call vamp0_delete_grid (g%grids)
 deallocate (g%grids, g%weights, g%num_calls)
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
 else
 allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
 call vamp_create_empty_grid (g%grids)
 end if
end if
call vamp_broadcast_grid (g%grids, root, domain, error)
call mpi90_broadcast (g%weights, root, domain, error)
call mpi90_broadcast (g%num_calls, root, domain, error)
end subroutine vamp_broadcast_grids

```

190a *<Declaration of vampi procedures 168a>+≡* (167b) <186c

```

public :: vamp_send_history
public :: vamp_receive_history

```

190b *<Implementation of vampi procedures 168c>+≡* (167b) <189b 191>

```

subroutine vamp_send_history (g, target, tag, domain, error)
 type(vamp_history), intent(in) :: g
 integer, intent(in) :: target, tag
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer, dimension(2) :: words
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call vamp_marshall_history_size (g, words(1), words(2))
 allocate (ibuf(words(1)), dbuf(words(2)))
 call vamp_marshall_history (g, ibuf, dbuf)
 call mpi90_send (words, target, tag, domain, error)
 call mpi90_send (ibuf, target, tag+1, domain, error)
 call mpi90_send (dbuf, target, tag+2, domain, error)
 deallocate (ibuf, dbuf)
end subroutine vamp_send_history

```

191 *⟨Implementation of vampi procedures 168c⟩+≡* (167b) <190b

```

subroutine vamp_receive_history (g, source, tag, domain, status, error)
 type(vamp_history), intent(inout) :: g
 integer, intent(in) :: source, tag
 integer, intent(in), optional :: domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 integer, dimension(2) :: words
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call mpi90_receive (words, source, tag, domain, status, error)
 allocate (ibuf(words(1)), dbuf(words(2)))
 call mpi90_receive (ibuf, source, tag+1, domain, status, error)
 call mpi90_receive (dbuf, source, tag+2, domain, status, error)
 call vamp_unmarshal_history (g, ibuf, dbuf)
 deallocate (ibuf, dbuf)
end subroutine vamp_receive_history

```



# —6—

## SELF TEST

### 6.1 No Mapping Mode

In this chapter we perform a test of the major features of Vamp. A function with many peaks is integrated with the traditional Vegas algorithm, using a multi-channel approach and in parallel. The function is constructed to have a known analytical integral (which is chosen to be one) in order to be able to gauge the accuracy of the result and error estimate.

#### 6.1.1 Serial Test

```

192a <vamp_test.f90 192a>≡
! vamp_test.f90 --
<Copyleft notice 1>
<Module vamp_test_functions 192b>
<Module vamp_tests 196b>
200c>

192b <Module vamp_test_functions 192b>≡
module vamp_test_functions
 use kinds
 use constants, only: PI
 use coordinates
 use vamp, only: vamp_grid, vamp_multi_channel
 use vamp, only: vamp_data_t
 implicit none
 private
 public :: f, j, phi, ihp, w
 public :: lorentzian
 private :: lorentzian_normalized
 real(kind=default), public :: width
contains
 <Implementation of vamp_test_functions procedures 193a>

```

```
end module vamp_test_functions
```

$$\int_{x_1}^{x_2} dx \frac{1}{(x - x_0)^2 + a^2} = \frac{1}{a} \left( \operatorname{atan} \left( \frac{x_2 - x_0}{a} \right) - \operatorname{atan} \left( \frac{x_1 - x_0}{a} \right) \right) = N(x_0, x_1, x_2, a) \quad (6.1)$$

193a  $\langle$ Implementation of vamp\_test\_functions procedures 193a $\rangle \equiv$  (192b) 193b $\rangle$

```
pure function lorentzian_normalized (x, x0, x1, x2, a) result (f)
 real(kind=default), intent(in) :: x, x0, x1, x2, a
 real(kind=default) :: f
 if (x1 <= x .and. x <= x2) then
 f = 1 / ((x - x0)**2 + a**2) &
 * a / (atan2 (x2 - x0, a) - atan2 (x1 - x0, a))
 else
 f = 0
 end if
end function lorentzian_normalized
```

$$\int d^n x f(x) = \int d\Omega_n r^{n-1} dr f(x) = 1 \quad (6.2)$$

193b  $\langle$ Implementation of vamp\_test\_functions procedures 193a $\rangle + \equiv$  (192b)  $\langle$ 193a 193c $\rangle$

```
pure function lorentzian (x, x0, x1, x2, r0, a) result (f)
 real(kind=default), dimension(:), intent(in) :: x, x0, x1, x2
 real(kind=default), intent(in) :: r0, a
 real(kind=default) :: f
 real(kind=default) :: r, r1, r2
 integer :: n
 n = size (x)
 if (n > 1) then
 r = sqrt (dot_product (x-x0, x-x0))
 r1 = 0.4_default
 r2 = min (minval (x2-x0), minval (x0-x1))
 if (r1 <= r .and. r <= r2) then
 f = lorentzian_normalized (r, r0, r1, r2, a) * r**(1-n) / surface (n)
 else
 f = 0
 end if
 else
 f = lorentzian_normalized (x(1), x0(1), x1(1), x2(1), a)
 endif
end function lorentzian
```

193c  $\langle$ Implementation of vamp\_test\_functions procedures 193a $\rangle + \equiv$  (192b)  $\langle$ 193b 194 $\rangle$

```
pure function f (x, data, weights, channel, grids) result (f_x)
 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
```

```

real(kind=default), dimension(:), intent(in), optional :: weights
integer, intent(in), optional :: channel
type(vamp_grid), dimension(:), intent(in), optional :: grids
real(kind=default) :: f_x
real(kind=default), dimension(size(x)) :: minus_one, plus_one, zero, w_i, f_i
integer :: n, i
n = size(x)
minus_one = -1
zero = 0
plus_one = 1
w_i = 1
do i = 1, n
 if (all (abs (x(i+1:)) <= 1)) then
 f_i = lorentzian (x(1:i), zero(1:i), minus_one(1:i), plus_one(1:i), &
 0.7_default, width) &
 / 2.0_default**(n-i)
 else
 f_i = 0
 end if
end do
f_x = dot_product (w_i, f_i) / sum (w_i)
end function f

```

194  $\langle$ Implementation of vamp\_test functions procedures 193a $\rangle + \equiv$  (192b)  $\langle$ 193c 195a $\rangle$

```

pure function phi (xi, channel) result (x)
real(kind=default), dimension(:), intent(in) :: xi
integer, intent(in) :: channel
real(kind=default), dimension(size(xi)) :: x
real(kind=default) :: r
real(kind=default), dimension(0) :: dummy
integer :: n
n = size(x)
if (channel == 1) then
 x = xi
else if (channel == 2) then
 r = (xi(1) + 1) / 2 * sqrt (2.0_default)
 x(1:2) = spherical_cos_to_cartesian (r, PI * xi(2), dummy)
 x(3:) = xi(3:)
else if (channel < n) then
 r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))
 x(1:channel) = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:channel))
 x(channel+1:) = xi(channel+1:)
else if (channel == n) then
 r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))

```

```

 x = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:))
 else
 x = 0
 end if
end function phi
195a <Implementation of vamp_test_functions procedures 193a>+≡ (192b) <194 195b>
pure function ihp (x, channel) result (xi)
 real(kind=default), dimension(:), intent(in) :: x
 integer, intent(in) :: channel
 real(kind=default), dimension(size(x)) :: xi
 real(kind=default) :: r, phi
 integer :: n
 n = size(x)
 if (channel == 1) then
 xi = x
 else if (channel == 2) then
 call cartesian_to_spherical_cos (x(1:2), r, phi)
 xi(1) = 2 * r / sqrt (2.0_default) - 1
 xi(2) = phi / PI
 xi(3:) = x(3:)
 else if (channel < n) then
 call cartesian_to_spherical_cos (x(1:channel), r, phi, xi(3:channel))
 xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
 xi(2) = phi / PI
 xi(channel+1:) = x(channel+1:)
 else if (channel == n) then
 call cartesian_to_spherical_cos (x, r, phi, xi(3:))
 xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
 xi(2) = phi / PI
 else
 xi = 0
 end if
end function ihp
195b <Implementation of vamp_test_functions procedures 193a>+≡ (192b) <195a 196a>
pure function j (x, data, channel) result (j_x)
 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
 integer, intent(in) :: channel
 real(kind=default) :: j_x
 if (channel == 1) then
 j_x = 1
 else if (channel > 1) then
 j_x = 2 / sqrt (real (channel, kind=default)) ! 1/|dr/dξ1|
 end if
end function j

```

```

 j_x = j_x / PI ! 1/|dφ/dξ2|
 j_x = j_x * cartesian_to_spherical_cos_j (x(1:channel))
 else
 j_x = 0
 end if
end function j

```

196a  $\langle$ Implementation of `vamp_test_functions` procedures 193a $\rangle \equiv$  (192b)  $\triangleleft$  195b

```

function w (x, data, weights, channel, grids) result (w_x)
 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: w_x
 w_x = vamp_multi_channel (f, data, phi, ihp, j, x, weights, channel, grids)
end function w

```

196b  $\langle$ Module `vamp_tests` 196b $\rangle \equiv$  (192a)

```

module vamp_tests
 use kinds
 use exceptions
 use histograms
 use tao_random_numbers
 use coordinates
 use vamp
 use vamp_test_functions !NODEP!
 implicit none
 private
 \langle Declaration of procedures in vamp_tests 196c \rangle
contains
 \langle Implementation of procedures in vamp_tests 197a \rangle
end module vamp_tests

```

### Verification

196c  $\langle$ Declaration of procedures in `vamp_tests` 196c $\rangle \equiv$  (196b 202b) 198a $\triangleright$

```

! public :: check_jacobians, check_inverses, check_inverses3
public :: check_inverses, check_inverses3

```

196d  $\langle$ Implementation of procedures in `vamp_tests` (broken?) 196d $\rangle \equiv$

```

subroutine check_jacobians (rng, region, weights, samples)
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), dimension(:, :), intent(in) :: region
 real(kind=default), dimension(:), intent(in) :: weights

```

```

integer, intent(in) :: samples
real(kind=default), dimension(size(region,dim=2)) :: x
real(kind=default) :: d
integer :: ch
do ch = 1, size(weights)
 call vamp_check_jacobian (rng, samples, j, NO_DATA, phi, ch, region, d, x)
 print *, "channel", ch, ": delta(j)/j=", real(d), ", @x=", real (x)
end do
end subroutine check_jacobians

```

197a *<Implementation of procedures in vamp\_tests 197a>≡ (196b 202b) 197b>*

```

subroutine check_inverses (rng, region, weights, samples)
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), dimension(:,,:), intent(in) :: region
 real(kind=default), dimension(:), intent(in) :: weights
 integer, intent(in) :: samples
 real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx
 real(kind=default) :: dx, dx_max
 integer :: ch, i
 dx_max = 0
 x_dx = 0
 do ch = 1, size(weights)
 do i = 1, samples
 call tao_random_number (rng, x1)
 x2 = ihp (phi (x1, ch), ch)
 dx = sqrt (dot_product (x1-x2, x1-x2))
 if (dx > dx_max) then
 dx_max = dx
 x_dx = x1
 end if
 end do
 print *, "channel", ch, ": |x-x|=", real(dx), ", @x=", real (x_dx)
 end do
end subroutine check_inverses

```

197b *<Implementation of procedures in vamp\_tests 197a>+≡ (196b 202b) <197a 198b>*

```

subroutine check_inverses3 (rng, region, samples)
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), dimension(:,,:), intent(in) :: region
 integer, intent(in) :: samples
 real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx, x_dj
 real(kind=default) :: r, phi, jac, caj, dx, dx_max, dj, dj_max
 real(kind=default), dimension(size(x1)-2) :: cos_theta
 integer :: i
 dx_max = 0

```

```

x_dx = 0
dj_max = 0
x_dj = 0
do i = 1, samples
 call tao_random_number (rng, x1)
 call cartesian_to_spherical_cos_2 (x1, r, phi, cos_theta, jac)
 call spherical_cos_to_cartesian_2 (r, phi, cos_theta, x2, caj)
 dx = sqrt (dot_product (x1-x2, x1-x2))
 dj = jac*caj - 1
 if (dx > dx_max) then
 dx_max = dx
 x_dx = x1
 end if
 if (dj > dj_max) then
 dj_max = dj
 x_dj = x1
 end if
end do
print *, "channel 3 : j*j-1=", real(dj), ", @x=", real (x_dj)
print *, "channel 3 : |x-x|=", real(dx), ", @x=", real (x_dx)
end subroutine check_inverses3

```

### Integration

- 198a *<Declaration of procedures in vamp\_tests 196c>+≡ (196b 202b) <196c 200a>*  
 public :: single\_channel, multi\_channel
- 198b *<Implementation of procedures in vamp\_tests 197a>+≡ (196b 202b) <197b 199a>*  
 subroutine single\_channel (rng, region, samples, iterations, &  
 integral, standard\_dev, chi\_squared)  
 type(tao\_random\_state), intent(inout) :: rng  
 real(kind=default), dimension(:,:), intent(in) :: region  
 integer, dimension(:), intent(in) :: samples, iterations  
 real(kind=default), intent(out) :: integral, standard\_dev, chi\_squared  
 type(vamp\_grid) :: gr  
 type(vamp\_history), dimension(iterations(1)+iterations(2)) :: history  
 call vamp\_create\_history (history)  
 call vamp\_create\_grid (gr, region, samples(1))  
 call vamp\_sample\_grid (rng, gr, f, NO\_DATA, iterations(1), history = history)  
 call vamp\_discard\_integral (gr, samples(2))  
 call vamp\_sample\_grid &  
 (rng, gr, f, NO\_DATA, iterations(2), &  
 integral, standard\_dev, chi\_squared, &  
 history = history(iterations(1)+1:))

```

 call vamp_write_grid (gr, "vamp_test.grid")
 call vamp_delete_grid (gr)
 call vamp_print_history (history, "single")
 call vamp_delete_history (history)
end subroutine single_channel
199a <Implementation of procedures in vamp_tests 197a>+≡ (196b 202b) <198b 200b>
subroutine multi_channel (rng, region, weights, samples, iterations, powers, &
 integral, standard_dev, chi_squared)
type(tao_random_state), intent(inout) :: rng
real(kind=default), dimension(:, :), intent(in) :: region
real(kind=default), dimension(:), intent(inout) :: weights
integer, dimension(:), intent(in) :: samples, iterations
real(kind=default), dimension(:), intent(in) :: powers
real(kind=default), intent(out) :: integral, standard_dev, chi_squared
type(vamp_grids) :: grs
<Body of multi_channel 199b>
end subroutine multi_channel
199b <Body of multi_channel 199b>≡ (199a 212b) 213>
type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
 history
type(vamp_history), dimension(size(history),size(weights)) :: histories
integer :: it, nit
nit = size (powers)
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weights)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
 history = history, histories = histories)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
do it = 1, nit
 call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
 history = history(iterations(1)+it-1:), &
 histories = histories(iterations(1)+it-1:,:))
 call vamp_print_history (history(iterations(1)+it-1:), "multi")
 call vamp_print_history (histories(iterations(1)+it-1:,:), "multi")
 call vamp_refine_weights (grs, powers(it))
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
 (rng, grs, w, NO_DATA, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+nit:), &

```



```

 histories = histories(iterations(1)+nit:, :)
call vamp_print_history (history(iterations(1)+nit:), "multi")
call vamp_print_history (histories(iterations(1)+nit:, :), "multi")
call vamp_write_grids (grs, "vamp_test.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)

```

### *Input/Output*

- 200a *<Declaration of procedures in vamp\_tests 196c>+≡ (196b 202b) <198a*  
public :: print\_results
- 200b *<Implementation of procedures in vamp\_tests 197a>+≡ (196b 202b) <199a*  
subroutine print\_results (prefix, prev\_ticks, &  
integral, std\_dev, chi2, acceptable, failures)  
character(len=\*), intent(in) :: prefix  
integer, intent(in) :: prev\_ticks  
real(kind=default), intent(in) :: integral, std\_dev, chi2, acceptable  
integer, intent(inout) :: failures  
integer :: ticks, ticks\_per\_second  
real(kind=default) :: pull  
call system\_clock (ticks, ticks\_per\_second)  
pull = (integral - 1) / std\_dev  
print "(1X,A,A,F6.2,A)", prefix, &  
": time = ", real (ticks - prev\_ticks) / ticks\_per\_second, " secs"  
print \*, prefix, ": int, err, chi2: ", &  
real (integral), real (std\_dev), real (chi2)  
if (abs (pull) > acceptable) then  
failures = failures + 1  
print \*, prefix, ": unacceptable pull:", real (pull)  
else  
print \*, prefix, ": acceptable pull:", real (pull)  
end if  
end subroutine print\_results

### *Main Program*

- 200c *<vamp\_test.f90 192a>+≡ <192a*  
program vamp\_test  
use kinds  
use tao\_random\_numbers

```

use coordinates
use vamp
use vamp_test_functions !NODEP!
use vamp_tests !NODEP!
implicit none
integer :: start_ticks, status
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
failures = 0
call tao_random_create (rng, 0)
call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
if (status == 0) then
 call system_clock (start_ticks)
else
 start_ticks = 42
end if
call tao_random_seed (rng, start_ticks)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
print *, "Starting VAMP 1.0 self test..."
print *, "serial code"
call system_clock (start_ticks)
call single_channel (rng, region, samples, iterations, &
 single_integral, single_standard_dev, single_chi_squared)
call print_results ("SINGLE", start_ticks, &
 single_integral, single_standard_dev, single_chi_squared, &
 10*ACCEPTABLE, failures)
weight_vector = 1
powers = 0.25_default
call system_clock (start_ticks)
call multi_channel (rng, region, weight_vector, samples, iterations, &
 powers, multi_integral, multi_standard_dev, multi_chi_squared)
call print_results ("MULTI", start_ticks, &

```

```

 multi_integral, multi_standard_dev, multi_chi_squared, &
 ACCEPTABLE, failures)
 call system_clock (start_ticks)
! call check_jacobians (rng, region, weight_vector, samples(1))
 call check_inverses (rng, region, weight_vector, samples(1))
 call check_inverses3 (rng, region, samples(1))
 if (failures == 0) then
 stop 0
 else if (failures == 1) then
 stop 1
 else
 stop 2
 end if
end program vamp_test

```

### 6.1.2 Parallel Test

202a `<vampi_test.f90 202a>≡` 202b>  
`! vampi_test.f90 --`  
`<Copyleft notice 1>`  
`<Module vamp_test_functions 192b>`

The following is identical to `vamp_tests`, except for use `vampi`:

202b `<vampi_test.f90 202a>+≡` <202a 202c>  
`module vampi_tests`  
`use kinds`  
`use exceptions`  
`use histograms`  
`use tao_random_numbers`  
`use coordinates`  
`use vampi`  
`use vamp_test_functions !NODEP!`  
`implicit none`  
`private`  
`<Declaration of procedures in vamp_tests 196c>`  
`contains`  
`<Implementation of procedures in vamp_tests 197a>`  
`end module vampi_tests`

202c `<vampi_test.f90 202a>+≡` <202b  
`program vampi_test`  
`use kinds`  
`use tao_random_numbers`  
`use coordinates`

```

use vampi
use mpi90
use vamp_test_functions !NODEP!
use vampi_tests !NODEP!
implicit none
integer :: num_proc, proc_id, start_ticks
logical :: perform_io
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
integer :: iostat, command
character(len=72) :: command_line
integer, parameter :: &
 CMD_ERROR = -1, CMD_END = 0, &
 CMD_NOP = 1, CMD_SINGLE = 2, CMD_MULTI = 3, CMD_CHECK = 4
call tao_random_create (rng, 0)
call mpi90_init ()
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
perform_io = (proc_id == 0)
call system_clock (start_ticks)
call tao_random_seed (rng, start_ticks + proc_id)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
samples = (/ 200000, 2000000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
if (perform_io) then
 print *, "Starting VAMP 1.0 self test..."
 if (num_proc > 1) then
 print *, "parallel code running on ", num_proc, " processors"
 else
 print *, "parallel code running serially"
 end if
end if
command_loop: do
 Parse the commandline in vamp_test and set command (never defined)
 call mpi90_broadcast (command, 0)

```

```

 call system_clock (start_ticks)
 select case (command)
 <Execute command in vamp_test (never defined)>
 case (CMD_END)
 exit command_loop
 case (CMD_NOP)
 ! do nothing
 case (CMD_ERROR)
 ! do nothing
 end select
end do command_loop
call mpi90_finalize ()
end program vampi_test

```

### 6.1.3 Output

204a <vamp\_test.out 204a>≡

## 6.2 Mapped Mode

In this chapter we perform a test of the major features of Vamp. A function with many peaks is integrated with the traditional Vegas algorithm, using a multi-channel approach and in parallel. The function is constructed to have a known analytical integral (which is chosen to be one) in order to be able to gauge the accuracy of the result and error estimate.

### 6.2.1 Serial Test

204b <vamp\_test0.f90 204b>≡ 211a>  
 ! vamp\_test0.f90 --  
 <Copyleft notice 1>  
 <Module vamp\_test0\_functions 204c>

#### Single Channel

The functions to be integrated are shared by the serial and the parallel incarnation of the code.

204c <Module vamp\_test0\_functions 204c>≡ (204b 219e)  
 module vamp\_test0\_functions  
 use kinds  
 use vamp, only: vamp\_grid, vamp\_multi\_channel0

```

use vamp, only: vamp_data_t
implicit none
private
public :: f, g, phi, w
public :: create_sample, delete_sample
private :: f0, psi, g0, f_norm
real(kind=default), dimension(:), allocatable, private :: c, x_min, x_max
real(kind=default), dimension(:, :, :), allocatable, public :: x0, gamma
contains
 <Implementation of vamp_test0_functions procedures 205>
end module vamp_test0_functions

```

We start from a model of  $n_p$  interfering resonances in one variable (cf. section ??)

$$f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{N(x_{\min}, x_{\max}, x_0, \gamma)} \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.3)$$

where

$$N(x_{\min}, x_{\max}, x_0, \gamma) = \int_{x_{\min}}^{x_{\max}} dx \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.4)$$

such that

$$\int_{x_{\min}}^{x_{\max}} dx f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = 1 \quad (6.5)$$

NB: the  $N(x_{\min}, x_{\max}, x_0, \gamma)$  should be calculated once and tabulated to save processing time, but we are lazy here.

$$\begin{aligned}
N(x_{\min}, x_{\max}, x_0, \gamma) &= \sum_{p=1}^{n_p} \int_{x_{\min}}^{x_{\max}} dx \left| \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \\
&\quad + 2 \operatorname{Re} \sum_{p=1}^{n_p} \sum_{q=1}^{n_p} \int_{x_{\min}}^{x_{\max}} dx \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} \quad (6.6)
\end{aligned}$$

```

205 <Implementation of vamp_test0_functions procedures 205>≡ (204c) 206>
pure function f0(x, x_min, x_max, x0, g) result(f_x)
 real(kind=default), intent(in) :: x, x_min, x_max
 real(kind=default), dimension(:), intent(in) :: x0, g
 real(kind=default) :: f_x
 complex(kind=default) :: amp

```

```

real(kind=default) :: norm
integer :: i, j
amp = sum (1.0 / cmplx (x - x0, g, kind=default))
norm = 0
do i = 1, size (x0)
 norm = norm + f_norm (x_min, x_max, x0(i), g(i), x0(i), g(i))
 do j = i + 1, size (x0)
 norm = norm + 2 * f_norm (x_min, x_max, x0(i), g(i), x0(j), g(j))
 end do
end do
f_x = amp * conjg (amp) / norm
end function f0

```

$$\int_{x_{\min}}^{x_{\max}} dx \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} = \frac{1}{x_{0,p} - x_{0,q} - i\gamma_p - i\gamma_q} \left( \ln \left( \frac{x_{\max} - x_{0,p} + i\gamma_p}{x_{\min} - x_{0,p} + i\gamma_p} \right) - \ln \left( \frac{x_{\max} - x_{0,q} - i\gamma_q}{x_{\min} - x_{0,q} - i\gamma_q} \right) \right) \quad (6.7)$$

Don't even think of merging the logarithms: it will screw up the Riemann sheet.

206  $\langle$ Implementation of `vamp_test0_functions` procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 205 207a $\rangle$

```

pure function f_norm (x_min, x_max, x0p, gp, x0q, gq) &
 result (norm)
real(kind=default), intent(in) :: x_min, x_max, x0p, gp, x0q, gq
real(kind=default) :: norm
norm = real ((log (cmplx (x_max - x0p, gp, kind=default) &
 / cmplx (x_min - x0p, gp, kind=default)) &
 - log (cmplx (x_max - x0q, - gq, kind=default) &
 / cmplx (x_min - x0q, - gq, kind=default))) &
 / cmplx (x0p - x0q, - gp - gq, kind=default), &
 kind=default)
end function f_norm

```

Since we want to be able to do the integral of  $f$  analytically, it is most convenient to take a weighted sum of products:

$$f(x_1, \dots, x_{n_d} | x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{\sum_{i=1}^{n_c} c_i} \sum_{i=1}^{n_c} c_i \prod_{j=1}^{n_d} f_0(x_j | x_{\min,j}, x_{\max,j}, x_{0,ij}, \gamma_{ij}) \quad (6.8)$$

Each summand is factorized and therefore very easily integrated by Vegas.  
A non-trivial sum is more realistic in this respect.

207a  $\langle$ Implementation of vamp\_test0.functions procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 206 207b $\rangle$   
pure function **f** (**x**, data, weights, channel, grids) result (f\_x)

```

 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: f_x
 real(kind=default) :: fi_x
 integer :: i, j
 f_x = 0.0
 do i = 1, size (c)
 fi_x = 1.0
 do j = 1, size (x)
 if (all (gamma(:,i,j) > 0)) then
 fi_x = fi_x * f0 (x(j), x_min(j), x_max(j), &
 x0(:,i,j), gamma(:,i,j))
 else
 fi_x = fi_x / (x_max(j) - x_min(j))
 end if
 end do
 f_x = f_x + c(i) * fi_x
 end do
 f_x = f_x / sum (c)
end function f

```

207b  $\langle$ Implementation of vamp\_test0.functions procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 207a 207c $\rangle$   
subroutine **delete\_sample** ()  
deallocate (c, x\_min, x\_max, x0, **gamma**)  
end subroutine **delete\_sample**

207c  $\langle$ Implementation of vamp\_test0.functions procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 207b 208 $\rangle$   
subroutine **create\_sample** (num\_poles, weights, region)  
integer, intent(in) :: num\_poles  
real(kind=default), dimension(:), intent(in) :: weights  
real(kind=default), dimension(:,:), intent(in) :: region  
integer :: nd, nc  
nd = size (region, dim=2)  
nc = size (weights)  
allocate (c(nc), x\_min(nd), x\_max(nd))  
allocate (x0(num\_poles,nc,nd), **gamma**(num\_poles,nc,nd))  
x\_min = region(1,:)



```

x_max = region(2,:)
c = weights
end subroutine create_sample

```

### Multi Channel

We start from the usual mapping for Lorentzian peaks

$$\begin{aligned} \psi(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ \xi \mapsto x = \psi(\xi|x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.9)$$

where

$$\begin{aligned} \psi(\xi|x_{\min}, x_{\max}, x_0, \gamma) = x_0 + \\ \gamma \cdot \tan \left( \frac{\xi - x_{\min}}{x_{\max} - x_{\min}} \cdot \operatorname{atan} \frac{x_{\max} - x_0}{\gamma} - \frac{x_{\max} - \xi}{x_{\max} - x_{\min}} \cdot \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma} \right) \end{aligned} \quad (6.10)$$

208  $\langle$ Implementation of `vamp_test0_functions` procedures 205 $\rangle + \equiv$  (204c)  $\triangleleft$ 207c 209a $\triangleright$

```

pure function psi (xi, x_min, x_max, x0, gamma) result (x)
 real(kind=default), intent(in) :: xi, x_min, x_max, x0, gamma
 real(kind=default) :: x
 x = x0 + gamma &
 * tan (((xi - x_min) * atan ((x_max - x0) / gamma) &
 - (x_max - xi) * atan ((x0 - x_min) / gamma)) &
 / (x_max - x_min))
end function psi

```

The inverse mapping is

$$\begin{aligned} \psi^{-1}(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ x \mapsto \xi = \psi^{-1}(x|x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.11)$$

with

$$\begin{aligned} \psi^{-1}(x|x_{\min}, x_{\max}, x_0, \gamma) = \\ \frac{x_{\max}(\operatorname{atan} \frac{x_0 - x_{\min}}{\gamma} + \operatorname{atan} \frac{x - x_0}{\gamma}) + x_{\min}(\operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x}{\gamma})}{\operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma}} \end{aligned} \quad (6.12)$$

with Jacobian

$$\frac{d(\psi^{-1}(x|x_{\min}, x_{\max}, x_0, \gamma))}{dx} = \frac{x_{\max} - x_{\min}}{\operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma}} \frac{\gamma}{(x - x_0)^2 + \gamma^2} \quad (6.13)$$

209a  $\langle$ Implementation of `vamp_test0_functions` procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 208 209c $\rangle$

```

pure function g0 (x, x_min, x_max, x0, gamma) result (g_x)
 real(kind=default), intent(in) :: x, x_min, x_max, x0, gamma
 real(kind=default) :: g_x
 g_x = gamma / (atan ((x_max - x0) / gamma) - atan ((x_min - x0) / gamma)) &
 * (x_max - x_min) / ((x - x0)**2 + gamma**2)
end function g0

```

The function  $f$  has  $n_c n_p^{n_d}$  peaks and we need a channel for each one, plus a constant function for the background. We encode the position on the grid linearly:

209b  $\langle$ Decode channel into `ch` and `p(:)` 209b $\rangle \equiv$  (209c 210a)

```

ch = channel - 1
do j = 1, size (x)
 p(j) = 1 + modulo (ch, np)
 ch = ch / np
end do
ch = ch + 1

```

The map  $\phi$  is the direct product of  $\psi$ s:

209c  $\langle$ Implementation of `vamp_test0_functions` procedures 205 $\rangle + \equiv$  (204c)  $\langle$ 209a 210a $\rangle$

```

pure function phi (xi, channel) result (x)
 real(kind=default), dimension(:), intent(in) :: xi
 integer, intent(in) :: channel
 real(kind=default), dimension(size(xi)) :: x
 integer, dimension(size(xi)) :: p
 integer :: j, ch, np, nch, nd, channels
 np = size (x0, dim = 1)
 nch = size (x0, dim = 2)
 nd = size (x0, dim = 3)
 channels = nch * np**nd
 if (channel >= 1 .and. channel <= channels) then
 \langle Decode channel into ch and p(:) 209b \rangle
 do j = 1, size (xi)
 if (all (gamma(:,ch,j) > 0)) then
 x(j) = psi (xi(j), x_min(j), x_max(j), &
 x0(p(j),ch,j), gamma(p(j),ch,j))
 else
 x = xi
 end if
 end do
 else if (channel == channels + 1) then
 x = xi
 else

```

```

 x = 0
 end if
end function phi

```

similarly for the Jacobians:

210a  $\langle$ Implementation of vamp\_test0\_functions procedures 205 $\rangle + \equiv$  (204c)  $\triangleleft$ 209c 210b $\triangleright$

```

pure recursive function g (x, data, channel) result (g_x)
 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
 integer, intent(in) :: channel
 real(kind=default) :: g_x
 integer, dimension(size(x)) :: p
 integer :: j, ch, np, nch, nd, channels
 np = size (x0, dim = 1)
 nch = size (x0, dim = 2)
 nd = size (x0, dim = 3)
 channels = nch * np**nd
 if (channel >= 1 .and. channel <= channels) then
 \langle Decode channel into ch and p(:) 209b \rangle
 g_x = 1.0
 do j = 1, size (x)
 if (all (gamma(:,ch,j) > 0)) then
 g_x = g_x * g0 (x(j), x_min(j), x_max(j), &
 x0(p(j),ch,j), gamma(p(j),ch,j))
 end if
 end do
 else if (channel == channels + 1) then
 g_x = 1.0
 else
 g_x = 0
 end if
end function g

```

210b  $\langle$ Implementation of vamp\_test0\_functions procedures 205 $\rangle + \equiv$  (204c)  $\triangleleft$ 210a

```

function w (x, data, weights, channel, grids) result (w_x)
 real(kind=default), dimension(:), intent(in) :: x
 class(vamp_data_t), intent(in) :: data
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: w_x
 w_x = vamp_multi_channel0 (f, data, phi, g, x, weights, channel)
end function w

```

## Driver Routines

211a  $\langle$ vamp\_test0.f90 204b $\rangle$ + $\equiv$   $\langle$ 204b 217 $\rangle$   
 module **vamp\_tests0**  
 $\langle$ Modules used by vamp\_tests0 211b $\rangle$   
 use **vamp**  
 implicit none  
 private  
 $\langle$ Declaration of procedures in vamp\_tests0 211e $\rangle$   
 contains  
 $\langle$ Implementation of procedures in vamp\_tests0 212a $\rangle$   
 end module **vamp\_tests0**

211b  $\langle$ Modules used by vamp\_tests0 211b $\rangle$  $\equiv$  (211a 219e)  
 use kinds  
 use **exceptions**  
 use **histograms**  
 use **tao\_random\_numbers**  
 use **vamp\_test0\_functions** !NODEP!

### Verification

211c  $\langle$ Declaration of procedures in vamp\_tests0 (broken?) 211c $\rangle$  $\equiv$   
 public :: **check\_jacobians**

211d  $\langle$ Implementation of procedures in vamp\_tests0 (broken?) 211d $\rangle$  $\equiv$   
**subroutine check\_jacobians** (do\_print, region, samples, rng)  
 logical, intent(in) :: do\_print  
 real(kind=default), dimension(:, :), intent(in) :: region  
 integer, dimension(:), intent(in) :: samples  
 type(**tao\_random\_state**), intent(inout) :: rng  
 real(kind=default), dimension(size(region,dim=2)) :: **x**  
 real(kind=default) :: d  
 integer :: ch  
 do ch = 1, size(x0,dim=2) \* size(x0,dim=1)\*\*size(x0,dim=3) + 1  
 call **vamp\_check\_jacobian** (rng, samples(1), **g**, **phi**, ch, region, d, **x**)  
 if (do\_print) then  
 print \*, ch, ": ", d, ", ", **x** = ", real (**x**)  
 end if  
 end do  
end **subroutine check\_jacobians**

### Integration

211e  $\langle$ Declaration of procedures in vamp\_tests0 211e $\rangle$  $\equiv$  (211a 219e) 214a $\rangle$   
 public :: **single\_channel**, **multi\_channel**

212a *⟨Implementation of procedures in vamp\_tests0 212a⟩*≡ (211a 219e) 212b▷

```

subroutine single_channel (do_print, region, iterations, samples, rng, &
 acceptable, failures)
 logical, intent(in) :: do_print
 real(kind=default), dimension(:,:), intent(in) :: region
 integer, dimension(:), intent(in) :: iterations, samples
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), intent(in) :: acceptable
 integer, intent(inout) :: failures
 type(vamp_grid) :: gr
 type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
 real(kind=default) :: integral, standard_dev, chi_squared, pull
 call vamp_create_history (history)
 call vamp_create_grid (gr, region, samples(1))
 call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
 call vamp_discard_integral (gr, samples(2))
 call vamp_sample_grid &
 (rng, gr, f, NO_DATA, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+1:))
 call vamp_write_grid (gr, "vamp_test0.grid")
 call vamp_delete_grid (gr)
 call vamp_print_history (history, "single")
 call vamp_delete_history (history)
 pull = (integral - 1) / standard_dev
 if (do_print) then
 print *, " int, err, chi2:", integral, standard_dev, chi_squared
 end if
 if (abs (pull) > acceptable) then
 failures = failures + 1
 print *, " unacceptable pull:", pull
 else
 print *, " acceptable pull:", pull
 end if
end subroutine single_channel

```

212b *⟨Implementation of procedures in vamp\_tests0 212a⟩*+≡ (211a 219e) ◁212a 214b▷

```

subroutine multi_channel (do_print, region, iterations, samples, rng, &
 acceptable, failures)
 logical, intent(in) :: do_print
 real(kind=default), dimension(:,:), intent(in) :: region
 integer, dimension(:), intent(in) :: iterations, samples
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), intent(in) :: acceptable

```

```

 type(vamp_grids) :: grs
 integer, intent(inout) :: failures
 <Body of multi_channel 199b>
end subroutine multi_channel
213 <Body of multi_channel 199b>+≡ (199a 212b) <199b
 real(kind=default), &
 dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
 weight_vector
 type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
 type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
 real(kind=default) :: integral, standard_dev, chi_squared, pull
 integer :: it
 weight_vector = 1.0
 call vamp_create_history (history)
 call vamp_create_history (histories)
 call vamp_create_grids (grs, region, samples(1), weight_vector)
 call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
 history = history, histories = histories)
do it = 1, 5
 call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
 history = history(iterations(1)+it-1:), &
 histories = histories(iterations(1)+it-1:,:))
 call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
 (rng, grs, w, NO_DATA, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+5:), &
 histories = histories(iterations(1)+5:,:))
call vamp_write_grids (grs, "vamp_test0.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
if (do_print) then
 print *, integral, standard_dev, chi_squared
end if
pull = (integral - 1) / standard_dev
if (abs (pull) > acceptable) then
 failures = failures + 1
 print *, " unacceptable pull:", pull

```

```

else
 print *, " acceptable pull:", pull
end if

```

### Event Generation

```

214a <Declaration of procedures in vamp_tests0 211e>+≡ (211a 219e) <211e
 public :: single_channel_generator, multi_channel_generator

214b <Implementation of procedures in vamp_tests0 212a>+≡ (211a 219e) <212b 215>
 subroutine single_channel_generator (do_print, region, iterations, samples, rng)
 logical, intent(in) :: do_print
 real(kind=default), dimension(:,:), intent(in) :: region
 integer, dimension(:), intent(in) :: iterations, samples
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid) :: gr
 type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
 type(histogram) :: unweighted, reweighted, weighted, weights
 type(exception) :: exc
 real(kind=default) :: weight, integral, standard_dev
 integer :: i
 real(kind=default), dimension(size(region,dim=2)) :: x
 call vamp_create_grid (gr, region, samples(1))
 call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
 call vamp_discard_integral (gr, samples(2))
 call vamp_warmup_grid &
 (rng, gr, f, NO_DATA, iterations(2), history = history(iterations(1)+1:))
 call vamp_print_history (history, "single")
 call vamp_delete_history (history)
 call create_histogram (unweighted, region(1,1), region(2,1), 100)
 call create_histogram (reweighted, region(1,1), region(2,1), 100)
 call create_histogram (weighted, region(1,1), region(2,1), 100)
 call create_histogram (weights, 0.0_default, 10.0_default, 100)
 ! do i = 1, 1000000
 do i = 1, 100
 call clear_exception (exc)
 call vamp_next_event (x, rng, gr, f, NO_DATA, exc = exc)
 call handle_exception (exc)
 call fill_histogram (unweighted, x(1))
 call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
 end do
 integral = 0.0
 standard_dev = 0.0
 do i = 1, 10000

```

```

 call clear_exception (exc)
 call vamp_next_event (x, rng, gr, f, NO_DATA, weight, exc = exc)
 call handle_exception (exc)
 call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
 call fill_histogram (weights, x(1), weight)
 integral = integral + weight
 standard_dev = standard_dev + weight**2
end do
if (do_print) then
 print *, integral / (i-1), sqrt (standard_dev) / (i-1)
 call write_histogram (unweighted, "u_s.d")
 call write_histogram (reweighted, "r_s.d")
 call write_histogram (weighted, "w_s.d")
 call write_histogram (weights, "ws_s.d")
end if
call delete_histogram (unweighted)
call delete_histogram (reweighted)
call delete_histogram (weighted)
call delete_histogram (weights)
call vamp_delete_grid (gr)
end subroutine single_channel_generator

```

215 *Implementation of procedures in vamp\_tests0* 212a)+≡ (211a 219e) <214b

```

subroutine multi_channel_generator (do_print, region, iterations, samples, rng)
 logical, intent(in) :: do_print
 real(kind=default), dimension(:, :), intent(in) :: region
 integer, dimension(:), intent(in) :: iterations, samples
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grids) :: grs
 real(kind=default), &
 dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
 weight_vector
 type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
 type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
 type(histogram) :: unweighted, reweighted, weighted, weights
 type(exception) :: exc
 real(kind=default) :: weight, integral, standard_dev
 real(kind=default), dimension(size(region,dim=2)) :: x
 character(len=5) :: pfx
 integer :: it, i, j
 weight_vector = 1.0
 call vamp_create_history (history)
 call vamp_create_history (histories)
 call vamp_create_grids (grs, region, samples(1), weight_vector)

```



```

call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
 history = history, histories = histories)
do it = 1, 5
 call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
 history = history(iterations(1)+it-1:), &
 histories = histories(iterations(1)+it-1:,:))
 call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_warmup_grids &
 (rng, grs, w, NO_DATA, iterations(2), &
 history = history(iterations(1)+5:), &
 histories = histories(iterations(1)+5:,:))
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
!!! do i = 1, size (grs%grids)
!!! do j = 1, size (grs%grids(i)%div)
!!! write (pfx, "(I2.2,'/',I2.2)") i, j
!!! call dump_division (grs%grids(i)%div(j), pfx)
!!! end do
!!! end do
call create_histogram (unweighted, region(1,1), region(2,1), 100)
call create_histogram (reweighted, region(1,1), region(2,1), 100)
call create_histogram (weighted, region(1,1), region(2,1), 100)
call create_histogram (weights, 0.0_default, 10.0_default, 100)
! do i = 1, 1000000
do i = 1, 100
 call clear_exception (exc)
 call vamp_next_event (x, rng, grs, f, NO_DATA, phi, exc = exc)
 call handle_exception (exc)
 call fill_histogram (unweighted, x(1))
 call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
end do
integral = 0.0
standard_dev = 0.0
do i = 1, 10000
 call clear_exception (exc)
 call vamp_next_event (x, rng, grs, f, NO_DATA, phi, weight, exc = exc)
 call handle_exception (exc)
 call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
 call fill_histogram (weights, x(1), weight)

```

```

 integral = integral + weight
 standard_dev = standard_dev + weight**2
 end do
 if (do_print) then
 print *, integral / (i-1), sqrt (standard_dev) / (i-1)
 call write_histogram (unweighted, "u_m.d")
 call write_histogram (reweighted, "r_m.d")
 call write_histogram (weighted, "w_m.d")
 call write_histogram (weights, "ws_m.d")
 end if
 call delete_histogram (unweighted)
 call delete_histogram (reweighted)
 call delete_histogram (weighted)
 call delete_histogram (weights)
 call vamp_delete_grids (grs)
end subroutine multi_channel_generator

```

### *Main Program*

```

217 <vamp_test0.f90 204b>+≡ <211a
 program vamp_test0
 <Modules used by vamp_test0 219a>
 implicit none
 <Variables in vamp_test0 218f>
 do_print = .true.
 print *, "Starting VAMP 1.0 self test..."
 print *, "serial code"
 call tao_random_create (rng, 0)
 call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
 if (status == 0) then
 call system_clock (ticks0)
 else
 ticks0 = 42
 end if
 call tao_random_seed (rng, ticks0)
 <Set up integrand and region in vamp_test0 219c>
 <Execute tests in vamp_test0 218a>
 <Cleanup in vamp_test0 219d>
 if (failures == 0) then
 stop 0
 else if (failures == 1) then
 stop 1
 else

```

```

 stop 2
 end if
end program vamp_test0

218a <Execute tests in vamp_test0 218a>≡ (217) 218b>
 failures = 0
 call system_clock (ticks0)
 call single_channel (do_print, region, iterations, samples, rng, 10*ACCEPTABLE, failures)
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F6.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218b <Execute tests in vamp_test0 218a>+≡ (217) <218a 218c>
 call system_clock (ticks0)
 call single_channel_generator &
 (do_print, region, iterations, samples, rng)
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F6.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218c <Execute tests in vamp_test0 218a>+≡ (217) <218b 218d>
 call system_clock (ticks0)
 call multi_channel (do_print, region, iterations, samples, rng, ACCEPTABLE, failures)
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F6.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218d <Execute tests in vamp_test0 218a>+≡ (217) <218c 218e>
 call system_clock (ticks0)
 call multi_channel_generator &
 (do_print, region, iterations, samples, rng)
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F6.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218e <Execute tests in vamp_test0 218a>+≡ (217) <218d
 call system_clock (ticks0)
 ! call check_jacobians (do_print, region, samples, rng)
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F6.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218f <Variables in vamp_test0 218f>≡ (217 220) 219b>
 logical :: do_print

218g <Execute command 218g>≡ (220)

```

```

219a <Modules used by vamp_test0 219a>≡ (217 220)
 use kinds
 use tao_random_numbers
 use vamp_test0_functions !NODEP!
 use vamp_tests0 !NODEP!

219b <Variables in vamp_test0 218f>+≡ (217 220) <218f
 integer :: i, j, ticks, ticks_per_second, ticks0, status
 integer, dimension(2) :: iterations, samples
 real(kind=default), dimension(:,,:), allocatable :: region
 type(tao_random_state) :: rng
 real(kind=default), parameter :: ACCEPTABLE = 4
 integer :: failures

219c <Set up integrand and region in vamp_test0 219c>≡ (217 220)
 iterations = (/ 4, 3 /)
 samples = (/ 10000, 50000 /)
 allocate (region(2,2))
 region(1,:) = -1.0
 region(2,:) = 2.0
 call create_sample &
 (num_poles = 2, weights = (/ 1.0_default, 2.0_default /), region = region)
 do i = 1, size (x0, dim=2)
 do j = 1, size (x0, dim=3)
 call tao_random_number (rng, x0(:,i,j))
 end do
 end do
 gamma = 0.001
 x0(1, :, :) = 0.2
 x0(2, :, :) = 0.8

219d <Cleanup in vamp_test0 219d>≡ (217 220)
 call delete_sample ()
 deallocate (region)

```

### 6.2.2 Parallel Test

```

219e <vampi_test0.f90 219e>≡ 220>
 ! vampi_test0.f90 --
 <Copyleft notice 1>
 <Module vamp_test0_functions 204c>
 module vamp_tests0
 <Modules used by vamp_tests0 211b>
 use vampi
 use mpi90

```

```

 implicit none
 private
 <Declaration of procedures in vamp_tests0 211e>
contains
 <Implementation of procedures in vamp_tests0 212a>
end module vamp_tests0

220 <vampi_test0.f90 219e>+≡ ◁219e
 program vampi_test0
 <Modules used by vamp_test0 219a>
 use mpi90
 implicit none
 <Variables in vamp_test0 218f>
 integer :: num_proc, proc_id
 call mpi90_init ()
 call mpi90_size (num_proc)
 call mpi90_rank (proc_id)
 if (proc_id == 0) then
 do_print = .true.
 print *, "Starting VAMP 1.0 self test..."
 if (num_proc > 1) then
 print *, "parallel code running on ", num_proc, " processors"
 else
 print *, "parallel code running serially"
 end if
 else
 do_print = .false.
 end if
 call tao_random_create (rng, 0)
 call system_clock (ticks0)
 call tao_random_seed (rng, ticks0 + proc_id)
 <Set up integrand and region in vamp_test0 219c>
 call mpi90_broadcast (x0, 0)
 call mpi90_broadcast (gamma, 0)
 command_loop: do
 if (proc_id == 0) then
 <Read command line and decode it as command (never defined)>
 end if
 call mpi90_broadcast (command, 0)
 call system_clock (ticks0)
 <Execute command 218g>
 call system_clock (ticks, ticks_per_second)
 if (proc_id == 0) then
 print "(1X,A,F6.2,A)", &

```

```

 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
 end if
end do command_loop
<Cleanup in vamp_test0 219d>
call mpi90_finalize ()
if (proc_id == 0) then
 print *, "bye."
end if
end program vampi_test0

```

### 6.2.3 Output

221 <vamp\_test0.out 221>≡

# —7—

## APPLICATION

### 7.1 Cross section

```
222a <application.f90 222a>≡ 239▷
! application.f90 --
<Copyleft notice 1>
module cross_section
 use kinds
 use constants
 use utils
 use kinematics
 use tao_random_numbers
 use products, only: dot
 use helicity
 use vamp, only: vamp_grid, vamp_probability
 implicit none
 private
 <Declaration of cross_section procedures 223d>
 <Types in cross_section 228c>
 <Variables in cross_section 222b>
contains
 <Implementation of cross_section procedures 224a>
end module cross_section

222b <Variables in cross_section 222b>≡ (222a) 223c▷
 real(kind=default), private, parameter :: &
 MA_0 = 0.0, &
 MB_0 = 0.0, &
 M1_0 = 0.0, &
 M2_0 = 0.0, &
 M3_0 = 0.0, &
```

```
S_0 = 200.0 ** 2
```

223a  $\langle$ XXX Variables in cross\_section 223a $\rangle \equiv$  223b $\triangleright$

```
real(kind=default), private, parameter :: &
 MA_0 = 0.01, &
 MB_0 = 0.01, &
 M1_0 = 0.01, &
 M2_0 = 0.01, &
 M3_0 = 0.01, &
 S_0 = 200.0 ** 2
```

223b  $\langle$ XXX Variables in cross\_section 223a $\rangle + \equiv$   $\triangleleft$  223a

```
real(kind=default), private, parameter :: &
 S1_MIN_0 = 0.0 ** 2, &
 S2_MIN_0 = 0.0 ** 2, &
 S3_MIN_0 = 0.0 ** 2, &
 T1_MIN_0 = 0.0 ** 2, &
 T2_MIN_0 = 0.0 ** 2
```

223c  $\langle$ Variables in cross\_section 222b $\rangle + \equiv$  (222a)  $\triangleleft$  222b 223f $\triangleright$

```
real(kind=default), private, parameter :: &
 S1_MIN_0 = 1.0 ** 2, &
 S2_MIN_0 = 1.0 ** 2, &
 S3_MIN_0 = 1.0 ** 2, &
 T1_MIN_0 = 10.0 ** 2, &
 T2_MIN_0 = 10.0 ** 2
```

223d  $\langle$ Declaration of cross\_section procedures 223d $\rangle \equiv$  (222a) 225a $\triangleright$

```
private :: cuts
```

223e  $\langle$ XXX Implementation of cross\_section procedures 223e $\rangle \equiv$

```
pure function cuts (k1, k2, p1, p2, q) result (inside)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 logical :: inside
 inside = (abs (dot (k1 - q, k1 - q)) >= T1_MIN_0) &
 .and. (abs (dot (k2 - q, k2 - q)) >= T2_MIN_0) &
 .and. (abs (dot (p1 + q, p1 + q)) >= S1_MIN_0) &
 .and. (abs (dot (p2 + q, p2 + q)) >= S2_MIN_0) &
 .and. (abs (dot (p1 + p2, p1 + p2)) >= S3_MIN_0)
end function cuts
```

223f  $\langle$ Variables in cross\_section 222b $\rangle + \equiv$  (222a)  $\triangleleft$  223c

```
real(kind=default), private, parameter :: &
```



```

E_MIN = 1.0, &
COSTH_SEP_MAX = 0.99, &
COSTH_BEAM_MAX = 0.99

```

224a *⟨Implementation of cross\_section procedures 224a⟩*≡ (222a) 224b>

```

pure function cuts (k1, k2, p1, p2, q) result (inside)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 logical :: inside
 real(kind=default), dimension(3) :: p1n, p2n, qn
 inside = .false.
 if ((p1(0) < E_MIN) .or. (p2(0) < E_MIN) .or. (q(0) < E_MIN)) then
 return
 end if
 p1n = p1(1:3) / sqrt (dot_product (p1(1:3), p1(1:3)))
 p2n = p2(1:3) / sqrt (dot_product (p2(1:3), p2(1:3)))
 qn = q(1:3) / sqrt (dot_product (q(1:3), q(1:3)))
 if ((abs (qn(3)) > COSTH_BEAM_MAX) &
 .or. (abs (p1n(3)) > COSTH_BEAM_MAX)&
 .or. (abs (p2n(3)) > COSTH_BEAM_MAX)) then
 return
 end if
 if (dot_product (p1n, qn) > COSTH_SEP_MAX) then
 return
 end if
 if (dot_product (p2n, qn) > COSTH_SEP_MAX) then
 return
 end if
 if (dot_product (p1n, p2n) > COSTH_SEP_MAX) then
 return
 end if
 inside = .true.
end function cuts

```

224b *⟨Implementation of cross\_section procedures 224a⟩*+≡ (222a) <224a 226b>

```

function xsect (k1, k2, p1, p2, q) result (xs)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 real(kind=default) :: xs
 complex(kind=default), dimension(-1:1,-1:1,-1:1,-1:1,-1:1) :: amp
 !!! xs = 1.0_double / phase_space_volume (3, k1(0) + k2(0))
 !!! xs = 1.0_double / dot (p1 + q, p1 + q) &
 !!! + 1.0_double / dot (p2 + q, p2 + q)
 !!! return
 amp = nneeg (k1, k2, p1, p2, q)

```

```

 xs = sum (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2) &
 * conjg (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2)))
 end function xsect

```

225a  $\langle$ Declaration of cross\_section procedures 223d $\rangle + \equiv$  (222a)  $\langle$ 223d 227b $\rangle$

```

private :: xsect

$$\phi : [0, 1]^{\otimes 5} \rightarrow [(m_2 + m_3)^2, (\sqrt{s} - m_1)^2] \otimes [t_1^{\min}(s_2), t_1^{\max}(s_2)]$$

$$\otimes [0, 2\pi] \otimes [-1, 1] \otimes [0, 2\pi]$$

$$(x_1, \dots, x_5) \mapsto (s_2, t_1, \phi, \cos \theta_3, \phi_3)$$

$$= (s_2(x_1), x_2 t_1^{\max}(s_2) + (1 - x_2) t_1^{\min}(s_2), 2\pi x_3, 2x_4 - 1, 2\pi x_5)$$


```

(7.1)

where

$$t_1^{\max/\min}(s_2)$$

$$= m_a^2 + m_1^2 - \frac{(s + m_a^2 - m_b^2)(s - s_2 + m_1^2) \mp \sqrt{\lambda(s, m_a^2, m_b^2)\lambda(s, s_2, m_1^2)}}{2s}$$

(7.2)

225b  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  225b $\rangle \equiv$  (226b)

```

! s2_min = S1_MIN_0
s2_min = (m2 + m3)**2
s2_max = (sqrt(s) - m1)**2
s2 = s2_max * x(1) + s2_min * (1 - x(1))
t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
+ sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
- sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1 = t1_max * x(2) + t1_min * (1 - x(2))
phi = 2*PI * x(3)
cos_theta3 = 2 * x(4) - 1
phi3 = 2*PI * x(5)

```

225c  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 225c $\rangle \equiv$  (228b)

```

! s2_min = S1_MIN_0
s2_min = 0
s2_max = s
s2 = s2_max * x(1) + s2_min * (1 - x(1))
t1_min = - (s - s2)
t1_max = 0
t1 = t1_max * x(2) + t1_min * (1 - x(2))
phi = 2*PI * x(3)
cos_theta3 = 2 * x(4) - 1
phi3 = 2*PI * x(5)

```

$$J_\phi(x_1, \dots, x_5) = \left| \begin{array}{cc} \frac{\partial s_2}{\partial x_1} & \frac{\partial t_1}{\partial x_1} \\ \frac{\partial s_2}{\partial x_2} & \frac{\partial t_1}{\partial x_2} \end{array} \right| \cdot 8\pi^2 \quad (7.3)$$

i.e.

$$J_\phi(x_1, \dots, x_5) = 8\pi^2 \cdot \left| \frac{ds_2}{dx_1} \right| \cdot (t_1^{\max}(s_2) - t_1^{\min}(s_2)) \quad (7.4)$$

226a  $\langle \text{Adjust Jacobian } 226a \rangle \equiv$  (226b 228b)

```
p%jacobian = p%jacobian &
* (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
```

226b  $\langle \text{Implementation of cross\_section procedures } 224a \rangle + \equiv$  (222a)  $\langle 224b \ 227c \rangle$

```
pure function phase_space(x, channel) result(p)
 real(kind=default), dimension(:), intent(in) :: x
 integer, intent(in) :: channel
 type(LIPS3) :: p
 real(kind=default) :: &
 ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
 real(kind=default) :: s2_min, s2_max, t1_min, t1_max
 s = S_0
 $\langle m_a \leftrightarrow m_b, m_1 \leftrightarrow m_2 \text{ for channel \#1 } 226c \rangle$
 $\langle \text{Set } (s_2, t_1, \phi, \cos \theta_3, \phi_3) \text{ from } (x_1, \dots, x_5) \ 225b \rangle$
 p = two_to_three(s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
 $\langle \text{Adjust Jacobian } 226a \rangle$
 $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 } 227a \rangle$
end function phase_space
```

226c  $\langle m_a \leftrightarrow m_b, m_1 \leftrightarrow m_2 \text{ for channel \#1 } 226c \rangle \equiv$  (226b)

```
select case (channel)
case (1)
 ma = MA_0
 mb = MB_0
 m1 = M1_0
 m2 = M2_0
 m3 = M3_0
case (2)
 ma = MB_0
 mb = MA_0
 m1 = M2_0
 m2 = M1_0
 m3 = M3_0
case (3)
 ma = MA_0
 mb = MB_0
 m1 = M3_0
```

```

 m2 = M2_0
 m3 = M1_0
 case default
 ma = MA_0
 mb = MB_0
 m1 = M1_0
 m2 = M2_0
 m3 = M3_0
 end select

```

227a  $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 227a} \rangle \equiv$  (226b 228b)

```

 select case (channel)
 case (1)
 ! OK
 case (2)
 call swap (p%p(1,:), p%p(2,:))
 case (3)
 call swap (p%p(1,:), p%p(3,:))
 case default
 ! OK
 end select

```

227b  $\langle \text{Declaration of cross\_section procedures 223d} \rangle + \equiv$  (222a)  $\langle$ 225a 228a $\rangle$   
 private :: jacobian

227c  $\langle \text{Implementation of cross\_section procedures 224a} \rangle + \equiv$  (222a)  $\langle$ 226b 228b $\rangle$

```

pure function jacobian (k1, k2, p1, p2, q) result (jac)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 real(kind=default) :: jac
 real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
 real(kind=default) :: s, s2, s2_min, s2_max, t1_min, t1_max
 ma_2 = max (dot (k1, k1), 0.0_double)
 mb_2 = max (dot (k2, k2), 0.0_double)
 m1_2 = max (dot (p1, p1), 0.0_double)
 m2_2 = max (dot (p2, p2), 0.0_double)
 m3_2 = max (dot (q, q), 0.0_double)
 s = dot (k1 + k2, k1 + k2)
 s2 = dot (p2 + q, p2 + q)
 ! s2_min = S1_MIN_0
 s2_min = (sqrt (m2_2) + sqrt (m3_2))**2
 s2_max = (sqrt (s) - sqrt (m1_2))**2
 t1_min = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
 + sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
 t1_max = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
 - sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)

```

```

 jac = 1.0 / ((2*PI)**5 * 32 * s2) &
 * sqrt (lambda (s2, m2_2, m3_2) / lambda (s, ma_2, mb_2)) &
 * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
end function jacobian

```

228a  $\langle$ Declaration of cross\_section procedures 223d $\rangle + \equiv$  (222a)  $\langle$ 227b 228e $\rangle$   
 private :: phase\_space, phase\_space\_massless

228b  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 227c 228f $\rangle$   
 pure function phase\_space\_massless (x, channel) result (p)  
 real(kind=default), dimension(:), intent(in) :: x  
 integer, intent(in) :: channel  
 type(LIPS3) :: p  
 real(kind=default) :: s, t1, s2, phi, cos\_theta3, phi3  
 real(kind=default) :: s2\_min, s2\_max, t1\_min, t1\_max  
 s = S\_0  
 $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 225c $\rangle$   
 p = two\_to\_three (s, t1, s2, phi, cos\_theta3, phi3)  
 $\langle$ Adjust Jacobian 226a $\rangle$   
 $\langle$  $p_1 \leftrightarrow p_2$  for channel #2 227a $\rangle$   
 end function phase\_space\_massless

228c  $\langle$ Types in cross\_section 228c $\rangle \equiv$  (222a) 228d $\rangle$   
 type, public :: LIPS3\_m5i2a3  
 ! private  
 real(kind=default) :: ma, mb, m1, m2, m3  
 real(kind=default) :: s, s2, t1  
 real(kind=default) :: phi, cos\_theta3, phi3  
 real(kind=default) :: jacobian  
 end type LIPS3\_m5i2a3

228d  $\langle$ Types in cross\_section 228c $\rangle + \equiv$  (222a)  $\langle$ 228c $\rangle$   
 type, public :: x5  
 ! private  
 real(kind=default), dimension(5) :: x  
 real(kind=default) :: jacobian  
 end type x5

228e  $\langle$ Declaration of cross\_section procedures 223d $\rangle + \equiv$  (222a)  $\langle$ 228a 231a $\rangle$   
 private :: invariants\_from\_p, invariants\_to\_p  
 private :: invariants\_from\_x, invariants\_to\_x

228f  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 228b 229a $\rangle$   
 pure function invariants\_from\_p (p, k1, k2) result (q)  
 type(LIPS3), intent(in) :: p

```

real(kind=default), dimension(0:), intent(in) :: k1, k2
type(LIPS3_m5i2a3) :: q
real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
real(kind=default), dimension(0:3) :: k1k2, p2p3, k1p1, p3_23
k1k2 = k1 + k2
k1p1 = - k1 + p%p(1,:)
p2p3 = p%p(2,:) + p%p(3,:)
ma_2 = max (dot (k1, k1), 0.0_double)
mb_2 = max (dot (k2, k2), 0.0_double)
m1_2 = max (dot (p%p(1,:), p%p(1:)), 0.0_double)
m2_2 = max (dot (p%p(2,:), p%p(2:)), 0.0_double)
m3_2 = max (dot (p%p(3,:), p%p(3:)), 0.0_double)
q%ma = sqrt (ma_2)
q%mb = sqrt (mb_2)
q%m1 = sqrt (m1_2)
q%m2 = sqrt (m2_2)
q%m3 = sqrt (m3_2)
q%s = dot (k1k2, k1k2)
q%s2 = dot (p2p3, p2p3)
q%t1 = dot (k1p1, k1p1)
q%phi = atan2 (p%p(1,2), p%p(1,1))
if (q%phi < 0) then
 q%phi = q%phi + 2*PI
end if
p3_23 = boost_momentum (p%p(3,:), p2p3)
q%cos_theta3 = p3_23(3) / sqrt (dot_product (p3_23(1:3), p3_23(1:3)))
q%phi3 = atan2 (p3_23(2), p3_23(1))
if (q%phi3 < 0) then
 q%phi3 = q%phi3 + 2*PI
end if
q%jacobian = 1.0 / ((2*PI)**5 * 32 * q%s2) &
 * sqrt (lambda (q%s2, m2_2, m3_2) / lambda (q%s, ma_2, mb_2))
end function invariants_from_p

```

229a  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 228f 229b $\rangle$

```

pure function invariants_to_p (p) result (q)
type(LIPS3_m5i2a3), intent(in) :: p
type(LIPS3) :: q
q = two_to_three (p%s, p%t1, p%s2, p%phi, p%cos_theta3, p%phi3)
q%jacobian = q%jacobian * p%jacobian
end function invariants_to_p

```

229b  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 229a 230 $\rangle$

```

pure function invariants_from_x (x, s, ma, mb, m1, m2, m3) result (p)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), intent(in) :: s, ma, mb, m1, m2, m3
 type(LIPS3_m5i2a3) :: p
 real(kind=default) :: s2_min, s2_max, t1_min, t1_max
 p%ma = ma
 p%mb = mb
 p%m1 = m1
 p%m2 = m2
 p%m3 = m3
 p%s = s
 s2_min = (p%m2 + p%m3)**2
 s2_max = (sqrt (p%s) - p%m1)**2
 p%s2 = s2_max * x(1) + s2_min * (1 - x(1))
 t1_min = p%ma**2 + p%m1**2 &
 - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
 + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
 * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
 t1_max = p%ma**2 + p%m1**2 &
 - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
 - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
 * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
 p%t1 = t1_max * x(2) + t1_min * (1 - x(2))
 p%phi = 2*PI * x(3)
 p%cos_theta3 = 2 * x(4) - 1
 p%phi3 = 2*PI * x(5)
 p%jacobian = 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_from_x

```

230  $\langle$ Implementation of cross-section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 229b 231b $\rangle$

```

pure function invariants_to_x (p) result (x)
 type(LIPS3_m5i2a3), intent(in) :: p
 type(x5) :: x
 real(kind=default) :: s2_min, s2_max, t1_min, t1_max
 s2_min = (p%m2 + p%m3)**2
 s2_max = (sqrt (p%s) - p%m1)**2
 t1_min = p%ma**2 + p%m1**2 &
 - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
 + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
 * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
 t1_max = p%ma**2 + p%m1**2 &
 - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
 - sqrt (lambda (p%s, p%ma**2, p%mb**2) &

```

```

 * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
x%x(1) = (p%s2 - s2_min) / (s2_max - s2_min)
x%x(2) = (p%t1 - t1_min) / (t1_max - t1_min)
x%x(3) = p%phi / (2*PI)
x%x(4) = (p%cos_theta3 + 1) / 2
x%x(5) = p%phi3 / (2*PI)
x%jacobian = p%jacobian * 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_to_x

```

231a *<Declaration of cross\_section procedures 223d>+≡ (222a) <228e 232b>*  
public :: sigma, sigma\_raw, sigma\_massless

231b *<Implementation of cross\_section procedures 224a>+≡ (222a) <230 231c>*  
function sigma (x, weights, channel, grids) result (xs)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp\_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: xs
 real(kind=default), dimension(2,0:3) :: k
 type(LIPS3) :: p
 k(1,:) = (/ 100.0\_double, 0.0\_double, 0.0\_double, 100.0\_double /)
 k(2,:) = (/ 100.0\_double, 0.0\_double, 0.0\_double, -100.0\_double /)
 if (present (channel)) then
 p = phase\_space (x, channel)
 else
 p = phase\_space (x, 0)
 end if
 if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
 xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
 \* jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
 !!! \* p%jacobian
 else
 xs = 0.0
 end if
end function sigma

231c *<Implementation of cross\_section procedures 224a>+≡ (222a) <231b 232a>*  
function sigma\_raw (k1, k2, p1, p2, q) result (xs)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 real(kind=default) :: xs
 if (cuts (k1, k2, p1, p2, q)) then
 xs = xsect (k1, k2, p1, p2, q)



```

else
 xs = 0.0
end if
end function sigma_raw

```

232a  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 231c 232c $\rangle$

```

function sigma_massless (x, weights, channel, grids) result (xs)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: xs
 real(kind=default), dimension(2,0:3) :: k
 type(LIPS3) :: p
 k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 p = phase_space_massless (x, 0)
 if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
 xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
 * p%jacobian
 else
 xs = 0.0
 end if
end function sigma_massless

```

232b  $\langle$ Declaration of cross\_section procedures 223d $\rangle + \equiv$  (222a)  $\langle$ 231a 234a $\rangle$

```

public :: w

```



232c  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 232a 233 $\rangle$

```

function w (x, weights, channel, grids) result (w_x)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: w_x
 real(kind=default), dimension(size(weights)) :: g_x

```

```

real(kind=default), dimension(2,0:3) :: k
type(LIPS3) :: p
integer :: ch
if (present (channel)) then
 ch = channel
else
 ch = 0
end if
k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
p = phase_space (x, abs (ch))
g_x(1) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
g_x(2) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(2,:), p%p(1,:), p%p(3,:))
g_x(3) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(3,:), p%p(2,:), p%p(1,:))
if (ch > 0) then
 w_x = sigma_raw (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
 / sum (weights * g_x)
else if (ch < 0) then
 w_x = g_x(-ch) / sum (weights * g_x)
else
 w_x = -1
end if
end function w

```

233  $\langle$ Implementation of cross-section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 232c 234c $\rangle$

```

function sigma_rambo (x, weights, channel, grids) result (xs)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: xs
 real(kind=default), dimension(2,0:3) :: k
 real(kind=default), dimension(3,0:3) :: p
 k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 p = massless_isotropic_decay (sum (k(:,0)), reshape (x, (/ 3, 4 /)))
 if (cuts (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:))) then
 xs = xsect (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:)) &
 * phase_space_volume (size (p, dim = 1), sum (k(:,0)))
 else
 xs = 0.0
 end if
end function sigma_rambo

```

234a *<Declaration of cross\_section procedures 223d>+≡ (222a) <232b 234b>*  
public :: sigma\_rambo

234b *<Declaration of cross\_section procedures 223d>+≡ (222a) <234a 235a>*  
public :: check\_kinematics  
private :: print\_LIPS3\_m5i2a3

234c *<Implementation of cross\_section procedures 224a>+≡ (222a) <233 234d>*  
subroutine check\_kinematics (rng)  
type(tao\_random\_state), intent(inout) :: rng  
real(kind=default), dimension(5) :: x  
real(kind=default), dimension(0:3) :: k1, k2  
type(x5) :: x1, x2  
type(LIPS3) :: p1, p2  
type(LIPS3\_m5i2a3) :: q, q1, q2  
k1 = (/ 100.0\_double, 0.0\_double, 0.0\_double, 100.0\_double /)  
k2 = (/ 100.0\_double, 0.0\_double, 0.0\_double, -100.0\_double /)  
call tao\_random\_number (rng, x)  
q = invariants\_from\_x (x, S\_0, MA\_0, MB\_0, M1\_0, M2\_0, M3\_0)  
p1 = invariants\_to\_p (q)  
q1 = invariants\_from\_p (p1, k1, k2)  
p2 = phase\_space (x, 1)  
q2 = invariants\_from\_p (p2, k1, k2)  
x1 = invariants\_to\_x (q1)  
x2 = invariants\_to\_x (q2)  
print \*, p1%jacobian, p2%jacobian, x1%jacobian, x2%jacobian  
call print\_lips3\_m5i2a3 (q)  
call print\_lips3\_m5i2a3 (q1)  
call print\_lips3\_m5i2a3 (q2)  
end subroutine check\_kinematics

234d *<Implementation of cross\_section procedures 224a>+≡ (222a) <234c 235b>*  
subroutine print\_LIPS3\_m5i2a3 (p)  
type(LIPS3\_m5i2a3), intent(in) :: p  
print "(1x,5('m',a1,'=',e9.2,' '))", &  
'a', p%ma, 'b', p%mb, '1', p%m1, '2', p%m2, '3', p%m3  
print "(1x,'s=',e9.2,' s2=',e9.2,' t1=',e9.2)", &  
p%s, p%s2, p%t1  
print "(1x,'phi=',e9.2,' cos(th3)=',e9.2,' phi2=',e9.2)", &  
p%phi, p%cos\_theta3, p%phi3  
print "(1x,'j=',e9.2)", &  
p%jacobian  
end subroutine print\_LIPS3\_m5i2a3

235a *<Declaration of cross\_section procedures 223d>+≡ (222a) <234b 238a>*

```

public :: phi12, phi21, phi1, phi2
public :: g12, g21, g1, g2

```

235b *<Implementation of cross\_section procedures 224a>+≡ (222a) <234d 235c>*

```

pure function phi12 (x1, dummy) result (x2)
 real(kind=default), dimension(:), intent(in) :: x1
 integer, intent(in) :: dummy
 real(kind=default), dimension(size(x1)) :: x2
 type(LIPS3) :: p1, p2
 type(LIPS3_m5i2a3) :: q1, q2
 type(x5) :: x52
 real(kind=default), dimension(0:3) :: k1, k2
 k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
 p1 = invariants_to_p (q1)
 p2%p(1,:) = p1%p(2,:)
 p2%p(2,:) = p1%p(1,:)
 p2%p(3,:) = p1%p(3,:)
 if (dummy < 0) then
 q2 = invariants_from_p (p2, k2, k1)
 else
 q2 = invariants_from_p (p2, k1, k2)
 end if
 x52 = invariants_to_x (q2)
 x2 = x52%x
end function phi12

```

235c *<Implementation of cross\_section procedures 224a>+≡ (222a) <235b 236a>*

```

pure function phi21 (x2, dummy) result (x1)
 real(kind=default), dimension(:), intent(in) :: x2
 integer, intent(in) :: dummy
 real(kind=default), dimension(size(x2)) :: x1
 type(LIPS3) :: p1, p2
 type(LIPS3_m5i2a3) :: q1, q2
 type(x5) :: x51
 real(kind=default), dimension(0:3) :: k1, k2
 k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
 p2 = invariants_to_p (q2)
 p1%p(1,:) = p2%p(2,:)
 p1%p(2,:) = p2%p(1,:)

```

```

p1%p(3,:) = p2%p(3,:)
if (dummy < 0) then
 q1 = invariants_from_p (p1, k2, k1)
else
 q1 = invariants_from_p (p1, k1, k2)
end if
x51 = invariants_to_x (q1)
x1 = x51%x
end function phi21

```

236a  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 235c 236b $\rangle$

```

pure function phi1 (x1) result (p1)
 real(kind=default), dimension(:), intent(in) :: x1
 type(LIPS3) :: p1
 type(LIPS3_m5i2a3) :: q1
 q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
 p1 = invariants_to_p (q1)
end function phi1

```

236b  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 236a 236c $\rangle$

```

pure function phi2 (x2) result (p2)
 real(kind=default), dimension(:), intent(in) :: x2
 type(LIPS3) :: p2
 type(LIPS3_m5i2a3) :: q2
 q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
 p2 = invariants_to_p (q2)
end function phi2

```

236c  $\langle$ Implementation of cross\_section procedures 224a $\rangle + \equiv$  (222a)  $\langle$ 236b 237a $\rangle$

```

pure function g12 (x1) result (g)
 real(kind=default), dimension(:), intent(in) :: x1
 real(kind=default) :: g
 type(LIPS3) :: p1, p2
 type(LIPS3_m5i2a3) :: q1, q2
 type(x5) :: x52
 real(kind=default), dimension(0:3) :: k1, k2
 k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
 p1 = invariants_to_p (q1)
 p2%p(1,:) = p1%p(2,:)
 p2%p(2,:) = p1%p(1,:)

```

```

p2%p(3,:) = p1%p(3,:)
q2 = invariants_from_p (p2, k2, k1)
x52 = invariants_to_x (q2)
g = x52%jacobian / p1%jacobian
end function g12

```

237a *<Implementation of cross\_section procedures 224a>+≡ (222a) <236c 237b>*

```

pure function g21 (x2) result (g)
 real(kind=default), dimension(:), intent(in) :: x2
 real(kind=default) :: g
 type(LIPS3) :: p1, p2
 type(LIPS3_m5i2a3) :: q1, q2
 type(x5) :: x51
 real(kind=default), dimension(0:3) :: k1, k2
 k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
 p2 = invariants_to_p (q2)
 p1%p(1,:) = p2%p(2,:)
 p1%p(2,:) = p2%p(1,:)
 p1%p(3,:) = p2%p(3,:)
 q1 = invariants_from_p (p1, k2, k1)
 x51 = invariants_to_x (q1)
 g = x51%jacobian / p2%jacobian
end function g21

```

237b *<Implementation of cross\_section procedures 224a>+≡ (222a) <237a 237c>*

```

pure function g1 (x1) result (g)
 real(kind=default), dimension(:), intent(in) :: x1
 real(kind=default) :: g
 type(LIPS3) :: p1
 type(LIPS3_m5i2a3) :: q1
 q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
 p1 = invariants_to_p (q1)
 g = 1 / p1%jacobian
end function g1

```

237c *<Implementation of cross\_section procedures 224a>+≡ (222a) <237b 238b>*

```

pure function g2 (x2) result (g)
 real(kind=default), dimension(:), intent(in) :: x2
 real(kind=default) :: g
 type(LIPS3) :: p2

```

```

type(LIPS3_m5i2a3) :: q2
q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
p2 = invariants_to_p (q2)
g = 1 / p2%jacobian
end function g2

```

238a *<Declaration of cross\_section procedures 223d>+≡* (222a) <235a  
public :: wx

238b *<Implementation of cross\_section procedures 224a>+≡* (222a) <237c  
function wx (x, weights, channel, grids) result (w\_x)  
  real(kind=default), dimension(:), intent(in) :: x  
  real(kind=default), dimension(:), intent(in) :: weights  
  integer, intent(in) :: channel  
  type(vamp\_grid), dimension(:), intent(in) :: grids  
  real(kind=default) :: w\_x  
  real(kind=default), dimension(size(weights)) :: g\_x, p\_q  
  real(kind=default), dimension(size(x)) :: x1, x2  
  real(kind=default), dimension(2,0:3) :: k  
  type(LIPS3) :: q  
  k(1,:) = (/ 100.0\_double, 0.0\_double, 0.0\_double, 100.0\_double /)  
  k(2,:) = (/ 100.0\_double, 0.0\_double, 0.0\_double, -100.0\_double /)  
  select case (abs (channel))  
  case (1)  
    x1 = x  
    x2 = phi12 (x, 0)  
    q = phi1 (x1)  
  case (2)  
    x1 = phi21 (x, 0)  
    x2 = x  
    q = phi2 (x2)  
  end select  
  p\_q(1) = vamp\_probability (grids(1), x1)  
  p\_q(2) = vamp\_probability (grids(2), x2)  
  g\_x(1) = p\_q(1) \* g1 (x1)  
  g\_x(2) = p\_q(2) \* g2 (x2)  
  g\_x = g\_x / p\_q(abs(channel))  
  if (channel > 0) then  
    w\_x = sigma\_raw (k(1,:), k(2,:), q%p(1,:), q%p(2,:), q%p(3,:)) &  
      / dot\_product (weights, g\_x)  
  else if (channel < 0) then  
    w\_x = vamp\_probability (grids(-channel), x) / dot\_product (weights, g\_x)  
  else  
    w\_x = 0  
  end if  
end function wx

```

 end if
 end function wx

```

```

239 <application.f90 222a>+≡ <222a
 program application
 use kinds
 use utils
 use vampi
 use mpi90
 use linalg
 use exceptions
 use kinematics, only: phase_space_volume
 use cross_section !NODEP!
 use tao_random_numbers
 implicit none
 type(vamp_grid) :: gr
 type(vamp_grids) :: grs
 real(kind=default), dimension(:,:), allocatable :: region
 real(kind=default) :: integral, standard_dev, chi_squared
 real(kind=default) :: &
 single_integral, single_standard_dev, &
 rambo_integral, rambo_standard_dev
 real(kind=default), dimension(2) :: weight_vector
 integer, dimension(2) :: calls, iterations
 type(vamp_history), dimension(100) :: history
 type(vamp_history), dimension(100,size(weight_vector)) :: histories
 type(exception) :: exc
 type(tao_random_state) :: rng
 real(kind=default), dimension(5) :: x
 real(kind=default) :: jac
 integer :: i
 integer :: num_proc, proc_id, ticks, ticks0, ticks_per_second, command
 character(len=72) :: command_line
 integer, parameter :: &
 CMD_SINGLE = 1, &
 CMD_MULTI = 2, &
 CMD_ROTATING = 3, &
 CMD_RAMBO = 4, &
 CMD_COMPARE = 5, &
 CMD_MASSLESS = 6, &
 CMD_ERROR = 0
 call mpi90_init ()
 call mpi90_size (num_proc)

```



```

call mpi90_rank (proc_id)
call system_clock (ticks0)
call tao_random_create (rng, 0)
call tao_random_seed (rng, ticks0 + proc_id)
!!! call tao_random_seed (rng, proc_id)
call vamp_create_history (history, verbose = .true.)
call vamp_create_history (histories, verbose = .true.)
iterations = (/ 3, 4 /)
calls = (/ 10000, 100000 /)
if (proc_id == 0) then
 read *, command_line
 if (command_line == "single") then
 command = CMD_SINGLE
 else if (command_line == "multi") then
 command = CMD_MULTI
 else if (command_line == "rotating") then
 command = CMD_ROTATING
 else if (command_line == "rambo") then
 command = CMD_RAMBO
 else if (command_line == "compare") then
 command = CMD_COMPARE
 else if (command_line == "massless") then
 command = CMD_MASSLESS
 else
 command = CMD_ERROR
 end if
end if
call mpi90_broadcast (command, 0)
call system_clock (ticks0)
select case (command)
case (CMD_SINGLE)
 Application in single channel mode 242a
case (CMD_MASSLESS)
 Application in massless single channel mode 242b
case (CMD_MULTI)
 Application in multi channel mode 243
case (CMD_ROTATING)
 allocate (region(2,5))
 region(1,:) = 0.0
 region(2,:) = 1.0
 if (proc_id == 0) then
 print *, "rotating N/A yet ..."
 end if

```

```

case (CMD_RAMBO)
 <Application in Rambo mode 244>
case (CMD_COMPARE)
 <Application in single channel mode 242a>
 single_integral = integral
 single_standard_dev = standard_dev
 <Application in Rambo mode 244>
 if (proc_id == 0) then
 rambo_integral = integral
 rambo_standard_dev = standard_dev
 integral = &
 (single_integral / single_standard_dev**2 &
 + rambo_integral / rambo_standard_dev**2) &
 / (1.0_double / single_standard_dev**2 &
 + 1.0_double / rambo_standard_dev**2)
 standard_dev = 1.0_double &
 / sqrt (1.0_double / single_standard_dev**2 &
 + 1.0_double / rambo_standard_dev**2)
 chi_squared = &
 ((single_integral - integral)**2 / single_standard_dev**2) &
 + ((rambo_integral - integral)**2 / rambo_standard_dev**2)
 print *, "S&R: ", integral, standard_dev, chi_squared
 end if
case default
 if (proc_id == 0) then
 print *, "???: ", command
 !!! TO BE REMOVED !!!
 call check_kinematics (rng)
 allocate (region(2,5))
 region(1,:) = 0
 region(2,:) = 1
 do i = 1, 10
 call tao_random_number (rng, x)
 call vamp_jacobian (phi12, 0, x, region, jac)
 print *, "12: ", jac, 1 / g12 (x), jac * g12 (x) - 1
 call vamp_jacobian (phi21, 0, x, region, jac)
 print *, "21: ", jac, 1 / g21 (x), jac * g21 (x) - 1
 print *, "1: ", real(x)
 print *, "2: ", real(phi12(phi21(x,0),0))
 print *, "2': ", real(phi12(phi21(x,-1),-1))
 print *, "3: ", real(phi21(phi12(x,0),0))
 print *, "3': ", real(phi21(phi12(x,-1),-1))
 print *, "2-1: ", real(phi12(phi21(x,0),0) - x)
 end do
 end if
end

```

```

 print *, "3-1: ", real(phi21(phi12(x,0),0) - x)
 print *, "a: ", real(phi12(x,0))
 print *, "a': ", real(phi12(x,-1))
 print *, "b: ", real(phi21(x,0))
 print *, "b': ", real(phi21(x,-1))
 end do
 deallocate (region)
 ! do i = 2, 5
 ! print *, i, phase_space_volume (i, 200.0_double)
 ! end do
end if
end select
if (proc_id == 0) then
 call system_clock (ticks, ticks_per_second)
 print "(1X,A,F8.2,A)", &
 "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
end if
call mpi90_finalize ()
end program application
242a <Application in single channel mode 242a>≡ (239)
 allocate (region(2,5))
 region(1,:) = 0.0
 region(2,:) = 1.0
 call vamp_create_grid (gr, region, calls(1))
 call clear_exception (exc)
 call vamp_sample_grid &
 (rng, gr, sigma, iterations(1), history = history, exc = exc)
 call handle_exception (exc)
 call vamp_discard_integral (gr, calls(2))
 call vamp_sample_grid &
 (rng, gr, sigma, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+1:), exc = exc)
 call handle_exception (exc)
 call vamp_print_history (history, "single")
 if (proc_id == 0) then
 print *, "SINGLE: ", integral, standard_dev, chi_squared
 end if
 call vamp_write_grid (gr, "application.grid")
 call vamp_delete_grid (gr)
 deallocate (region)
242b <Application in massless single channel mode 242b>≡ (239)
 allocate (region(2,5))

```

```

region(1,:) = 0.0
region(2,:) = 1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
 (rng, gr, sigma_massless, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
 (rng, gr, sigma_massless, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "single")
if (proc_id == 0) then
 print *, "M=0: ", integral, standard_dev, chi_squared
end if
call vamp_write_grid (gr, "application.grid")
call vamp_delete_grid (gr)
deallocate (region)

```

243    *Application in multi channel mode 243* ≡ (239)

```

allocate (region(2,5))
region(1,:) = 0.0
region(2,:) = 1.0
weight_vector = 1.0
if (proc_id == 0) then
 read *, weight_vector
end if
call mpi90_broadcast (weight_vector, 0)
weight_vector = weight_vector / sum (weight_vector)
call vamp_create_grids (grs, region, calls(1), weight_vector)
do i = 1, 3
 call clear_exception (exc)
 call vamp_sample_grids &
 (rng, grs, wx, iterations(1), &
 history = history(1+(i-1)*iterations(1):), &
 histories = histories(1+(i-1)*iterations(1):,:), exc = exc)
 call handle_exception (exc)
 call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, calls(2))
call vamp_sample_grids &
 (rng, grs, wx, iterations(2), &

```

```

 integral, standard_dev, chi_squared, &
 history = history(3*iterations(1)+1:), &
 histories = histories(3*iterations(1)+1:,:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
if (proc_id == 0) then
 print *, "MULTI: ", integral, standard_dev, chi_squared
end if
call vamp_write_grids (grs, "application.grids")
call vamp_delete_grids (grs)
deallocate (region)

```

244 *Application in Rambo mode 244*≡

(239)

```

allocate (region(2,12))
region(1,:) = 0.0
region(2,:) = 1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
 (rng, gr, sigma_rambo, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
 (rng, gr, sigma_rambo, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "rambo")
if (proc_id == 0) then
 print *, "RAMBO: ", integral, standard_dev, chi_squared
end if
call vamp_delete_grid (gr)
deallocate (region)

```

# —A—

## CONSTANTS

### *A.1 Kinds*

This borders on overkill, but it is the most portable way to get double precision in standard Fortran without relying on `kind (1.0D0)`. Currently, it is possible to change `double` to any other supported real kind. The MPI interface is a potential trouble source for such things, however.

```
245a <vamp_kinds.f90 245a>≡
 ! vamp_kinds.f90 --
 <Copyleft notice 1>
 module kinds
 implicit none
 integer, parameter, private :: single = &
 & selected_real_kind (precision(1.0), range(1.0))
 integer, parameter, private :: double = &
 & selected_real_kind (precision(1.0_single) + 1, range(1.0_single) + 1)
 integer, parameter, private :: extended = &
 & selected_real_kind (precision (1.0_double) + 1, range (1.0_double))
 integer, parameter, public :: default = double
 end module kinds
```

### *A.2 Mathematical and Physical Constants*

```
245b <constants.f90 245b>≡
 ! constants.f90 --
 <Copyleft notice 1>
 module constants
 use kinds
 implicit none
```

```
private
real(kind=default), public, parameter :: &
 PI = 3.1415926535897932384626433832795028841972_default
end module constants
```

## —B—

# ERRORS AND EXCEPTIONS

Fortran95 does not allow *any* I/O in pure and elemental procedures, not even output to the unit \*. A `stop` statement is verboten as well. Therefore we have to use condition codes

```
247a <exceptions.f90 247a>≡
 ! exceptions.f90 --
 <Copyleft notice 1>
 module exceptions
 use kinds
 implicit none
 private
 <Declaration of exceptions procedures 248b>
 <Interfaces of exceptions procedures (never defined)>
 <Variables in exceptions 247c>
 <Declaration of exceptions types 247b>
 contains
 <Implementation of exceptions procedures 248c>
 end module exceptions

247b <Declaration of exceptions types 247b>≡ (247a)
 type, public :: exception
 integer :: level = EXC_NONE
 character(len=NAME_LENGTH) :: message = ""
 character(len=NAME_LENGTH) :: origin = ""
 end type exception

247c <Variables in exceptions 247c>≡ (247a) 248a▷
 integer, public, parameter :: &
 EXC_NONE = 0, &
 EXC_INFO = 1, &
 EXC_WARN = 2, &
 EXC_ERROR = 3, &
 EXC_FATAL = 4
```



248a *<Variables in exceptions 247c>+≡* (247a) *<247c*  
integer, private, parameter :: EXC\_DEFAULT = EXC\_ERROR  
integer, private, parameter :: NAME\_LENGTH = 64

248b *<Declaration of exceptions procedures 248b>≡* (247a) 248d*>*  
public :: **handle\_exception**

248c *<Implementation of exceptions procedures 248c>≡* (247a) 248e*>*  
**subroutine handle\_exception** (exc)  
type(**exception**), intent(inout) :: exc  
character(len=10) :: name  
if (exc%level > 0) then  
select case (exc%level)  
case (**EXC\_NONE**)  
name = "(none)"  
case (**EXC\_INFO**)  
name = "info"  
case (**EXC\_WARN**)  
name = "warning"  
case (**EXC\_ERROR**)  
name = "error"  
case (**EXC\_FATAL**)  
name = "fatal"  
case default  
name = "invalid"  
end select  
print \*, trim (exc%origin), ": ", trim(name), ": ", trim (exc%message)  
if (exc%level >= **EXC\_FATAL**) then  
print \*, "terminated."  
stop  
end if  
end if  
end **subroutine handle\_exception**

248d *<Declaration of exceptions procedures 248b>+≡* (247a) *<248b*  
public :: **raise\_exception, clear\_exception, gather\_exceptions**  
Raise an exception, but don't overwrite the messages in **exc** if it holds a more severe exception. This way we can accumulate error codes across procedure calls. We have **exc** optional to simplify life for the cslling procedures, which might have it optional themselves.

248e *<Implementation of exceptions procedures 248c>+≡* (247a) *<248c 249a>*  
**elemental subroutine raise\_exception** (exc, level, origin, message)  
type(**exception**), intent(inout), optional :: exc  
integer, intent(in), optional :: level

```

character(len=*), intent(in), optional :: origin, message
integer :: local_level
if (present (exc)) then
 if (present (level)) then
 local_level = level
 else
 local_level = EXC_DEFAULT
 end if
 if (exc%level < local_level) then
 exc%level = local_level
 if (present (origin)) then
 exc%origin = origin
 else
 exc%origin = "[vamp]"
 end if
 if (present (message)) then
 exc%message = message
 else
 exc%message = "[vamp]"
 end if
 end if
end if
end subroutine raise_exception

```

249a *<Implementation of exceptions procedures 248c>+≡* (247a) <248e 249b>

```

elemental subroutine clear_exception (exc)
 type(exception), intent(inout) :: exc
 exc%level = 0
 exc%message = ""
 exc%origin = ""
end subroutine clear_exception

```

249b *<Implementation of exceptions procedures 248c>+≡* (247a) <249a

```

pure subroutine gather_exceptions (exc, excs)
 type(exception), intent(inout) :: exc
 type(exception), dimension(:), intent(in) :: excs
 integer :: i
 i = sum (maxloc (excs%level))
 if (exc%level < excs(i)%level) then
 call raise_exception (exc, excs(i)%level, excs(i)%origin, &
 excs(i)%message)
 end if
end subroutine gather_exceptions

```

Here's how to use `gather_exceptions`. elemental\_procedure

249c  $\langle \textit{Idioms } 101a \rangle + \equiv$

$\triangleleft 101a$

```
call clear_exception (excs)
call elemental_procedure_1 (y, x, excs)
call elemental_procedure_2 (b, a, excs)
if (any (excs%level > 0)) then
 call gather_exceptions (exc, excs)
 return
end if
```

# —C—

## THE ART OF RANDOM NUMBERS

Volume two of Donald E. Knuth’ *The Art of Computer Programming* [16] has always been celebrated as a prime reference for random number generation. Recently, the third edition has been published and it contains a gem of a *portable* random number generator. It generates 30-bit integers with the following desirable properties

- they pass all the tests from George Marsaglia’s “diehard” suite of tests for random number generators [24] (but see [16] for a caveat regarding the “birthday-spacing” test)
- they can be generated with portable signed 32-bit arithmetic (Fortran can’t do unsigned arithmetic)
- it is faster than other lagged Fibonacci generators
- it can create at least  $2^{30} - 2$  independent sequences

We implement the improved versions available as FORTRAN77 code from

<http://www-cs-faculty.stanford.edu/~uno/programs.html#rng>

that contain a streamlined seeding algorithm with better independence of substreams.

### *C.1 Application Program Interface*

A function returning single reals and integers. Note that the static version without the `tao_random_state` argument does not require initialization. It will behave as if call `tao_random_seed(0)` had been executed. On the other hand, the parallelizable version with the explicit `tao_random_state` will fail if none of the `tao_random_create` have been called for the state. (This is a deficiency of Fortran90 that can be fixed in Fortran95).

251 *<API documentation 251>*≡ 252a>

```
call tao_random_number (r)
call tao_random_number (s, r)
```

The state of the random number generator comes in two varieties: buffered and raw. The former is much more efficient, but it can be beneficial to flush the buffers and to pass only the raw state in order to save of interprocess communication (IPC) costs.

252a *<API documentation 251>*+≡ <251 252b>

```
type(tao_random_state) :: s
type(tao_random_raw_state) :: rs
```

Subroutines filling arrays of reals and integers:

252b *<API documentation 251>*+≡ <252a 252c>

```
call tao_random_number (a, num = n)
call tao_random_number (s, a, num = n)
```

Subroutine for changing the seed:

252c *<API documentation 251>*+≡ <252b 252d>

```
call tao_random_seed (seed = seed)
call tao_random_seed (s, seed = seed)
```

Subroutine for changing the luxury. Per default, use all random numbers:

252d *<API documentation 251>*+≡ <252c 252e>

```
call tao_random_luxury ()
call tao_random_luxury (s)
```

With an integer argument, use the first n of each fill of the buffer:

252e *<API documentation 251>*+≡ <252d 252f>

```
call tao_random_luxury (n)
call tao_random_luxury (s, n)
```

With a floating point argument, use that fraction of each fill of the buffer:

252f *<API documentation 251>*+≡ <252e 252g>

```
call tao_random_luxury (x)
call tao_random_luxury (s, x)
```

Create a **tao\_random\_state**

252g *<API documentation 251>*+≡ <252f 252h>

```
call tao_random_create (s, seed, buffer_size = buffer_size)
call tao_random_create (s, raw_state, buffer_size = buffer_size)
call tao_random_create (s, state)
```

Create a **tao\_random\_raw\_state**

252h *<API documentation 251>*+≡ <252g 253a>

```
call tao_random_create (rs, seed)
call tao_random_create (rs, raw_state)
call tao_random_create (rs, state)
```

Destroy a `tao_random_state` or `tao_random_raw_state`

253a  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 252h 253b $\rangle$

```
 call tao_random_destroy (s)
```

Copy `tao_random_state` and `tao_random_raw_state` in all four combinations

253b  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253a 253c $\rangle$

```
 call tao_random_copy (lhs, rhs)
 lhs = rhs
```

253c  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253b 253d $\rangle$

```
 call tao_random_flush (s)
```

253d  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253c 253e $\rangle$

```
 call tao_random_read (s, unit)
 call tao_random_write (s, unit)
```

253e  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253d 253f $\rangle$

```
 call tao_random_test (name = name)
```

Here is a sample application of random number states:

253f  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253e 253g $\rangle$

```
 subroutine threads (args, y, state)
 real, dimension(:), intent(in) :: args
 real, dimension(:), intent(out) :: y
 type(tao_random_state) :: state
 integer :: seed
 type(tao_random_raw_state), dimension(size(y)) :: states
 integer :: s
 call tao_random_number (state, seed)
 call tao_random_create (states, (/ (s, s=seed,size(y)-1) /))
 y = thread (args, states)
 end function thread
```

In this example, we could equivalently pass an integer seed, instead of `raw_state`. But in more complicated cases it can be beneficial to have the option of reusing `raw_state` in the calling routine.

253g  $\langle$ API documentation 251 $\rangle + \equiv$   $\langle$ 253f

```
 elemental function thread (arg, raw_state) result (y)
 real, dimension, intent(in) :: arg
 type(tao_random_raw_state) :: raw_state
 real :: y
 type(tao_random_state) :: state
 real :: r
 call tao_random_create (state, raw_state)
 do
 ...
```

```

 call tao_random_number (state, r)
 ...
 end do
end function thread

```

## C.2 Low Level Routines

Here the low level routines are *much* more interesting than the high level routines. The latter contain a lot of duplication (made necessary by Fortran’s lack of parametric polymorphism) and consist mostly of bookkeeping. We will therefore start with the former.

### C.2.1 Generation of 30-bit Random Numbers

The generator is a subtractive lagged Fibonacci

$$X_j = (X_{j-K} - X_{j-L}) \mod 2^{30} \quad (\text{C.1})$$

with lags  $K = 100$  and  $L = 37$ .

254a  $\langle$ Parameters in tao\_random\_numbers 254a $\rangle \equiv$  (273) 254d $\triangleright$   
integer, parameter, private :: K = 100, L = 37

Other good choices for  $K$  and  $L$  are (cf. [16], table 1 in section 3.2.2, p. 29)

254b  $\langle$ Parameters in tao\_random\_numbers (alternatives) 254b $\rangle \equiv$   
integer, parameter, private :: K = 55, L = 24  
integer, parameter, private :: K = 89, L = 38  
integer, parameter, private :: K = 100, L = 37  
integer, parameter, private :: K = 127, L = 30  
integer, parameter, private :: K = 258, L = 83  
integer, parameter, private :: K = 378, L = 107  
integer, parameter, private :: K = 607, L = 273

A modulus of  $2^{30}$  is the largest we can handle in *portable* (i.e. *signed*) 32-bit arithmetic

254c  $\langle$ Variables in 30-bit tao\_random\_numbers 254c $\rangle \equiv$  (273c) 256a $\triangleright$   
integer(kind=tao\_i32), parameter, private :: M = 2\*\*30

**generate** fills the array  $a_1, \dots, a_n$  with random integers  $0 \leq a_i < 2^{30}$ . We *must* have at least  $n \geq K$ . Higher values don’t change the results, but make **generate** more efficient (about a factor of two, asymptotically). For  $K = 100$ , DEK recommends  $n \geq 1000$ . Best results are obtained using the first 100 random numbers out of 1009. Let’s therefore use 1009 as a default buffer size. The user can call **tao\_random\_luxury** (100) him/herself:

254d  $\langle$ Parameters in `tao_random_numbers` 254a $\rangle + \equiv$  (273)  $\triangleleft$ 254a  
integer, parameter, private :: `DEFAULT_BUFFER_SIZE` = 1009

Since users are not expected to call `generate` directly, we do *not* check for  $n \geq K$  and assume that the caller knows what (s)he's doing ...

255a  $\langle$ Implementation of 30-bit `tao_random_numbers` 255a $\rangle \equiv$  (273c) 256d $\triangleright$   
pure subroutine `generate` (a, state)  
integer(kind=tao\_i32), dimension(:), intent(inout) :: a, state  
integer :: j, n  
n = size (a)  
 $\langle$ Load a and refresh state 255c $\rangle$   
end subroutine `generate`

255b  $\langle$ Declaration of `tao_random_numbers` 255b $\rangle \equiv$  (273) 258g $\triangleright$   
private :: `generate`

`state(1:K)` is already set up properly:

255c  $\langle$ Load a and refresh state 255c $\rangle \equiv$  (255a) 255d $\triangleright$   
a(1:K) = state(1:K)

The remaining  $n - K$  random numbers can be gotten directly from the recursion (C.1). Note that Fortran90's `modulo` intrinsic does the right thing, since it guarantees (unlike Fortran77's `mod`) that  $0 \leq \text{modulo}(a, m) < a$  if  $m > 0$ ).

255d  $\langle$ Load a and refresh state 255c $\rangle + \equiv$  (255a)  $\triangleleft$ 255c 255e $\triangleright$   
do j = K+1, n  
a(j) = modulo (a(j-K) - a(j-L), M)  
end do

Do the recursion (C.1)  $K$  more times to prepare `state(1:K)` for the next invocation of `generate`.

255e  $\langle$ Load a and refresh state 255c $\rangle + \equiv$  (255a)  $\triangleleft$ 255d $\triangleright$   
state(1:L) = modulo (a(n+1-K:n+L-K) - a(n+1-L:n), M)  
do j = L+1, K  
state(j) = modulo (a(n+j-K) - state(j-L), M)  
end do

### C.2.2 Initialization of 30-bit Random Numbers

The non-trivial and most beautiful part is the algorithm to initialize the random number generator state `state` with the first  $K$  numbers. I haven't studied algebra over finite fields in sufficient depth to consider the mathematics behind it straightforward. The commentary below is rather verbose and reflects my understanding of DEK's rather terse remarks (solution to exercise 3.6-9 [16]).

255f  $\langle$ Implementation of `tao_random_numbers` 255f $\rangle \equiv$  (273) 256b $\triangleright$



```

subroutine seed_static (seed)
 integer, optional, intent(in) :: seed
 call seed_stateless (s_state, seed)
 s_virginal = .false.
 s_last = size (s_buffer)
end subroutine seed_static

```

The static version of `tao_random_raw_state`:

256a *⟨Variables in 30-bit tao\_random\_numbers 254c⟩+≡ (273c) <254c 275b>*  

```

integer(kind=tao_i32), dimension(K), save, private :: s_state
logical, save, private :: s_virginal = .true.

```

256b *⟨Implementation of tao\_random\_numbers 255f⟩+≡ (273) <255f 256c>*  

```

elemental subroutine seed_raw_state (s, seed)
 type(tao_random_raw_state), intent(inout) :: s
 integer, optional, intent(in) :: seed
 call seed_stateless (s%x, seed)
end subroutine seed_raw_state

```

256c *⟨Implementation of tao\_random\_numbers 255f⟩+≡ (273) <256b 262b>*  

```

elemental subroutine seed_state (s, seed)
 type(tao_random_state), intent(inout) :: s
 integer, optional, intent(in) :: seed
 call seed_raw_state (s%state, seed)
 s%last = size (s%buffer)
end subroutine seed_state

```

This incarnation of the procedure is pure.

256d *⟨Implementation of 30-bit tao\_random\_numbers 255a⟩+≡ (273c) <255a 267b>*  

```

pure subroutine seed_stateless (state, seed)
 integer(kind=tao_i32), dimension(:), intent(out) :: state
 integer, optional, intent(in) :: seed
 ⟨Parameters local to tao_random_seed 257a⟩
 integer :: seed_value, j, s, t
 integer(kind=tao_i32), dimension(2*K-1) :: x
 ⟨Set up seed_value from seed or DEFAULT_SEED 257c⟩
 ⟨Bootstrap the x buffer 257d⟩
 ⟨Set up s and t 257f⟩
 do
 ⟨p(z) → p(z)2 (modulo zK + zL + 1) 257g⟩
 ⟨p(z) → zp(z) (modulo zK + zL + 1) 258b⟩
 ⟨Shift s or t and exit if t ≤ 0 258c⟩
 end do
 ⟨Fill state from x 258d⟩
 ⟨Warm up state 258e⟩
end subroutine seed_stateless

```

Any default will do

257a  $\langle$ Parameters local to tao\_random\_seed 257a $\rangle \equiv$  (256d 259e) 257b $\triangleright$   
integer, parameter :: DEFAULT\_SEED = 0

These must not be changed:

257b  $\langle$ Parameters local to tao\_random\_seed 257a $\rangle + \equiv$  (256d 259e)  $\triangleleft$ 257a  
integer, parameter :: MAX\_SEED = 2\*\*30 - 3  
integer, parameter :: TT = 70

257c  $\langle$ Set up seed\_value from seed or DEFAULT\_SEED 257c $\rangle \equiv$  (256d 259e)  
if (present (seed)) then  
seed\_value = modulo (seed, MAX\_SEED + 1)  
else  
seed\_value = DEFAULT\_SEED  
end if

Fill the array  $x_1, \dots, x_K$  with even integers, shifted cyclically by 29 bits.

257d  $\langle$ Bootstrap the x buffer 257d $\rangle \equiv$  (256d) 257e $\triangleright$   
s = seed\_value - modulo (seed\_value, 2) + 2  
do j = 1, K  
x(j) = s  
s = 2\*s  
if (s >= M) then  
s = s - M + 2  
end if  
end do  
x(K+1:2\*K-1) = 0

Make  $x_2$  (and only  $x_2$ ) odd:

257e  $\langle$ Bootstrap the x buffer 257d $\rangle + \equiv$  (256d)  $\triangleleft$ 257d  
x(2) = x(2) + 1

257f  $\langle$ Set up s and t 257f $\rangle \equiv$  (256d 259e)  
s = seed\_value  
t = TT - 1

Consider the polynomial

$$p(z) = \sum_{n=1}^K x_n z^{n-1} = x_K z^{K-1} + \dots + x_2 z + x_1 \quad (\text{C.2})$$

We have  $p(z)^2 = p(z^2) \pmod{2}$  because cross terms have an even coefficient and  $x_n^2 = x_n \pmod{2}$ . Therefore we can square the polynomial by shifting the coefficients. The coefficients for  $n > K$  will be reduced.

257g  $\langle p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1} \rangle \equiv$  (256d) 258a $\triangleright$   
x(3:2\*K-1:2) = x(2:K)  
x(2:2\*K-2:2) = 0

Let's return to the coefficients for  $n > K$  generated by the shifting above. Subtract  $z^n(z^K + z^L + 1) = z^n z^K(1 + z^{-(K-L)} + z^{-K})$ . The coefficient of  $z^n z^K$  is left alone, because it doesn't belong to  $p(z)$  anyway.

```

258a <p(z) → p(z)2 (modulo $z^K + z^L + 1$) 257g>+≡ (256d) <257g
 do j = 2*K-1, K+1, -1
 x(j-(K-L)) = modulo (x(j-(K-L))-x(j), M)
 x(j-K)=modulo (x(j-K)-x(j), M)
 end do

258b <p(z) → zp(z) (modulo $z^K + z^L + 1$) 258b>≡ (256d)
 if (modulo (s, 2) == 1) then
 x(2:K+1) = x(1:K)
 x(1) = x(K+1)
 x(L+1) = modulo (x(L+1) - x(K+1), M)
 end if

258c <Shift s or t and exit if t ≤ 0 258c>≡ (256d 259e)
 if (s /= 0) then
 s = s / 2
 else
 t = t - 1
 end if
 if (t <= 0) then
 exit
 end if

258d <Fill state from x 258d>≡ (256d 259e)
 state(1:K-L) = x(L+1:K)
 state(K-L+1:K) = x(1:L)

258e <Warm up state 258e>≡ (256d 259e)
 do j = 1, 10
 call generate (x, state)
 end do

258f <Interfaces of tao_random_numbers 258f>≡ (273) 261e>
 interface tao_random_seed
 module procedure <Specific procedures for tao_random_seed 258h>
 end interface

258g <Declaration of tao_random_numbers 255b>+≡ (273) <255b 260a>
 private :: <Specific procedures for tao_random_seed 258h>

258h <Specific procedures for tao_random_seed 258h>≡ (258)
 seed_static, seed_state, seed_raw_state

```

### C.2.3 Generation of 52-bit Random Numbers

$$X_j = (X_{j-K} + X_{j-L}) \mod 1 \quad (\text{C.3})$$

259a *<Variables in 52-bit tao\_random\_numbers 259a>*≡ (273d) 259b>  
`real(kind=tao_r64), parameter, private :: M = 1.0_tao_r64`

The state of the internal routines

259b *<Variables in 52-bit tao\_random\_numbers 259a>*+≡ (273d) <259a 276a>  
`real(kind=tao_r64), dimension(K), save, private :: s_state`  
`logical, save, private :: s_virginal = .true.`

259c *<Implementation of 52-bit tao\_random\_numbers 259c>*≡ (273d) 259e>  
`pure subroutine generate (a, state)`  
`real(kind=tao_r64), dimension(:), intent(inout) :: a`  
`real(kind=tao_r64), dimension(:), intent(inout) :: state`  
`integer :: j, n`  
`n = size (a)`  
*<Load 52-bit a and refresh state 259d>*  
`end subroutine generate`

That's almost identical to the 30-bit version, except that the relative sign is flipped:

259d *<Load 52-bit a and refresh state 259d>*≡ (259c)  
`a(1:K) = state(1:K)`  
`do j = K+1, n`  
`a(j) = modulo (a(j-K) + a(j-L), M)`  
`end do`  
`state(1:L) = modulo (a(n+1-K:n+L-K) + a(n+1-L:n), M)`  
`do j = L+1, K`  
`state(j) = modulo (a(n+j-K) + state(j-L), M)`  
`end do`

### C.2.4 Initialization of 52-bit Random Numbers

This incarnation of the procedure is pure.

259e *<Implementation of 52-bit tao\_random\_numbers 259c>*+≡ (273d) <259c 267f>  
`pure subroutine seed_stateless (state, seed)`  
`real(kind=tao_r64), dimension(:), intent(out) :: state`  
`integer, optional, intent(in) :: seed`  
*<Parameters local to tao\_random\_seed 257a>*  
*<Variables local to 52-bit tao\_random\_seed 260b>*  
*<Set up seed\_value from seed or DEFAULT\_SEED 257c>*  
*<Bootstrap the 52-bit x buffer 260d>*  
*<Set up s and t 257f>*

```

do
 <52-bit $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$ 260f>
 <52-bit $p(z) \rightarrow zp(z) \pmod{z^K + z^L + 1}$ 260h>
 <Shift s or t and exit if $t \leq 0$ 258c>
end do
<Fill state from x 258d>
<Warm up state 258e>
end subroutine seed_stateless

260a <Declaration of tao_random_numbers 255b>+≡ (273) <258g 261f>
private :: seed_stateless

260b <Variables local to 52-bit tao_random_seed 260b>≡ (259e) 260c>
real(kind=tao_r64), parameter :: ULP = 2.0_tao_r64**(-52)

260c <Variables local to 52-bit tao_random_seed 260b>+≡ (259e) <260b>
real(kind=tao_r64), dimension(2*K-1) :: x
real(kind=tao_r64) :: ss
integer :: seed_value, t, s, j

260d <Bootstrap the 52-bit x buffer 260d>≡ (259e) 260e>
ss = 2*ULP * (seed_value + 2)
do j = 1, K
 x(j) = ss
 ss = 2*ss
 if (ss >= 1) then
 ss = ss - 1 + 2*ULP
 end if
end do
x(K+1:2*K-1) = 0.0

260e <Bootstrap the 52-bit x buffer 260d>+≡ (259e) <260d>
x(2) = x(2) + ULP

260f <52-bit $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$ 260f>≡ (259e) 260g>
x(3:2*K-1:2) = x(2:K)
x(2:2*K-2:2) = 0

This works because 2*K-1 is odd

260g <52-bit $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$ 260f>+≡ (259e) <260f>
do j = 2*K-1, K+1, -1
 x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
 x(j-K) = modulo (x(j-K) + x(j), M)
end do

260h <52-bit $p(z) \rightarrow zp(z) \pmod{z^K + z^L + 1}$ 260h>≡ (259e)
if (modulo (s, 2) == 1) THEN
 x(2:K+1) = x(1:K)

```

```

x(1) = x(K+1)
x(L+1) = modulo (x(L+1) + x(K+1), M)
end if

```

### C.3 The State

- 261a  $\langle$ Declaration of 30-bit tao\_random\_numbers types 261a $\rangle \equiv$  (273c) 261b $\triangleright$
- ```

type, public :: tao_random_raw_state
private
integer(kind=tao_i32), dimension(K) :: x
end type tao_random_raw_state

```
- 261b \langle Declaration of 30-bit tao_random_numbers types 261a $\rangle + \equiv$ (273c) \triangleleft 261a
- ```

type, public :: tao_random_state
private
type(tao_random_raw_state) :: state
integer(kind=tao_i32), dimension(:), pointer :: buffer => null ()
integer :: buffer_end, last
end type tao_random_state

```
- 261c  $\langle$ Declaration of 52-bit tao\_random\_numbers types 261c $\rangle \equiv$  (273d) 261d $\triangleright$
- ```

type, public :: tao_random_raw_state
private
real(kind=tao_r64), dimension(K) :: x
end type tao_random_raw_state

```
- 261d \langle Declaration of 52-bit tao_random_numbers types 261c $\rangle + \equiv$ (273d) \triangleleft 261c
- ```

type, public :: tao_random_state
private
type(tao_random_raw_state) :: state
real(kind=tao_r64), dimension(:), pointer :: buffer => null ()
integer :: buffer_end, last
end type tao_random_state

```

#### C.3.1 Creation

- 261e  $\langle$ Interfaces of tao\_random\_numbers 258f $\rangle + \equiv$  (273)  $\triangleleft$ 258f 263d $\triangleright$
- ```

interface tao_random_create
module procedure  $\langle$ Specific procedures for tao_random_create 262a $\rangle$ 
end interface

```
- 261f \langle Declaration of tao_random_numbers 255b $\rangle + \equiv$ (273) \triangleleft 260a 263e \triangleright
- ```

private :: \langle Specific procedures for tao_random_create 262a \rangle

```

262a *<Specific procedures for tao\_random\_create 262a>*≡ (261)

```

create_state_from_seed, create_raw_state_from_seed, &
create_state_from_state, create_raw_state_from_state, &
create_state_from_raw_state, create_raw_state_from_raw_st

```

There are no procedures for copying the state of the static generator to or from an explicit `tao_random_state`. Users needing this functionality can be expected to handle explicit states anyway. Since the direction of the copying can not be obvious from the type of the argument, such functions would spoil the simplicity of the generic procedure interface.

262b *<Implementation of tao\_random\_numbers 255f>*+≡ (273) <256c 262c>

```

elemental subroutine create_state_from_seed (s, seed, buffer_size)
 type(tao_random_state), intent(out) :: s
 integer, intent(in) :: seed
 integer, intent(in), optional :: buffer_size
 call create_raw_state_from_seed (s%state, seed)
 if (present (buffer_size)) then
 s%buffer_end = max (buffer_size, K)
 else
 s%buffer_end = DEFAULT_BUFFER_SIZE
 end if
 allocate (s%buffer(s%buffer_end))
 call tao_random_flush (s)
end subroutine create_state_from_seed

```

262c *<Implementation of tao\_random\_numbers 255f>*+≡ (273) <262b 262d>

```

elemental subroutine create_state_from_state (s, state)
 type(tao_random_state), intent(out) :: s
 type(tao_random_state), intent(in) :: state
 call create_raw_state_from_raw_st (s%state, state%state)
 allocate (s%buffer(size(state%buffer)))
 call tao_random_copy (s, state)
end subroutine create_state_from_state

```

262d *<Implementation of tao\_random\_numbers 255f>*+≡ (273) <262c 263a>

```

elemental subroutine create_state_from_raw_state &
 (s, raw_state, buffer_size)
 type(tao_random_state), intent(out) :: s
 type(tao_random_raw_state), intent(in) :: raw_state
 integer, intent(in), optional :: buffer_size
 call create_raw_state_from_raw_st (s%state, raw_state)
 if (present (buffer_size)) then
 s%buffer_end = max (buffer_size, K)
 else
 s%buffer_end = DEFAULT_BUFFER_SIZE

```

```

 end if
 allocate (s%buffer(s%buffer_end))
 call tao_random_flush (s)
 end subroutine create_state_from_raw_state
263a <Implementation of tao_random_numbers 255f>+≡ (273) <262d 263b>
 elemental subroutine create_raw_state_from_seed (s, seed)
 type(tao_random_raw_state), intent(out) :: s
 integer, intent(in) :: seed
 call seed_raw_state (s, seed)
 end subroutine create_raw_state_from_seed
263b <Implementation of tao_random_numbers 255f>+≡ (273) <263a 263c>
 elemental subroutine create_raw_state_from_state (s, state)
 type(tao_random_raw_state), intent(out) :: s
 type(tao_random_state), intent(in) :: state
 call copy_state_to_raw_state (s, state)
 end subroutine create_raw_state_from_state
263c <Implementation of tao_random_numbers 255f>+≡ (273) <263b 263f>
 elemental subroutine create_raw_state_from_raw_st (s, raw_state)
 type(tao_random_raw_state), intent(out) :: s
 type(tao_random_raw_state), intent(in) :: raw_state
 call copy_raw_state (s, raw_state)
 end subroutine create_raw_state_from_raw_st

```

### C.3.2 Destruction

```

263d <Interfaces of tao_random_numbers 258f>+≡ (273) <261e 264a>
 interface tao_random_destroy
 module procedure destroy_state, destroy_raw_state
 end interface
263e <Declaration of tao_random_numbers 255b>+≡ (273) <261f 264c>
 private :: destroy_state, destroy_raw_state
263f <Implementation of tao_random_numbers 255f>+≡ (273) <263c 263g>
 elemental subroutine destroy_state (s)
 type(tao_random_state), intent(inout) :: s
 deallocate (s%buffer)
 end subroutine destroy_state

```

Currently, this is a no-op, but we might need a non-trivial destruction method in the future

```

263g <Implementation of tao_random_numbers 255f>+≡ (273) <263f 264e>
 elemental subroutine destroy_raw_state (s)

```



```

 type(tao_random_raw_state), intent(inout) :: s
end subroutine destroy_raw_state

```

### C.3.3 Copying

- 264a *⟨Interfaces of tao\_random\_numbers 258f⟩+≡* (273) *◁263d 264b▷*  

```

 interface tao_random_copy
 module procedure ⟨Specific procedures for tao_random_copy 264d⟩
 end interface

```
- 264b *⟨Interfaces of tao\_random\_numbers 258f⟩+≡* (273) *◁264a 265d▷*  

```

 interface assignment(=)
 module procedure ⟨Specific procedures for tao_random_copy 264d⟩
 end interface

```
- 264c *⟨Declaration of tao\_random\_numbers 255b⟩+≡* (273) *◁263e 265e▷*  

```

 public :: assignment(=)
 private :: ⟨Specific procedures for tao_random_copy 264d⟩

```
- 264d *⟨Specific procedures for tao\_random\_copy 264d⟩≡* (264)  

```

 copy_state, copy_raw_state, &
 copy_raw_state_to_state, copy_state_to_raw_state

```
- 264e *⟨Implementation of tao\_random\_numbers 255f⟩+≡* (273) *◁263g 264f▷*  

```

 elemental subroutine copy_state (lhs, rhs)
 type(tao_random_state), intent(inout) :: lhs
 type(tao_random_state), intent(in) :: rhs
 call copy_raw_state (lhs%state, rhs%state)
 if (size (lhs%buffer) /= size (rhs%buffer)) then
 deallocate (lhs%buffer)
 allocate (lhs%buffer(size(rhs%buffer)))
 end if
 lhs%buffer = rhs%buffer
 lhs%buffer_end = rhs%buffer_end
 lhs%last = rhs%last
 end subroutine copy_state

```
- 264f *⟨Implementation of tao\_random\_numbers 255f⟩+≡* (273) *◁264e 265a▷*  

```

 elemental subroutine copy_raw_state (lhs, rhs)
 type(tao_random_raw_state), intent(out) :: lhs
 type(tao_random_raw_state), intent(in) :: rhs
 lhs%x = rhs%x
 end subroutine copy_raw_state

```

265a *<Implementation of tao\_random\_numbers 255f>+≡* (273) *<264f 265b>*  
 elemental subroutine copy\_raw\_state\_to\_state (lhs, rhs)  
   type(tao\_random\_state), intent(inout) :: lhs  
   type(tao\_random\_raw\_state), intent(in) :: rhs  
   call copy\_raw\_state (lhs%state, rhs)  
   call tao\_random\_flush (lhs)  
 end subroutine copy\_raw\_state\_to\_state

265b *<Implementation of tao\_random\_numbers 255f>+≡* (273) *<265a 265c>*  
 elemental subroutine copy\_state\_to\_raw\_state (lhs, rhs)  
   type(tao\_random\_raw\_state), intent(out) :: lhs  
   type(tao\_random\_state), intent(in) :: rhs  
   call copy\_raw\_state (lhs, rhs%state)  
 end subroutine copy\_state\_to\_raw\_state

### C.3.4 Flushing

265c *<Implementation of tao\_random\_numbers 255f>+≡* (273) *<265b 266b>*  
 elemental subroutine tao\_random\_flush (s)  
   type(tao\_random\_state), intent(inout) :: s  
   s%last = size (s%buffer)  
 end subroutine tao\_random\_flush

### C.3.5 Input and Output

265d *<Interfaces of tao\_random\_numbers 258f>+≡* (273) *<264b 265f>*  
 interface tao\_random\_write  
   module procedure &  
     write\_state\_unit, write\_state\_name, &  
     write\_raw\_state\_unit, write\_raw\_state\_name  
 end interface

265e *<Declaration of tao\_random\_numbers 255b>+≡* (273) *<264c 266a>*  
 private :: write\_state\_unit, write\_state\_name  
 private :: write\_raw\_state\_unit, write\_raw\_state\_name

265f *<Interfaces of tao\_random\_numbers 258f>+≡* (273) *<265d 270a>*  
 interface tao\_random\_read  
   module procedure &  
     read\_state\_unit, read\_state\_name, &  
     read\_raw\_state\_unit, read\_raw\_state\_name  
 end interface

266a *<Declaration of tao\_random\_numbers 255b>+≡* (273) <265e 269b>  
 private :: read\_state\_unit, read\_state\_name  
 private :: read\_raw\_state\_unit, read\_raw\_state\_name

266b *<Implementation of tao\_random\_numbers 255f>+≡* (273) <265c 266c>  
 subroutine write\_state\_unit (s, unit)  
   type(tao\_random\_state), intent(in) :: s  
   integer, intent(in) :: unit  
   write (unit = unit, fmt = \*) "BEGIN TAO\_RANDOM\_STATE"  
   call write\_raw\_state\_unit (s%state, unit)  
   write (unit = unit, fmt = "(2(1x,a16,1x,i10/),1x,a16,1x,i10)") &  
     "BUFFER\_SIZE", size (s%buffer), &  
     "BUFFER\_END", s%buffer\_end, &  
     "LAST", s%last  
   write (unit = unit, fmt = \*) "BEGIN BUFFER"  
   call write\_state\_array (s%buffer, unit)  
   write (unit = unit, fmt = \*) "END BUFFER"  
   write (unit = unit, fmt = \*) "END TAO\_RANDOM\_STATE"  
 end subroutine write\_state\_unit

266c *<Implementation of tao\_random\_numbers 255f>+≡* (273) <266b 266d>  
 subroutine read\_state\_unit (s, unit)  
   type(tao\_random\_state), intent(inout) :: s  
   integer, intent(in) :: unit  
   integer :: buffer\_size  
   read (unit = unit, fmt = \*)  
   call read\_raw\_state\_unit (s%state, unit)  
   read (unit = unit, fmt = "(2(1x,16x,1x,i10/),1x,16x,1x,i10)") &  
     buffer\_size, s%buffer\_end, s%last  
   read (unit = unit, fmt = \*)  
   if (buffer\_size /= size (s%buffer)) then  
     deallocate (s%buffer)  
     allocate (s%buffer(buffer\_size))  
   end if  
   call read\_state\_array (s%buffer, unit)  
   read (unit = unit, fmt = \*)  
   read (unit = unit, fmt = \*)  
 end subroutine read\_state\_unit

266d *<Implementation of tao\_random\_numbers 255f>+≡* (273) <266c 267a>  
 subroutine write\_raw\_state\_unit (s, unit)  
   type(tao\_random\_raw\_state), intent(in) :: s  
   integer, intent(in) :: unit  
   write (unit = unit, fmt = \*) "BEGIN TAO\_RANDOM\_RAW\_STATE"  
   call write\_state\_array (s%x, unit)

```

 write (unit = unit, fmt = *) "END TAO_RANDOM_RAW_STATE"
 end subroutine write_raw_state_unit
267a <Implementation of tao_random_numbers 255f>+≡ (273) <266d 268d>
 subroutine read_raw_state_unit (s, unit)
 type(tao_random_raw_state), intent(inout) :: s
 integer, intent(in) :: unit
 read (unit = unit, fmt = *)
 call read_state_array (s%x, unit)
 read (unit = unit, fmt = *)
 end subroutine read_raw_state_unit
267b <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <256d 267d>
 subroutine write_state_array (a, unit)
 integer(kind=tao_i32), dimension(:), intent(in) :: a
 integer, intent(in) :: unit
 integer :: i
 do i = 1, size (a)
 write (unit = unit, fmt = "(1x,i10,1x,i10)") i, a(i)
 end do
 end subroutine write_state_array
267c <Declaration of 30-bit tao_random_numbers 267c>≡ (273c) 267e>
 private :: write_state_array
267d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <267b 270c>
 subroutine read_state_array (a, unit)
 integer(kind=tao_i32), dimension(:), intent(inout) :: a
 integer, intent(in) :: unit
 integer :: i, idum
 do i = 1, size (a)
 read (unit = unit, fmt = *) idum, a(i)
 end do
 end subroutine read_state_array
267e <Declaration of 30-bit tao_random_numbers 267c>+≡ (273c) <267c 280f>
 private :: read_state_array

```

Reading and writing 52-bit floating point numbers accurately is beyond most Fortran runtime libraries. Their job is simplified considerably if we rescale by  $2^{52}$  before writing. Then the temptation to truncate will not be as overwhelming as before ...

```

267f <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <259e 268b>
 subroutine write_state_array (a, unit)
 real(kind=tao_r64), dimension(:), intent(in) :: a
 integer, intent(in) :: unit
 integer :: i

```

```

do i = 1, size (a)
 write (unit = unit, fmt = "(1x,i10,1x,f30.0)") i, 2.0_tao_r64**52 * a(i)
end do
end subroutine write_state_array

268a <Declaration of 52-bit tao_random_numbers 268a>≡ (273d) 268c>
private :: write_state_array

268b <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <267f 272a>
subroutine read_state_array (a, unit)
 real(kind=tao_r64), dimension(:), intent(inout) :: a
 integer, intent(in) :: unit
 real(kind=tao_r64) :: x
 integer :: i, idum
do i = 1, size (a)
 read (unit = unit, fmt = *) idum, x
 a(i) = 2.0_tao_r64**(-52) * x
end do
end subroutine read_state_array

268c <Declaration of 52-bit tao_random_numbers 268a>+≡ (273d) <268a 281d>
private :: read_state_array

268d <Implementation of tao_random_numbers 255f>+≡ (273) <267a 269c>
subroutine find_free_unit (u, iostat)
 integer, intent(out) :: u
 integer, intent(out), optional :: iostat
 logical :: exists, is_open
 integer :: i, status
do i = MIN_UNIT, MAX_UNIT
 inquire (unit = i, exist = exists, opened = is_open, &
 iostat = status)
 if (status == 0) then
 if (exists .and. .not. is_open) then
 u = i
 if (present (iostat)) then
 iostat = 0
 end if
 return
 end if
 end if
end do
if (present (iostat)) then
 iostat = -1
end if
u = -1

```

```

end subroutine find_free_unit

269a <Variables in tao_random_numbers 269a>≡ (273)
 integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99

269b <Declaration of tao_random_numbers 255b>+≡ (273) <266a 270b>
 private :: find_free_unit

269c <Implementation of tao_random_numbers 255f>+≡ (273) <268d 269d>
 subroutine write_state_name (s, name)
 type(tao_random_state), intent(in) :: s
 character(len=*), intent(in) :: name
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", file = name)
 call write_state_unit (s, unit)
 close (unit = unit)
 end subroutine write_state_name

269d <Implementation of tao_random_numbers 255f>+≡ (273) <269c 269e>
 subroutine write_raw_state_name (s, name)
 type(tao_random_raw_state), intent(in) :: s
 character(len=*), intent(in) :: name
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "write", status = "replace", file = name)
 call write_raw_state_unit (s, unit)
 close (unit = unit)
 end subroutine write_raw_state_name

269e <Implementation of tao_random_numbers 255f>+≡ (273) <269d 269f>
 subroutine read_state_name (s, name)
 type(tao_random_state), intent(inout) :: s
 character(len=*), intent(in) :: name
 integer :: unit
 call find_free_unit (unit)
 open (unit = unit, action = "read", status = "old", file = name)
 call read_state_unit (s, unit)
 close (unit = unit)
 end subroutine read_state_name

269f <Implementation of tao_random_numbers 255f>+≡ (273) <269e 281f>
 subroutine read_raw_state_name (s, name)
 type(tao_random_raw_state), intent(inout) :: s
 character(len=*), intent(in) :: name
 integer :: unit

```

```

call find_free_unit (unit)
open (unit = unit, action = "read", status = "old", file = name)
call read_raw_state_unit (s, unit)
close (unit = unit)
end subroutine read_raw_state_name

```

### C.3.6 Marshaling and Unmarshaling

Note that we can not use the `transfer` intrinsic function for marshalling types that contain pointers that substitute for allocatable array components. `transfer` will copy the pointers in this case and not where they point to!

- 270a  $\langle$ Interfaces of `tao_random_numbers` 258f $\rangle + \equiv$  (273)  $\langle$ 265f
- ```

interface tao_random_marshall_size
  module procedure marshal_state_size, marshal_raw_state_size
end interface
interface tao_random_marshall
  module procedure marshal_state, marshal_raw_state
end interface
interface tao_random_unmarshal
  module procedure unmarshal_state, unmarshal_raw_state
end interface

```
- 270b \langle Declaration of `tao_random_numbers` 255b $\rangle + \equiv$ (273) \langle 269b 274a \rangle
- ```

public :: tao_random_marshall
private :: marshal_state, marshal_raw_state
public :: tao_random_marshall_size
private :: marshal_state_size, marshal_raw_state_size
public :: tao_random_unmarshal
private :: unmarshal_state, unmarshal_raw_state

```
- 270c  $\langle$ Implementation of 30-bit `tao_random_numbers` 255a $\rangle + \equiv$  (273c)  $\langle$ 267d 271a $\rangle$
- ```

pure subroutine marshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  integer :: buf_size
  buf_size = size (s%buffer)
  ibuf(1) = s%buffer_end
  ibuf(2) = s%last
  ibuf(3) = buf_size
  ibuf(4:3+buf_size) = s%buffer
  call marshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
end subroutine marshal_state

```

271a *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <270c 271b>*

```

pure subroutine marshal_state_size (s, iwords, dwords)
  type(tao_random_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  call marshal_raw_state_size (s%state, iwords, dwords)
  iwords = iwords + 3 + size (s%buffer)
end subroutine marshal_state_size

```

271b *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271a 271c>*

```

pure subroutine unmarshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  s%buffer_end = ibuf(1)
  s%last = ibuf(2)
  buf_size = ibuf(3)
  s%buffer = ibuf(4:3+buf_size)
  call unmarshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
end subroutine unmarshal_state

```

271c *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271b 271d>*

```

pure subroutine marshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  ibuf(1) = size (s%x)
  ibuf(2:1+size(s%x)) = s%x
end subroutine marshal_raw_state

```

271d *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271c 271e>*

```

pure subroutine marshal_raw_state_size (s, iwords, dwords)
  type(tao_random_raw_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  iwords = 1 + size (s%x)
  dwords = 0
end subroutine marshal_raw_state_size

```

271e *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271d 274b>*

```

pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  buf_size = ibuf(1)
  s%x = ibuf(2:1+buf_size)

```



```

end subroutine unmarshal_raw_state

272a <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <268b 272b>
pure subroutine marshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  integer :: buf_size
  buf_size = size (s%buffer)
  ibuf(1) = s%buffer_end
  ibuf(2) = s%last
  ibuf(3) = buf_size
  dbuf(1:buf_size) = s%buffer
  call marshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine marshal_state

272b <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <272a 272c>
pure subroutine marshal_state_size (s, iwords, dwords)
  type(tao_random_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  call marshal_raw_state_size (s%state, iwords, dwords)
  iwords = iwords + 3
  dwords = dwords + size(s%buffer)
end subroutine marshal_state_size

272c <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <272b 272d>
pure subroutine unmarshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  s%buffer_end = ibuf(1)
  s%last = ibuf(2)
  buf_size = ibuf(3)
  s%buffer = dbuf(1:buf_size)
  call unmarshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine unmarshal_state

272d <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <272c 273a>
pure subroutine marshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  ibuf(1) = size (s%x)
  dbuf(1:size(s%x)) = s%x
end subroutine marshal_raw_state

```

273a *<Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <272d 273b>*

```

pure subroutine marshal_raw_state_size (s, iwords, dwords)
  type(tao_random_raw_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  iwords = 1
  dwords = size (s%x)
end subroutine marshal_raw_state_size

```

273b *<Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <273a 275e>*

```

pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  buf_size = ibuf(1)
  s%x = dbuf(1:buf_size)
end subroutine unmarshal_raw_state

```

C.4 High Level Routines

273c *<tao_random_numbers.f90 273c>≡*

```

! tao_random_numbers.f90 --
<Copyleft notice 1>
module tao_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
  <Declaration of tao_random_numbers 255b>
  <Declaration of 30-bit tao_random_numbers 267c>
  <Interfaces of tao_random_numbers 258f>
  <Interfaces of 30-bit tao_random_numbers 280d>
  <Parameters in tao_random_numbers 254a>
  <Variables in tao_random_numbers 269a>
  <Variables in 30-bit tao_random_numbers 254c>
  <Declaration of 30-bit tao_random_numbers types 261a>
contains
  <Implementation of tao_random_numbers 255f>
  <Implementation of 30-bit tao_random_numbers 255a>
end module tao_random_numbers

```

273d *<tao52_random_numbers.f90 273d>≡*

```

! tao52_random_numbers.f90 --

```

⟨Copyleft notice 1⟩

```
module tao52_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
  ⟨Declaration of tao_random_numbers 255b⟩
  ⟨Declaration of 52-bit tao_random_numbers 268a⟩
  ⟨Interfaces of tao_random_numbers 258f⟩
  ⟨Interfaces of 52-bit tao_random_numbers 281b⟩
  ⟨Parameters in tao_random_numbers 254a⟩
  ⟨Variables in tao_random_numbers 269a⟩
  ⟨Variables in 52-bit tao_random_numbers 259a⟩
  ⟨Declaration of 52-bit tao_random_numbers types 261c⟩
contains
  ⟨Implementation of tao_random_numbers 255f⟩
  ⟨Implementation of 52-bit tao_random_numbers 259c⟩
end module tao52_random_numbers
```

Ten functions are exported

```
274a ⟨Declaration of tao_random_numbers 255b⟩+≡ (273) ◁270b
  public :: tao_random_number
  public :: tao_random_seed
  public :: tao_random_create
  public :: tao_random_destroy
  public :: tao_random_copy
  public :: tao_random_read
  public :: tao_random_write
  public :: tao_random_flush
  ! public :: tao_random_luxury
  public :: tao_random_test
```

C.4.1 Single Random Numbers

A random integer r with $0 \leq r < 2^{30} = 1073741824$:

```
274b ⟨Implementation of 30-bit tao_random_numbers 255a⟩+≡ (273c) ◁271e 275d▷
  pure subroutine integer_stateless &
    (state, buffer, buffer_end, last, r)
    integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    integer, intent(out) :: r
    integer, parameter :: NORM = 1
```

```

    <Body of tao_random.* 275a>
end subroutine integer_stateless
275a <Body of tao_random.* 275a>≡ (274 275)
    <Step last and reload buffer iff necessary 275c>
    r = NORM * buffer(last)

```

The low level routine `generate` will fill an array a_1, \dots, a_n , which will be consumed and refilled like an input buffer. We need at least $n \geq K$ for the call to `generate`.

```

275b <Variables in 30-bit tao_random_numbers 254c>+≡ (273c) <256a
    integer(kind=tao_i32), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
    integer, save, private :: s_buffer_end = size(s_buffer)
    integer, save, private :: s_last = size(s_buffer)

```

Increment the index `last` and reload the array `buffer`, iff this buffer is exhausted. Throughout these routines, `last` will point to random number that has just been consumed. For the array filling routines below, this is simpler than pointing to the next waiting number.

```

275c <Step last and reload buffer iff necessary 275c>≡ (275a)
    last = last + 1
    if (last > buffer_end) then
        call generate(buffer, state)
        last = 1
    end if

```

A random real $r \in [0, 1)$. This is almost identical to `tao_random_integer`, but we duplicate the code to avoid the function call overhead for speed.

```

275d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <274b 276b>
    pure subroutine real_stateless(state, buffer, buffer_end, last, r)
        integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
        integer, intent(in) :: buffer_end
        integer, intent(inout) :: last
        real(kind=default), intent(out) :: r
        real(kind=default), parameter :: NORM = 1.0_default / M
        <Body of tao_random.* 275a>
    end subroutine real_stateless

```

A random real $r \in [0, 1)$.

```

275e <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <273b 277e>
    pure subroutine real_stateless(state, buffer, buffer_end, last, r)
        real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer
        integer, intent(in) :: buffer_end
        integer, intent(inout) :: last
        real(kind=default), intent(out) :: r
        integer, parameter :: NORM = 1

```

⟨Body of tao_random. 275a⟩*

end subroutine real_stateless

The low level routine **generate** will fill an array a_1, \dots, a_N , which will be consumed and refilled like an input buffer.

276a *⟨Variables in 52-bit tao_random_numbers 259a⟩*+≡ (273d) <259b
 real(kind=tao_r64), dimension(DEFAULT_BUFFER_SIZE), save, private :: **s_buffer**
 integer, save, private :: **s_buffer_end** = size (**s_buffer**)
 integer, save, private :: **s_last** = size (**s_buffer**)

C.4.2 Arrays of Random Numbers

Fill the array j_1, \dots, j_ν with random integers $0 \leq j_i < 2^{30} = 1073741824$. This has to be done such that the underlying array length in **generate** is transparent to the user. At the same time we want to avoid the overhead of calling `tao_random_real` ν times.

276b *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) <275d 277d>
 pure subroutine integer_array_stateless &
 (state, buffer, **buffer_end**, **last**, v, num)
 integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
 integer, intent(in) :: **buffer_end**
 integer, intent(inout) :: **last**
 integer, dimension(:), intent(out) :: v
 integer, optional, intent(in) :: num
 integer, parameter :: NORM = 1
 *⟨Body of tao_random.*_array 276c⟩*
 end subroutine integer_array_stateless

276c *⟨Body of tao_random.*_array 276c⟩*≡ (276 277)

integer :: nu, done, todo, chunk
⟨Set nu to num or size(v) 276d⟩
⟨Prepare array buffer and done, todo, chunk 277a⟩
 v(1:chunk) = NORM * buffer(**last**+1:**last**+chunk)
 do
 ⟨Update last, done and todo and set new chunk 277b⟩
 ⟨Reload buffer or exit 277c⟩
 v(done+1:done+chunk) = NORM * buffer(1:chunk)
 end do

276d *⟨Set nu to num or size(v) 276d⟩*≡ (276c)

if (present (num)) then
 nu = num
else
 nu = size (v)
end if

`last` is used as an offset into the buffer `buffer`, as usual. `done` is an offset into the target. We still have to process all `nu` numbers. The first chunk can only use what's left in the buffer.

```
277a <Prepare array buffer and done, todo, chunk 277a>≡ (276c)
    if (last >= buffer_end) then
        call generate (buffer, state)
        last = 0
    end if
    done = 0
    todo = nu
    chunk = min (todo, buffer_end - last)
```

This logic is a bit weird, but after the first chunk, `todo` will either vanish (in which case we're done) or we have consumed all of the buffer and must reload. In any case we can pretend that the next chunk can use the whole buffer.

```
277b <Update last, done and todo and set new chunk 277b>≡ (276c)
    last = last + chunk
    done = done + chunk
    todo = todo - chunk
    chunk = min (todo, buffer_end)
```

```
277c <Reload buffer or exit 277c>≡ (276c)
    if (chunk <= 0) then
        exit
    end if
    call generate (buffer, state)
    last = 0
```

```
277d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <276b 278a>
    pure subroutine real_array_stateless &
        (state, buffer, buffer_end, last, v, num)
        integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
        integer, intent(in) :: buffer_end
        integer, intent(inout) :: last
        real(kind=default), dimension(:), intent(out) :: v
        integer, optional, intent(in) :: num
        real(kind=default), parameter :: NORM = 1.0_default / M
        <Body of tao_random.*_array 276c>
    end subroutine real_array_stateless
```

Fill the array v_1, \dots, v_ν with uniform deviates $v_i \in [0, 1)$.

```
277e <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <275e 278c>
    pure subroutine real_array_stateless &
        (state, buffer, buffer_end, last, v, num)
```

```

real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer
integer, intent(in) :: buffer_end
integer, intent(inout) :: last
real(kind=default), dimension(:), intent(out) :: v
integer, optional, intent(in) :: num
integer, parameter :: NORM = 1
<Body of tao_random.*_array 276c>
end subroutine real_array_stateless

```

C.4.3 Procedures With Explicit *tao_random_state*

Unfortunately, this is very boring, but Fortran's lack of parametric polymorphism forces this duplication on us:

- 278a <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <277d 278b>
 elemental subroutine integer_state (s, r)
 type(tao_random_state), intent(inout) :: s
 integer, intent(out) :: r
 call integer_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine integer_state
- 278b <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278a 278d>
 elemental subroutine real_state (s, r)
 type(tao_random_state), intent(inout) :: s
 real(kind=default), intent(out) :: r
 call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine real_state
- 278c <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <277e 279b>
 elemental subroutine real_state (s, r)
 type(tao_random_state), intent(inout) :: s
 real(kind=default), intent(out) :: r
 call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine real_state
- 278d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278b 279a>
 pure subroutine integer_array_state (s, v, num)
 type(tao_random_state), intent(inout) :: s
 integer, dimension(:), intent(out) :: v
 integer, optional, intent(in) :: num
 call integer_array_stateless &
 (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine integer_array_state

279a *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) <278d 279d>

```
pure subroutine real_array_state (s, v, num)
  type(tao_random_state), intent(inout) :: s
  real(kind=default), dimension(:), intent(out) :: v
  integer, optional, intent(in) :: num
  call real_array_stateless &
    (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine real_array_state
```

279b *⟨Implementation of 52-bit tao_random_numbers 259c⟩*+≡ (273d) <278c 279f>

```
pure subroutine real_array_state (s, v, num)
  type(tao_random_state), intent(inout) :: s
  real(kind=default), dimension(:), intent(out) :: v
  integer, optional, intent(in) :: num
  call real_array_stateless &
    (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine real_array_state
```

C.4.4 Static Procedures

First make sure that `tao_random_seed` has been called to initialize the generator state:

279c *⟨Initialize a virginal random number generator 279c⟩*≡ (279 280 282)

```
if (s_virginal) then
  call tao_random_seed ()
end if
```

279d *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) <279a 279e>

```
subroutine integer_static (r)
  integer, intent(out) :: r
  ⟨Initialize a virginal random number generator 279c⟩
  call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine integer_static
```

279e *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) <279d 280a>

```
subroutine real_static (r)
  real(kind=default), intent(out) :: r
  ⟨Initialize a virginal random number generator 279c⟩
  call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static
```

279f *⟨Implementation of 52-bit tao_random_numbers 259c⟩*+≡ (273d) <279b 280c>

```
subroutine real_static (r)
  real(kind=default), intent(out) :: r
  ⟨Initialize a virginal random number generator 279c⟩
```



```

        call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
    end subroutine real_static

280a  <Implementation of 30-bit tao_random_numbers 255a>+≡      (273c) <279e 280b>
        subroutine integer_array_static (v, num)
            integer, dimension(:), intent(out) :: v
            integer, optional, intent(in) :: num
            <Initialize a virginal random number generator 279c>
            call integer_array_stateless &
                (s_state, s_buffer, s_buffer_end, s_last, v, num)
        end subroutine integer_array_static

280b  <Implementation of 30-bit tao_random_numbers 255a>+≡      (273c) <280a 283a>
        subroutine real_array_static (v, num)
            real(kind=default), dimension(:), intent(out) :: v
            integer, optional, intent(in) :: num
            <Initialize a virginal random number generator 279c>
            call real_array_stateless &
                (s_state, s_buffer, s_buffer_end, s_last, v, num)
        end subroutine real_array_static

280c  <Implementation of 52-bit tao_random_numbers 259c>+≡      (273d) <279f 285b>
        subroutine real_array_static (v, num)
            real(kind=default), dimension(:), intent(out) :: v
            integer, optional, intent(in) :: num
            <Initialize a virginal random number generator 279c>
            call real_array_stateless &
                (s_state, s_buffer, s_buffer_end, s_last, v, num)
        end subroutine real_array_static

```

C.4.5 Generic Procedures

```

280d  <Interfaces of 30-bit tao_random_numbers 280d>≡          (273c)
        interface tao_random_number
            module procedure <Specific procedures for 30-bit tao_random_number 280e>
        end interface

280e  <Specific procedures for 30-bit tao_random_number 280e>≡      (280d 281a)
        integer_static, integer_state, &
        integer_array_static, integer_array_state, &
        real_static, real_state, real_array_static, real_array_state

These are not exported

280f  <Declaration of 30-bit tao_random_numbers 267c>+≡          (273c) <267e 281a>
        private :: &
            integer_stateless, integer_array_stateless, &

```

```

        real_stateless, real_array_stateless
281a  <Declaration of 30-bit tao_random_numbers 267c>+≡ (273c) <280f
        private :: <Specific procedures for 30-bit tao_random_number 280e>
281b  <Interfaces of 52-bit tao_random_numbers 281b>≡ (273d)
        interface tao_random_number
            module procedure <Specific procedures for 52-bit tao_random_number 281c>
        end interface
281c  <Specific procedures for 52-bit tao_random_number 281c>≡ (281)
        real_static, real_state, real_array_static, real_array_state
Thes are not exported
281d  <Declaration of 52-bit tao_random_numbers 268a>+≡ (273d) <268c 281e>
        private :: real_stateless, real_array_stateless
281e  <Declaration of 52-bit tao_random_numbers 268a>+≡ (273d) <281d
        private :: <Specific procedures for 52-bit tao_random_number 281c>

```

C.4.6 Luxury

```

281f  <Implementation of tao_random_numbers 255f>+≡ (273) <269f 281g>
        pure subroutine luxury_stateless &
            (buffer_size, buffer_end, last, consumption)
            integer, intent(in) :: buffer_size
            integer, intent(inout) :: buffer_end
            integer, intent(inout) :: last
            integer, intent(in) :: consumption
            if (consumption >= 1 .and. consumption <= buffer_size) then
                buffer_end = consumption
                last = min (last, buffer_end)
            else
                !!! print *, "tao_random_luxury: ", "invalid consumption ", &
                !!!      consumption, ", not in [ 1,", buffer_size, "]. "
                buffer_end = buffer_size
            end if
        end subroutine luxury_stateless
281g  <Implementation of tao_random_numbers 255f>+≡ (273) <281f 282a>
        elemental subroutine luxury_state (s)
            type(tao_random_state), intent(inout) :: s
            call luxury_state_integer (s, size (s%buffer))
        end subroutine luxury_state

```

282a \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273) \triangleleft 281g 282b \triangleright
 elemental subroutine luxury_state_integer (s, consumption)
 type(tao_random_state), intent(inout) :: s
 integer, intent(in) :: consumption
 call luxury_stateless (size (s%buffer), s%buffer_end, s%last, consumption)
 end subroutine luxury_state_integer

282b \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273) \triangleleft 282a 282c \triangleright
 elemental subroutine luxury_state_real (s, consumption)
 type(tao_random_state), intent(inout) :: s
 real(kind=default), intent(in) :: consumption
 call luxury_state_integer (s, int (consumption * size (s%buffer)))
 end subroutine luxury_state_real

282c \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273) \triangleleft 282b 282d \triangleright
 subroutine luxury_static ()
 \langle Initialize a virginal random number generator 279c \rangle
 call luxury_static_integer (size (s_buffer))
 end subroutine luxury_static

282d \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273) \triangleleft 282c 282e \triangleright
 subroutine luxury_static_integer (consumption)
 integer, intent(in) :: consumption
 \langle Initialize a virginal random number generator 279c \rangle
 call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
 end subroutine luxury_static_integer

282e \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273) \triangleleft 282d \triangleright
 subroutine luxury_static_real (consumption)
 real(kind=default), intent(in) :: consumption
 \langle Initialize a virginal random number generator 279c \rangle
 call luxury_static_integer (int (consumption * size (s_buffer)))
 end subroutine luxury_static_real

282f \langle Interfaces of tao_random_numbers (unused luxury) 282f $\rangle \equiv$
 interface tao_random_luxury
 module procedure *\langle Specific procedures for tao_random_luxury 282i \rangle*
 end interface

282g \langle Declaration of tao_random_numbers (unused luxury) 282g $\rangle \equiv$ 282h \triangleright
 private :: luxury_stateless

282h \langle Declaration of tao_random_numbers (unused luxury) 282g $\rangle + \equiv$ \triangleleft 282g \triangleright
 private :: *\langle Specific procedures for tao_random_luxury 282i \rangle*

282i \langle Specific procedures for tao_random_luxury 282i $\rangle \equiv$ (282)
 luxury_static, luxury_state, &
 luxury_static_integer, luxury_state_integer, &
 luxury_static_real, luxury_state_real

C.5 Testing

C.5.1 30-bit

283a \langle Implementation of 30-bit tao_random_numbers 255a $\rangle + \equiv$ (273c) \triangleleft 280b

```
subroutine tao_random_test (name)
  character(len=*), optional, intent(in) :: name
  character (len = *), parameter :: &
    OK = "(1x,i10,' is ok.')\langleParameters in tao_random_test 283b $\rangle$ 
  integer, parameter :: &
    A_2027082 = 995235265
  integer, dimension(N) :: a
  type(tao_random_state) :: s, t
  integer, dimension(:), allocatable :: ibuf
  real(kind=tao_r64), dimension(:), allocatable :: dbuf
  integer :: i, ibuf_size, dbuf_size
  print *, "testing the 30-bit tao_random_numbers ..."
   $\langle$ Perform simple tests of tao_random_numbers 283c $\rangle$ 
   $\langle$ Perform more tests of tao_random_numbers 284b $\rangle$ 
end subroutine tao_random_test
```

283b \langle Parameters in tao_random_test 283b $\rangle \equiv$ (283a 285b)

```
integer, parameter :: &
  SEED = 310952, &
  N = 2009, M = 1009, &
  N_SHORT = 1984
```

DEK's "official" test expects $a_{1009:2009+1} = a_{2027082} = 995235265$:

283c \langle Perform simple tests of tao_random_numbers 283c $\rangle \equiv$ (283a 285b) 284a \triangleright

```
! call tao_random_luxury ()
call tao_random_seed (SEED)
do i = 1, N+1
  call tao_random_number (a, M)
end do
 $\langle$ Test a(1) = A_2027082 283d $\rangle$ 
```

283d \langle Test a(1) = A_2027082 283d $\rangle \equiv$ (283-85)

```
if (a(1) == A_2027082) then
  print OK, a(1)
else
  print NOT_OK, a(1), A_2027082
stop 1
```

end if

Deja vu all over again, but 2027081 is factored the other way around this time

```
284a <Perform simple tests of tao_random_numbers 283c>+≡ (283a 285b) <283c
      call tao_random_seed (SEED)
      do i = 1, M+1
        call tao_random_number (a)
      end do
      <Test a(1) = A_2027082 283d>
```

Now checkpoint the random number generator after $N_{\text{short}} \cdot M$ numbers

```
284b <Perform more tests of tao_random_numbers 284b>≡ (283a 285b) 284c>
      print *, "testing the stateless stuff ..."
      call tao_random_create (s, SEED)
      do i = 1, N_SHORT
        call tao_random_number (s, a, M)
      end do
      call tao_random_create (t, s)
      do i = 1, N+1 - N_SHORT
        call tao_random_number (s, a, M)
      end do
      <Test a(1) = A_2027082 283d>
```

and restart the saved generator

```
284c <Perform more tests of tao_random_numbers 284b>+≡ (283a 285b) <284b 284d>
      do i = 1, N+1 - N_SHORT
        call tao_random_number (t, a, M)
      end do
      <Test a(1) = A_2027082 283d>
```

The same story again, but this time saving the copy to a file

```
284d <Perform more tests of tao_random_numbers 284b>+≡ (283a 285b) <284c 285a>
      if (present (name)) then
        print *, "testing I/O ..."
        call tao_random_seed (s, SEED)
        do i = 1, N_SHORT
          call tao_random_number (s, a, M)
        end do
        call tao_random_write (s, name)
        do i = 1, N+1 - N_SHORT
          call tao_random_number (s, a, M)
        end do
        <Test a(1) = A_2027082 283d>
        call tao_random_read (s, name)
```

```

do i = 1, N+1 - N_SHORT
  call tao_random_number (s, a, M)
end do
<Test a(1) = A_2027082 283d>
end if

```

And finally using marshaling/unmarshaling:

```

285a <Perform more tests of tao_random_numbers 284b>+≡ (283a 285b) <284d
  print *, "testing marshaling/unmarshaling ..."
  call tao_random_seed (s, SEED)
  do i = 1, N_SHORT
    call tao_random_number (s, a, M)
  end do
  call tao_random_marshall_size (s, ibuf_size, dbuf_size)
  allocate (ibuf(ibuf_size), dbuf(dbuf_size))
  call tao_random_marshall (s, ibuf, dbuf)
  do i = 1, N+1 - N_SHORT
    call tao_random_number (s, a, M)
  end do
  <Test a(1) = A_2027082 283d>
  call tao_random_unmarshal (s, ibuf, dbuf)
  do i = 1, N+1 - N_SHORT
    call tao_random_number (s, a, M)
  end do
  <Test a(1) = A_2027082 283d>

```

C.5.2 52-bit

DEK's "official" test expects $x_{1009 \cdot 2009 + 1} = x_{2027082} = 0.36410514377569680455$:

```

285b <Implementation of 52-bit tao_random_numbers 259c>+≡ (273d) <280c
  subroutine tao_random_test (name)
    character(len=*), optional, intent(in) :: name
    character(len=*), parameter :: &
      OK = "(1x,f22.20,' is ok.')

```

```

    print *, "testing the 52-bit tao_random_numbers ..."
    <Perform simple tests of tao_random_numbers 283c>
    <Perform more tests of tao_random_numbers 284b>
end subroutine tao_random_test

```

C.5.3 Test Program

```

286 <tao_test.f90 286>≡
    program tao_test
        use tao_random_numbers, only: test30 => tao_random_test
        use tao52_random_numbers, only: test52 => tao_random_test
        implicit none
        call test30 ("tmp.tao")
        call test52 ("tmp.tao")
        stop 0
    end program tao_test

```

—D—

SPECIAL FUNCTIONS

```

287a  <specfun.f90 287a>≡
      ! specfun.f90 --
      <Copyleft notice 1>
      module specfun
        use kinds
        ! use constants
        implicit none
        private
        <Declaration of specfun procedures 287b>
        real(kind=default), public, parameter :: &
          PI = 3.1415926535897932384626433832795028841972_default
        contains
        <Implementation of specfun procedures 288b>
      end module specfun

```

The algorithm is stolen from the FORTRAN version in routine C303 of the CERN library [25]. It has an accuracy which is approximately one digit less than machine precision.

```

287b  <Declaration of specfun procedures 287b>≡ (287a)
      public :: gamma

```

The so-called reflection formula is used for negative arguments:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \quad (\text{D.1})$$

Here's the identity transformation that pulls the argument of Γ into $[3, 4]$:

$$\Gamma(u) = \begin{cases} (u-1)\Gamma(u-1) & \text{for } u > 4 \\ \frac{1}{u}\Gamma(u+1) & \text{for } u < 3 \end{cases} \quad (\text{D.2})$$

```

287c  <Pull u into the intervall [3, 4] 287c>≡ (288b)
      f = 1

```



```

if (u < 3) then
  do i = 1, int (4 - u)
    f = f / u
    u = u + 1
  end do
else
  do i = 1, int (u - 3)
    u = u - 1
    f = f * u
  end do
end if

```

A Chebyshev approximation for $\Gamma(x)$ is used after mapping $x \in [3, 4]$ linearly to $h \in [-1, 1]$. The series is evaluated by Clenshaw's recurrence formula:

$$\begin{aligned}
 d_m &= d_{m+1} = 0 \\
 d_j &= 2xd_{j+1} - d_{j+2} + c_j \text{ for } 0 < j < m - 1 \\
 f(x) &= d_0 = xd_1 - d_2 + \frac{1}{2}c_0
 \end{aligned} \tag{D.3}$$

288a \langle Clenshaw's recurrence formula 288a $\rangle \equiv$ (288b)

```

alpha = 2*g
b1 = 0
b2 = 0
do i = 15, 0, -1
  b0 = c(i) + alpha * b1 - b2
  b2 = b1
  b1 = b0
end do
g = f * (b0 - g * b2)

```

Note that we're assuming that $c(0)$ is in fact $c_0/2$. This is for compatibility with the CERN library routines.

288b \langle Implementation of specfun procedures 288b $\rangle \equiv$ (287a)

```

pure function gamma (x) result (g)
  real(kind=default), intent(in) :: x
  real(kind=default) :: g
  integer :: i
  real(kind=default) :: u, f, alpha, b0, b1, b2
  real(kind=default), dimension(0:15), parameter :: &
    c =  $\langle c_0/2, c_1, c_2, \dots, c_{15} \text{ for } \Gamma(x) \text{ 289a} \rangle$ 
  u = x
  if (u <= 0.0) then
    if (u == int (u)) then
      g = huge (g)
    end if
  end if

```

```

        return
    else
        u = 1 - u
    end if
endif
<Pull u into the intervall [3, 4] 287c>
g = 2*u - 7
<Clenshaw's recurrence formula 288a>
if (x < 0) then
    g = PI / (sin (PI * x) * g)
end if
end function gamma
289a <c0/2, c1, c2, ..., c15 for  $\Gamma(x)$  289a>≡ (288b)
(/ 3.65738772508338244_default, &
  1.95754345666126827_default, &
  0.33829711382616039_default, &
  0.04208951276557549_default, &
  0.00428765048212909_default, &
  0.00036521216929462_default, &
  0.00002740064222642_default, &
  0.00000181240233365_default, &
  0.00000010965775866_default, &
  0.00000000598718405_default, &
  0.00000000030769081_default, &
  0.00000000001431793_default, &
  0.00000000000065109_default, &
  0.00000000000002596_default, &
  0.00000000000000111_default, &
  0.00000000000000004_default /)

```

D.1 Test

```

289b <stest.f90 289b>≡ (290c>
! stest.f90 --
<Copyleft notice 1>
module stest_functions
  use kinds
  use constants
  use specfun
  private
  <Declaration of stest_functions procedures 290a>

```

```

contains
  <Implementation of stest_functions procedures 290b>
end module stest_functions

290a <Declaration of stest_functions procedures 290a>≡ (289b)
  public :: gauss_multiplication
  Gauss' multiplication fomula can serve as a non-trivial test


$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \quad (\text{D.4})$$


290b <Implementation of stest_functions procedures 290b>≡ (289b)
  pure function gauss_multiplication (x, n) result (delta)
    real(kind=default), intent(in) :: x
    integer, intent(in) :: n
    real(kind=default) :: delta
    real(kind=default) :: gxn
    integer :: k
    gxn = (2*PI)**(0.5_double*(1-n)) * n**(n*x-0.5_double)
    do k = 0, n - 1
      gxn = gxn * gamma (x + real (k, kind=default) / n)
    end do
    delta = abs ((gamma (n*x) - gxn) / gamma (n*x))
  end function gauss_multiplication

290c <stest.f90 289b>+≡ <289b
  program stest
    use kinds
    use specfun
    use stest_functions !NODEP!
    implicit none
    integer :: i, steps
    real(kind=default) :: x, g, xmin, xmax
    xmin = -4.5
    xmax = 4.5
    steps = 100 ! 9
    do i = 0, steps
      x = xmin + ((xmax - xmin) / real (steps)) * i
      print "(f6.3,4(1x,e9.2))", x, &
        gauss_multiplication (x, 2), &
        gauss_multiplication (x, 3), &
        gauss_multiplication (x, 4), &
        gauss_multiplication (x, 5)
    end do
  end program stest

```

—E—

STATISTICS

291a $\langle \text{vamp_stat.f90 291a} \rangle \equiv$
`! vamp_stat.f90 --`
 $\langle \text{Copyleft notice 1} \rangle$
`module vamp_stat`
`use kinds`
`implicit none`
`private`
 $\langle \text{Declaration of vamp_stat procedures 291b} \rangle$
`contains`
 $\langle \text{Implementation of vamp_stat procedures 291c} \rangle$
`end module vamp_stat`

291b $\langle \text{Declaration of vamp_stat procedures 291b} \rangle \equiv$ (291a) 292c \triangleright
`public :: average, standard_deviation, value_spread`

$$\text{avg}(X) = \frac{1}{|X|} \sum_{x \in X} x \quad (\text{E.1})$$

291c $\langle \text{Implementation of vamp_stat procedures 291c} \rangle \equiv$ (291a) 292a \triangleright
`pure function average (x) result (a)`
`real(kind=default), dimension(:), intent(in) :: x`
`real(kind=default) :: a`
`integer :: n`
`n = size (x)`
`if (n == 0) then`
`a = 0.0`
`else`
`a = sum (x) / n`
`end if`
`end function average`

$$\text{stddev}(X) = \frac{1}{|X| - 1} \sum_{x \in X} (x - \text{avg}(X))^2 = \frac{1}{|X| - 1} \left(\frac{1}{|X|} \sum_{x \in X} x^2 - (\text{avg}(X))^2 \right) \quad (\text{E.2})$$

292a \langle Implementation of vamp_stat procedures 291c $\rangle + \equiv$ (291a) \triangleleft 291c 292b \triangleright

```

pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
    s = huge (s)
  else
    s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
                  0.0_default))
  end if
end function standard_deviation

```

$$\text{spread}(X) = \max_{x \in X}(x) - \min_{x \in X}(x) \quad (\text{E.3})$$

292b \langle Implementation of vamp_stat procedures 291c $\rangle + \equiv$ (291a) \triangleleft 292a 292d \triangleright

```

pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread

```

292c \langle Declaration of vamp_stat procedures 291b $\rangle + \equiv$ (291a) \triangleleft 291b

```

public :: standard_deviation_percent, value_spread_percent

```

292d \langle Implementation of vamp_stat procedures 291c $\rangle + \equiv$ (291a) \triangleleft 292b 292e \triangleright

```

pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
  else
    s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent

```

292e \langle Implementation of vamp_stat procedures 291c $\rangle + \equiv$ (291a) \triangleleft 292d

```

pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then

```

```
        s = huge (s)
    else
        s = 100.0 * value_spread (x) / abs_avg
    end if
end function value_spread_percent
```

—F—

HISTOGRAMMING

⚡ Merged WK's improvements for WHIZARD. TODO *after* merging:

1. bins3 is a bad undescriptive name
2. bins3 should be added to `histogram2`
3. `write_histogram2_unit` for symmetry.

⚡ There's almost no sanity checking. If you call one of these functions on a histogram that has not been initialized, you loose. — *Big time.*

```

294a <histograms.f90 294a>≡
    ! histograms.f90 --
    <Copyleft notice 1>
    module histograms
        use kinds
        use utils, only: find_free_unit
        implicit none
        private
        <Declaration of histograms procedures 295b>
        <Interfaces of histograms procedures 295c>
        <Variables in histograms 295e>
        <Declaration of histograms types 294b>
    contains
        <Implementation of histograms procedures 295f>
    end module histograms

294b <Declaration of histograms types 294b>≡ (294a) 295a>
    type, public :: histogram
    private
        integer :: n_bins
        real(kind=default) :: x_min, x_max
        real(kind=default), dimension(:), pointer :: bins => null ()
        real(kind=default), dimension(:), pointer :: bins2 => null ()

```

```

        real(kind=default), dimension(:), pointer :: bins3 => null ()
    end type histogram
295a  <Declaration of histograms types 294b>+≡ (294a) <294b
    type, public :: histogram2
        private
        integer, dimension(2) :: n_bins
        real(kind=default), dimension(2) :: x_min, x_max
        real(kind=default), dimension(:, :), pointer :: bins => null ()
        real(kind=default), dimension(:, :), pointer :: bins2 => null ()
    end type histogram2
295b  <Declaration of histograms procedures 295b>≡ (294a) 295d>
    public :: create_histogram
    public :: fill_histogram
    public :: delete_histogram
    public :: write_histogram
295c  <Interfaces of histograms procedures 295c>≡ (294a) 300b>
    interface create_histogram
        module procedure create_histogram1, create_histogram2
    end interface
    interface fill_histogram
        module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
    end interface
    interface delete_histogram
        module procedure delete_histogram1, delete_histogram2
    end interface
    interface write_histogram
        module procedure write_histogram1, write_histogram2
        module procedure write_histogram1_unit
    end interface
295d  <Declaration of histograms procedures 295b>+≡ (294a) <295b 299a>
    private :: create_histogram1, create_histogram2
    private :: fill_histogram1, fill_histogram2s, fill_histogram2v
    private :: delete_histogram1, delete_histogram2
    private :: write_histogram1, write_histogram2
295e  <Variables in histograms 295e>≡ (294a)
    integer, parameter, private :: N_BINS_DEFAULT = 10
295f  <Implementation of histograms procedures 295f>≡ (294a) 296a>
    elemental subroutine create_histogram1 (h, x_min, x_max, nb)
        type(histogram), intent(out) :: h
        real(kind=default), intent(in) :: x_min, x_max
        integer, intent(in), optional :: nb

```



```

    if (present (nb)) then
        h%n_bins = nb
    else
        h%n_bins = N_BINS_DEFAULT
    end if
    h%x_min = x_min
    h%x_max = x_max
    allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
    h%bins = 0
    h%bins2 = 0
    allocate (h%bins3(0:h%n_bins+1))
    h%bins3 = 0
end subroutine create_histogram1
296a <Implementation of histograms procedures 295f>+≡ (294a) <295f 296b>
pure subroutine create_histogram2 (h, x_min, x_max, nb)
    type(histogram2), intent(out) :: h
    real(kind=default), dimension(:), intent(in) :: x_min, x_max
    integer, intent(in), dimension(:), optional :: nb
    if (present (nb)) then
        h%n_bins = nb
    else
        h%n_bins = N_BINS_DEFAULT
    end if
    h%x_min = x_min
    h%x_max = x_max
    allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
        h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
    h%bins = 0
    h%bins2 = 0
end subroutine create_histogram2
296b <Implementation of histograms procedures 295f>+≡ (294a) <296a 297a>
elemental subroutine fill_histogram1 (h, x, weight, excess)
    type(histogram), intent(inout) :: h
    real(kind=default), intent(in) :: x
    real(kind=default), intent(in), optional :: weight
    real(kind=default), intent(in), optional :: excess
    integer :: i
    if (x < h%x_min) then
        i = 0
    else if (x > h%x_max) then
        i = h%n_bins + 1
    else
        i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)

```

```

!WK! i = min (max (i, 0), h%n_bins + 1)
end if
if (present (weight)) then
  h%bins(i) = h%bins(i) + weight
  h%bins2(i) = h%bins2(i) + weight*weight
else
  h%bins(i) = h%bins(i) + 1
  h%bins2(i) = h%bins2(i) + 1
end if
if (present (excess)) h%bins3(i) = h%bins3(i) + excess
end subroutine fill_histogram1
297a <Implementation of histograms procedures 295f>+≡ (294a) <296b 297b>
elemental subroutine fill_histogram2s (h, x1, x2, weight)
  type(histogram2), intent(inout) :: h
  real(kind=default), intent(in) :: x1, x2
  real(kind=default), intent(in), optional :: weight
  call fill_histogram2v (h, (/ x1, x2 /), weight)
end subroutine fill_histogram2s
297b <Implementation of histograms procedures 295f>+≡ (294a) <297a 297c>
pure subroutine fill_histogram2v (h, x, weight)
  type(histogram2), intent(inout) :: h
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(in), optional :: weight
  integer, dimension(2) :: i
  i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
  i = min (max (i, 0), h%n_bins + 1)
  if (present (weight)) then
    h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight
    h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight*weight
  else
    h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1
    h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1
  end if
end subroutine fill_histogram2v
297c <Implementation of histograms procedures 295f>+≡ (294a) <297b 297d>
elemental subroutine delete_histogram1 (h)
  type(histogram), intent(inout) :: h
  deallocate (h%bins, h%bins2)
  deallocate (h%bins3)
end subroutine delete_histogram1
297d <Implementation of histograms procedures 295f>+≡ (294a) <297c 298>
elemental subroutine delete_histogram2 (h)

```

```

    type(histogram2), intent(inout) :: h
    deallocate (h%bins, h%bins2)
end subroutine delete_histogram2
298 <Implementation of histograms procedures 295f>+≡ (294a) <297d 299b>
subroutine write_histogram1 (h, name, over)
    type(histogram), intent(in) :: h
    character(len=*), intent(in), optional :: name
    logical, intent(in), optional :: over
    integer :: i, iounit
    if (present (name)) then
        call find_free_unit (iounit)
        if (iounit > 0) then
            open (unit = iounit, action = "write", status = "replace", &
                file = name)
            if (present (over)) then
                if (over) then
                    write (unit = iounit, fmt = *) &
                        "underflow", h%bins(0), sqrt (h%bins2(0))
                end if
            end if
            do i = 1, h%n_bins
                write (unit = iounit, fmt = *) &
                    midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
            end do
            if (present (over)) then
                if (over) then
                    write (unit = iounit, fmt = *) &
                        "overflow", h%bins(h%n_bins+1), &
                        sqrt (h%bins2(h%n_bins+1))
                end if
            end if
            close (unit = iounit)
        else
            print *, "write_histogram: Can't find a free unit!"
        end if
    else
        if (present (over)) then
            if (over) then
                print *, "underflow", h%bins(0), sqrt (h%bins2(0))
            end if
        end if
        do i = 1, h%n_bins
            print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
        end do
    end if
end subroutine write_histogram1

```

```

        end do
        if (present (over)) then
            if (over) then
                print *, "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1))
            end if
        end if
    end if
end subroutine write_histogram1

```

299a *<Declaration of histograms procedures 295b>+≡ (294a) <295d 300a>*
 !WK! public :: write_histogram1_unit



I don't like the `format` statement with the line number. Use a character constant instead (after we have merged with WHIZARD's branch).

299b *<Implementation of histograms procedures 295f>+≡ (294a) <298 300d>*
 subroutine write_histogram1_unit (h, iounit, over, show_excess)
 type(histogram), intent(in) :: h
 integer, intent(in) :: iounit
 logical, intent(in), optional :: over, show_excess
 integer :: i
 logical :: show_exc
 show_exc = .false.; if (present(show_excess)) show_exc = show_excess
 if (present (over)) then
 if (over) then
 if (show_exc) then
 write (unit = iounit, fmt = 1) &
 "underflow", h%bins(0), sqrt (h%bins2(0)), h%bins3(0)
 else
 write (unit = iounit, fmt = 1) &
 "underflow", h%bins(0), sqrt (h%bins2(0))
 end if
 end if
 end if
 do i = 1, h%n_bins
 if (show_exc) then
 write (unit = iounit, fmt = 1) &
 midpoint (h, i), h%bins(i), sqrt (h%bins2(i)), h%bins3(i)
 else
 write (unit = iounit, fmt = 1) &
 midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
 end if
 end do
 end subroutine

```

    if (present (over)) then
        if (over) then
            if (show_exc) then
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1)), &
                    h%bins3(h%n_bins+1)
            else
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1))
            end if
        end if
    end if
    1 format (1x,4(G16.9,2x))
end subroutine write_histogram1_unit
300a <Declaration of histograms procedures 295b>+≡ (294a) <299a 300c>
    private :: midpoint
300b <Interfaces of histograms procedures 295c>+≡ (294a) <295c>
    interface midpoint
        module procedure midpoint1, midpoint2
    end interface
300c <Declaration of histograms procedures 295b>+≡ (294a) <300a>
    private :: midpoint1, midpoint2
300d <Implementation of histograms procedures 295f>+≡ (294a) <299b 300e>
    elemental function midpoint1 (h, bin) result (x)
        type(histogram), intent(in) :: h
        integer, intent(in) :: bin
        real(kind=default) :: x
        x = h%x_min + (h%x_max - h%x_min) * (bin - 0.5) / h%n_bins
    end function midpoint1
300e <Implementation of histograms procedures 295f>+≡ (294a) <300d 300f>
    elemental function midpoint2 (h, bin, d) result (x)
        type(histogram2), intent(in) :: h
        integer, intent(in) :: bin, d
        real(kind=default) :: x
        x = h%x_min(d) + (h%x_max(d) - h%x_min(d)) * (bin - 0.5) / h%n_bins(d)
    end function midpoint2
300f <Implementation of histograms procedures 295f>+≡ (294a) <300e>
    subroutine write_histogram2 (h, name, over)
        type(histogram2), intent(in) :: h

```

```

character(len=*), intent(in), optional :: name
logical, intent(in), optional :: over
integer :: i1, i2, iounit
if (present (name)) then
  call find_free_unit (iounit)
  if (iounit > 0) then
    open (unit = iounit, action = "write", status = "replace", &
          file = name)
    if (present (over)) then
      if (over) then
        write (unit = iounit, fmt = *) &
          "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
        do i2 = 1, h%n_bins(2)
          write (unit = iounit, fmt = *) &
            "x1 underflow", midpoint (h, i2, 2), &
            h%bins(0,i2), sqrt (h%bins2(0,i2))
        end do
        do i1 = 1, h%n_bins(1)
          write (unit = iounit, fmt = *) &
            "x2 underflow", midpoint (h, i1, 1), &
            h%bins(i1,0), sqrt (h%bins2(i1,0))
        end do
      end if
    end if
    do i1 = 1, h%n_bins(1)
      do i2 = 1, h%n_bins(2)
        write (unit = iounit, fmt = *) &
          midpoint (h, i1, 1), midpoint (h, i2, 2), &
          h%bins(i1,i2), sqrt (h%bins2(i1,i2))
      end do
    end do
  end do
  if (present (over)) then
    if (over) then
      do i2 = 1, h%n_bins(2)
        write (unit = iounit, fmt = *) &
          "x1 overflow", midpoint (h, i2, 2), &
          h%bins(h%n_bins(1)+1,i2), &
          sqrt (h%bins2(h%n_bins(1)+1,i2))
      end do
      do i1 = 1, h%n_bins(1)
        write (unit = iounit, fmt = *) &
          "x2 overflow", midpoint (h, i1, 1), &
          h%bins(i1,h%n_bins(2)+1), &

```

```

        sqrt (h%bins2(i1,h%n_bins(2)+1))
    end do
    write (unit = iounit, fmt = *) "double overflow", &
        h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
        sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
    end if
end if
close (unit = iounit)
else
    print *, "write_histogram: Can't find a free unit!"
end if
else
    if (present (over)) then
        if (over) then
            print *, "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
            do i2 = 1, h%n_bins(2)
                print *, "x1 underflow", midpoint (h, i2, 2), &
                    h%bins(0,i2), sqrt (h%bins2(0,i2))
            end do
            do i1 = 1, h%n_bins(1)
                print *, "x2 underflow", midpoint (h, i1, 1), &
                    h%bins(i1,0), sqrt (h%bins2(i1,0))
            end do
        end if
    end if
    do i1 = 1, h%n_bins(1)
        do i2 = 1, h%n_bins(2)
            print *, midpoint (h, i1, 1), midpoint (h, i2, 2), &
                h%bins(i1,i2), sqrt (h%bins2(i1,i2))
        end do
    end do
    if (present (over)) then
        if (over) then
            do i2 = 1, h%n_bins(2)
                print *, "x1 overflow", midpoint (h, i2, 2), &
                    h%bins(h%n_bins(1)+1,i2), &
                    sqrt (h%bins2(h%n_bins(1)+1,i2))
            end do
            do i1 = 1, h%n_bins(1)
                print *, "x2 overflow", midpoint (h, i1, 1), &
                    h%bins(i1,h%n_bins(2)+1), &
                    sqrt (h%bins2(i1,h%n_bins(2)+1))
            end do
        end if
    end if
end if

```

```

        print *, "double overflow", &
            h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
            sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
    end if
end if
end if
end subroutine write_histogram2

```


—G—

MISCELLANEOUS UTILITIES

```

304a  <utils.f90 304a>≡
      ! utils.f90 --
      <Copyleft notice 1>
      module utils
        use kinds
        implicit none
        private
        <Declaration of utils procedures 304b>
        <Parameters in utils 311c>
        <Variables in utils 312b>
        <Interfaces of utils procedures 304c>
        contains
        <Implementation of utils procedures 305c>
      end module utils

```

G.1 Memory Management

```

304b  <Declaration of utils procedures 304b>≡                                     (304a) 306d>
      public :: create_array_pointer
      private :: create_integer_array_pointer
      private :: create_real_array_pointer
      private :: create_integer_array2_pointer
      private :: create_real_array2_pointer

304c  <Interfaces of utils procedures 304c>≡                                     (304a) 306e>
      interface create_array_pointer
        module procedure &
          create_integer_array_pointer, &
          create_real_array_pointer, &
          create_integer_array2_pointer, &
          create_real_array2_pointer

```

```

end interface

305a  <Body of create_*_array_pointer 305a>≡ (305c 306a)
  if (associated (lhs)) then
    if (size (lhs) /= n) then
      deallocate (lhs)
      if (present (lb)) then
        allocate (lhs(lb:n+lb-1))
      else
        allocate (lhs(n))
      end if
    end if
  else
    if (present (lb)) then
      allocate (lhs(lb:n+lb-1))
    else
      allocate (lhs(n))
    end if
  end if
  lhs = 0

305b  <Body of create_*_array2_pointer 305b>≡ (306)
  if (associated (lhs)) then
    if (any (ubound (lhs) /= n)) then
      deallocate (lhs)
      if (present (lb)) then
        allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
      else
        allocate (lhs(n(1),n(2)))
      end if
    end if
  else
    if (present (lb)) then
      allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
    else
      allocate (lhs(n(1),n(2)))
    end if
  end if
  lhs = 0

305c  <Implementation of utils procedures 305c>≡ (304a) 306a>
  pure subroutine create_integer_array_pointer (lhs, n, lb)
    integer, dimension(:), pointer :: lhs
    integer, intent(in) :: n
    integer, intent(in), optional :: lb

```

```

    <Body of create_*_array_pointer 305a>
end subroutine create_integer_array_pointer

306a <Implementation of utils procedures 305c>+≡ (304a) <305c 306b>
    pure subroutine create_real_array_pointer (lhs, n, lb)
        real(kind=default), dimension(:), pointer :: lhs
        integer, intent(in) :: n
        integer, intent(in), optional :: lb
        <Body of create_*_array_pointer 305a>
    end subroutine create_real_array_pointer

306b <Implementation of utils procedures 305c>+≡ (304a) <306a 306c>
    pure subroutine create_integer_array2_pointer (lhs, n, lb)
        integer, dimension(:, :), pointer :: lhs
        integer, dimension(:), intent(in) :: n
        integer, dimension(:), intent(in), optional :: lb
        <Body of create_*_array2_pointer 305b>
    end subroutine create_integer_array2_pointer

306c <Implementation of utils procedures 305c>+≡ (304a) <306b 307a>
    pure subroutine create_real_array2_pointer (lhs, n, lb)
        real(kind=default), dimension(:, :), pointer :: lhs
        integer, dimension(:), intent(in) :: n
        integer, dimension(:), intent(in), optional :: lb
        <Body of create_*_array2_pointer 305b>
    end subroutine create_real_array2_pointer

Copy an allocatable array component of a derived type, reshaping the target
if necessary. The target can be disassociated, but its association must not
be undefined.

306d <Declaration of utils procedures 304b>+≡ (304a) <304b 307e>
    public :: copy_array_pointer
    private :: copy_integer_array_pointer
    private :: copy_real_array_pointer
    private :: copy_integer_array2_pointer
    private :: copy_real_array2_pointer

306e <Interfaces of utils procedures 304c>+≡ (304a) <304c 308a>
    interface copy_array_pointer
        module procedure &
            copy_integer_array_pointer, &
            copy_real_array_pointer, &
            copy_integer_array2_pointer, &
            copy_real_array2_pointer
    end interface

```

307a *<Implementation of utils procedures 305c>+≡* (304a) *<306c 307b>*
 pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
 integer, dimension(:), pointer :: lhs
 integer, dimension(:), intent(in) :: rhs
 integer, intent(in), optional :: lb
 call create_integer_array_pointer (lhs, size (rhs), lb)
 lhs = rhs
 end subroutine copy_integer_array_pointer

307b *<Implementation of utils procedures 305c>+≡* (304a) *<307a 307c>*
 pure subroutine copy_real_array_pointer (lhs, rhs, lb)
 real(kind=default), dimension(:), pointer :: lhs
 real(kind=default), dimension(:), intent(in) :: rhs
 integer, intent(in), optional :: lb
 call create_real_array_pointer (lhs, size (rhs), lb)
 lhs = rhs
 end subroutine copy_real_array_pointer

307c *<Implementation of utils procedures 305c>+≡* (304a) *<307b 307d>*
 pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
 integer, dimension(:, :), pointer :: lhs
 integer, dimension(:, :), intent(in) :: rhs
 integer, dimension(:), intent(in), optional :: lb
 call create_integer_array2_pointer &
 (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
 lhs = rhs
 end subroutine copy_integer_array2_pointer

307d *<Implementation of utils procedures 305c>+≡* (304a) *<307c 308b>*
 pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
 real(kind=default), dimension(:, :), pointer :: lhs
 real(kind=default), dimension(:, :), intent(in) :: rhs
 integer, dimension(:), intent(in), optional :: lb
 call create_real_array2_pointer &
 (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
 lhs = rhs
 end subroutine copy_real_array2_pointer

G.2 Sorting

307e *<Declaration of utils procedures 304b>+≡* (304a) *<306d 309d>*
 public :: swap
 private :: swap_integer, swap_real

308a *<Interfaces of utils procedures 304c>+≡* (304a) <306e 310a>

```
interface swap
  module procedure swap_integer, swap_real
end interface
```

308b *<Implementation of utils procedures 305c>+≡* (304a) <307d 308c>

```
elemental subroutine swap_integer (a, b)
  integer, intent(inout) :: a, b
  integer :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_integer
```

308c *<Implementation of utils procedures 305c>+≡* (304a) <308b 308d>

```
elemental subroutine swap_real (a, b)
  real(kind=default), intent(inout) :: a, b
  real(kind=default) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_real
```

Straight insertion:

308d *<Implementation of utils procedures 305c>+≡* (304a) <308c 309b>

```
pure subroutine sort_real (key, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  <Set rev to reverse or .false. 308e>
  do i = 1, size (key) - 1
    <Set j to minloc(key) 309a>
    if (j /= i) then
      call swap (key(i), key(j))
    end if
  end do
end subroutine sort_real
```

308e *<Set rev to reverse or .false. 308e>≡* (308 309)

```
if (present (reverse)) then
  rev = reverse
else
  rev = .false.
end if
```

```

309a  <Set j to minloc(key) 309a>≡ (308 309)
      if (rev) then
        j = sum (maxloc (key(i:))) + i - 1
      else
        j = sum (minloc (key(i:))) + i - 1
      end if

309b  <Implementation of utils procedures 305c>+≡ (304a) <308d 309c>
      pure subroutine sort_real_and_real_array (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        real(kind=default), dimension(:, :), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(:, i), table(:, j))
          end if
        end do
      end subroutine sort_real_and_real_array

309c  <Implementation of utils procedures 305c>+≡ (304a) <309b 310c>
      pure subroutine sort_real_and_integer (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        integer, dimension(:), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(i), table(j))
          end if
        end do
      end subroutine sort_real_and_integer

309d  <Declaration of utils procedures 304b>+≡ (304a) <307e 310b>
      public :: sort
      private :: sort_real, sort_real_and_real_array, sort_real_and_integer

```

310a \langle Interfaces of utils procedures 304c $\rangle + \equiv$ (304a) \triangleleft 308a

```

interface sort
  module procedure &
    sort_real, sort_real_and_real_array, &
    sort_real_and_integer
end interface

```

G.3 Mathematics

310b \langle Declaration of utils procedures 304b $\rangle + \equiv$ (304a) \triangleleft 309d 310d \rangle

```

public :: outer_product

```

Admittedly, one has to get used to this notation for the tensor product:

310c \langle Implementation of utils procedures 305c $\rangle + \equiv$ (304a) \triangleleft 309c 310e \rangle

```

pure function outer_product (x, y) result (xy)
  real(kind=default), dimension(:), intent(in) :: x, y
  real(kind=default), dimension(size(x),size(y)) :: xy
  xy = spread (x, dim=2, ncopies=size(y)) &
    * spread (y, dim=1, ncopies=size(x))
end function outer_product

```

Greatest common divisor and least common multiple

310d \langle Declaration of utils procedures 304b $\rangle + \equiv$ (304a) \triangleleft 310b 312a \rangle

```

public :: factorize, gcd, lcm
private :: gcd_internal

```

For our purposes, a straightforward implementation of Euclid's algorithm suffices:

310e \langle Implementation of utils procedures 305c $\rangle + \equiv$ (304a) \triangleleft 310c 310f \rangle

```

pure recursive function gcd_internal (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
  if (n <= 0) then
    gcd_m_n = m
  else
    gcd_m_n = gcd_internal (n, modulo (m, n))
  end if
end function gcd_internal

```

Wrap an elemental procedure around the recursive procedure:

310f \langle Implementation of utils procedures 305c $\rangle + \equiv$ (304a) \triangleleft 310e 311a \rangle

```

elemental function gcd (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n

```

```

gcd_m_n = gcd_internal (m, n)
end function gcd

```

As long as $m \cdot n$ does not overflow, we can use $\text{gcd}(m, n) \text{lcm}(m, n) = mn$:

311a *<Implementation of utils procedures 305c>+≡ (304a) <310f 311b>*

```

elemental function lcm (m, n) result (lcm_m_n)
  integer, intent(in) :: m, n
  integer :: lcm_m_n
  lcm_m_n = (m * n) / gcd (m, n)
end function lcm

```

A very simple minded factorization procedure, that is not fool proof at all. It maintains $n == \text{product}(\text{factors}(1:i))$, however, and will work in all cases of practical relevance.

311b *<Implementation of utils procedures 305c>+≡ (304a) <311a 312c>*

```

pure subroutine factorize (n, factors, i)
  integer, intent(in) :: n
  integer, dimension(:), intent(out) :: factors
  integer, intent(out) :: i
  integer :: nn, p
  nn = n
  i = 0
  do p = 1, size (PRIMES)
    try: do
      if (modulo (nn, PRIMES(p)) == 0) then
        i = i + 1
        factors(i) = PRIMES(p)
        nn = nn / PRIMES(p)
        if (i >= size (factors)) then
          factors(i) = nn
          return
        end if
      else
        exit try
      end if
    end do try
    if (nn == 1) then
      return
    end if
  end do
end subroutine factorize

```

311c *<Parameters in utils 311c>≡ (304a)*

```

integer, dimension(13), parameter, private :: &
  PRIMES = (/ 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41 /)

```


G.4 I/O

312a *<Declaration of utils procedures 304b>+≡* (304a) <310d
 public :: **find_free_unit**

312b *<Variables in utils 312b>≡* (304a)
 integer, parameter, private :: **MIN_UNIT** = 11, **MAX_UNIT** = 99

312c *<Implementation of utils procedures 305c>+≡* (304a) <311b
 subroutine find_free_unit (u, iostat)
 integer, intent(out) :: u
 integer, intent(out), optional :: iostat
 logical :: exists, is_open
 integer :: **i**, status
 do **i** = **MIN_UNIT**, **MAX_UNIT**
 inquire (**unit** = **i**, exist = exists, opened = is_open, &
 iostat = status)
 if (status == 0) then
 if (exists .and. .not. is_open) then
 u = **i**
 if (present (iostat)) then
 iostat = 0
 end if
 return
 end if
 end if
 end do
 if (present (iostat)) then
 iostat = -1
 end if
 u = -1
 end **subroutine find_free_unit**

—H—

LINEAR ALGEBRA

```

313a  <linalg.f90 313a>≡
      ! linalg.f90 --
      <Copyleft notice 1>
      module linalg
        use kinds
        use utils
        implicit none
        private
        <Declaration of linalg procedures 313b>
      contains
        <Implementation of linalg procedures 314>
      end module linalg

```

H.1 LU Decomposition

```

313b  <Declaration of linalg procedures 313b>≡ (313a) 315e>
      public :: lu_decompose

```

$$A = LU \tag{H.1a}$$

In more detail

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \dots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix} \tag{H.1b}$$

Rewriting (H.1) in block matrix notation

$$\begin{pmatrix} a_{11} & a_{1\cdot} \\ a_{\cdot 1} & A \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ l_{\cdot 1} & L \end{pmatrix} \begin{pmatrix} u_{11} & u_{1\cdot} \\ 0 & U \end{pmatrix} = \begin{pmatrix} u_{11} & u_{1\cdot} \\ l_{\cdot 1} u_{11} & l_{\cdot 1} \otimes u_{1\cdot} + LU \end{pmatrix} \tag{H.2}$$

we can solve it easily

$$u_{11} = a_{11} \quad (\text{H.3a})$$

$$u_{1\cdot} = a_{1\cdot} \quad (\text{H.3b})$$

$$l_{\cdot 1} = \frac{a_{\cdot 1}}{a_{11}} \quad (\text{H.3c})$$

$$LU = A - \frac{a_{\cdot 1} \otimes a_{1\cdot}}{a_{11}} \quad (\text{H.3d})$$

and (H.3c) and (H.3d) define a simple iterative algorithm if we work from the outside in. It just remains to add pivoting.

314 *Implementation of linalg procedures 314* \equiv (313a) 316 \triangleright

```

pure subroutine lu_decompose (a, pivots, eps, l, u)
  real(kind=default), dimension(:, :), intent(inout) :: a
  integer, dimension(:), intent(out), optional :: pivots
  real(kind=default), intent(out), optional :: eps
  real(kind=default), dimension(:, :), intent(out), optional :: l, u
  real(kind=default), dimension(size(a,dim=1)) :: vv
  integer, dimension(size(a,dim=1)) :: p
  integer :: j, pivot
  (eps = 1 315a)
  vv = maxval (abs (a), dim=2)
  if (any (vv == 0.0)) then
    a = 0.0
    (pivots = 0 and eps = 0 315c)
    return
  end if
  vv = 1.0 / vv
  do j = 1, size (a, dim=1)
    pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
    if (j /= pivot) then
      call swap (a(pivot,:), a(j,:))
      (eps = - eps 315b)
      vv(pivot) = vv(j)
    end if
    p(j) = pivot
    if (a(j,j) == 0.0) then
      a(j,j) = tiny (a(j,j))
    end if
    a(j+1:,j) = a(j+1:,j) / a(j,j)
    a(j+1:,j+1:) &
      = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
  end do

```

```

    <Return optional arguments in lu_decompose 315d>
end subroutine lu_decompose

315a <eps = 1 315a>≡ (314)
    if (present (eps)) then
        eps = 1.0
    end if

315b <eps = - eps 315b>≡ (314)
    if (present (eps)) then
        eps = - eps
    end if

315c <pivots = 0 and eps = 0 315c>≡ (314)
    if (present (pivots)) then
        pivots = 0
    end if
    if (present (eps)) then
        eps = 0
    end if

315d <Return optional arguments in lu_decompose 315d>≡ (314)
    if (present (pivots)) then
        pivots = p
    end if
    if (present (l)) then
        do j = 1, size (a, dim=1)
            l(1:j-1,j) = 0.0
            l(j,j) = 1.0
            l(j+1:,j) = a(j+1:,j)
        end do
        do j = size (a, dim=1), 1, -1
            call swap (l(j,:), l(p(j),:))
        end do
    end if
    if (present (u)) then
        do j = 1, size (a, dim=1)
            u(1:j,j) = a(1:j,j)
            u(j+1:,j) = 0.0
        end do
    end if
end if

```

H.2 Determinant

315e <Declaration of linalg procedures 313b>+≡ (313a) <313b 317a>

```
public :: determinant
```

This is a subroutine to comply with F's rules, otherwise, we would code it as a function.

316 \langle Implementation of linalg procedures 314 $\rangle + \equiv$ (313a) \langle 314 317b \rangle

```
pure subroutine determinant (a, det)
  real(kind=default), dimension(:, :), intent(in) :: a
  real(kind=default), intent(out) :: det
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu
  integer :: i
  lu = a
  call lu_decompose (lu, eps = det)
  do i = 1, size (a, dim = 1)
    det = det * lu(i,i)
  end do
end subroutine determinant
```

H.3 Diagonalization

The code is an implementation of the algorithm presented in [17, 18], but independent from the code presented in [19] to avoid legal problems.

A Jacobi rotation around the angle ϕ in row p and column q

$$P(\phi; p, q) = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos \phi & \cdots & \sin \phi & & \\ & & \vdots & 1 & \vdots & & \\ & & -\sin \phi & \cdots & \cos \phi & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \quad (\text{H.4})$$

results in

$$A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) = \begin{pmatrix} & & A'_{1p} & & A'_{1q} & & \\ & & \vdots & & \vdots & & \\ A'_{p1} & \cdots & A'_{pq} & \cdots & A'_{pq} & \cdots & A'_{pn} \\ & & \vdots & & \vdots & & \\ A'_{q1} & \cdots & A'_{qp} & \cdots & A'_{qq} & \cdots & A'_{qn} \\ & & \vdots & & \vdots & & \\ & & A'_{np} & & A'_{nq} & & \end{pmatrix} \quad (\text{H.5})$$

317a *<Declaration of linalg procedures 313b>+≡* (313a) <315e 320b>
public :: diagonalize_real_symmetric

317b *<Implementation of linalg procedures 314>+≡* (313a) <316 320a>
pure subroutine diagonalize_real_symmetric (a, eval, evec, num_rot)
real(kind=default), dimension(:, :), intent(in) :: a
real(kind=default), dimension(:), intent(out) :: eval
real(kind=default), dimension(:, :), intent(out) :: evec
integer, intent(out), optional :: num_rot
real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: aa
real(kind=default) :: off_diagonal_norm, threshold, &
c, g, h, s, t, tau, cot_2phi
logical, dimension(size(eval),size(eval)) :: upper_triangle
integer, dimension(size(eval)) :: one_to_ndim
integer :: p, q, ndim, j, sweep
integer, parameter :: MAX_SWEEPS = 50
ndim = size (eval)
one_to_ndim = (/ (j, j=1,ndim) /)
upper_triangle = &
spread (one_to_ndim, dim=1, ncopies=ndim) &
> spread (one_to_ndim, dim=2, ncopies=ndim)
aa = a
call unit (evec)
<Initialize num_rot 320d>
sweeps: do sweep = 1, MAX_SWEEPS
off_diagonal_norm = sum (abs (aa), mask=upper_triangle)
if (off_diagonal_norm == 0.0) then
eval = diag (aa)
return
end if
if (sweep < 4) then
threshold = 0.2 * off_diagonal_norm / ndim**2
else
threshold = 0.0
end if
do p = 1, ndim - 1
do q = p + 1, ndim
<Perform the Jacobi rotation resulting in $A'_{pq} = 0$ 318a>
end do
end do
end do sweeps
if (present (num_rot)) then
num_rot = -1
end if

```

!!! print *, "linalg::diagonalize_real_symmetric: exceeded sweep count"
end subroutine diagonalize_real_symmetric

318a ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  318a⟩≡ (317b)
  g = 100 * abs (aa (p,q))
  if ((sweep > 4) &
      .and. (g <= min (spacing (aa(p,p)), spacing (aa(q,q))))) then
    aa(p,q) = 0.0
  else if (abs (aa(p,q)) > threshold) then
    ⟨Determine  $\phi$  for the Jacobi rotation  $P(\phi; p, q)$  with  $A'_{pq} = 0$  318b⟩
    ⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  319b⟩
    ⟨ $V' = V \cdot P(\phi; p, q)$  320c⟩
    ⟨Update num_rot 320e⟩
  end if

```

We want

$$A'_{pq} = (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) = 0 \quad (\text{H.6})$$

and therefore

$$\cot 2\phi = \frac{1 - \tan^2 \phi}{2 \tan \phi} = \frac{\cos^2 \phi - \sin^2 \phi}{2 \sin \phi \cos \phi} = \frac{A_{pp} - A_{qq}}{2A_{pq}} \quad (\text{H.7})$$

i.e. with $t = \tan \phi = s/c$

$$t^2 + 2t \cot 2\phi - 1 = 0 \quad (\text{H.8})$$

This quadratic equation has the roots

$$t = -\cot 2\phi \pm \sqrt{1 + \cot^2 2\phi} = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| \pm \epsilon(\cot 2\phi)\sqrt{1 + \cot^2 2\phi}} \quad (\text{H.9})$$

and the smaller in magnitude of these is

$$t = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| + \sqrt{1 + \cot^2 2\phi}} \quad (\text{H.10})$$

and since $|t| \leq 1$, it corresponds to $|\phi| \leq \pi/4$. For very large $\cot 2\phi$ we will use

$$t = \frac{1}{2 \cot 2\phi} = \frac{A_{pq}}{A_{pp} - A_{qq}} \quad (\text{H.11})$$

$$h = A_{qq} - A_{pp} \quad (\text{H.12})$$

```

318b ⟨Determine  $\phi$  for the Jacobi rotation  $P(\phi; p, q)$  with  $A'_{pq} = 0$  318b⟩≡ (318a) 319a▷
  h = aa(q,q) - aa(p,p)
  if (g <= spacing (h)) then

```

```

    t = aa(p,q) / h
else
    cot_2phi = 0.5 * h / aa(p,q)
    t = sign (1.0_default, cot_2phi) &
        / (abs (cot_2phi) + sqrt (1.0 + cot_2phi**2))
end if
Trivia

```

$$\cos^2 \phi = \frac{\cos^2 \phi}{\cos^2 \phi + \sin^2 \phi} = \frac{1}{1 + \tan^2 \phi} \quad (\text{H.13a})$$

$$\sin \phi = \tan \phi \cos \phi \quad (\text{H.13b})$$

$$\tau \sin \phi = \frac{\sin^2}{1 + \cos \phi} = \frac{1 - \cos^2}{1 + \cos \phi} = 1 - \cos \phi \quad (\text{H.13c})$$

319a $\langle \text{Determine } \phi \text{ for the Jacobi rotation } P(\phi; p, q) \text{ with } A'_{pq} = 0 \text{ } \mathbf{318b} \rangle + \equiv \quad (\mathbf{318a}) \triangleleft \mathbf{318b}$

```

c = 1.0 / sqrt (1.0 + t**2)
s = t * c
tau = s / (1.0 + c)

```

$$\begin{aligned} A'_{pp} &= c^2 A_{pp} + s^2 A_{qq} - 2scA_{pq} = A_{pp} - tA_{pq} \\ A'_{qq} &= s^2 A_{pp} + c^2 A_{qq} + 2scA_{pq} = A_{qq} + tA_{pq} \\ A'_{pq} &= (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) \end{aligned} \quad (\text{H.14})$$

319b $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) \text{ } \mathbf{319b} \rangle \equiv \quad (\mathbf{318a}) \text{ } \mathbf{319c} \triangleright$

```

aa(p,p) = aa(p,p) - t * aa(p,q)
aa(q,q) = aa(q,q) + t * aa(p,q)
aa(p,q) = 0.0

```

$$\begin{aligned} r \neq p < q \neq r : A'_{rp} &= cA_{rp} - sA_{rq} \\ A'_{rq} &= sA_{rp} + cA_{rq} \end{aligned} \quad (\text{H.15})$$

Here's how we cover the upper triangular region using array notation:

$$\begin{pmatrix} & \mathbf{a(1:p-1,p)} & & \mathbf{a(1:p-1,q)} & \\ \cdots & A_{pq} & \mathbf{a(p,p+1:q-1)} & A_{pq} & \mathbf{a(p,q+1:ndim)} \\ & \vdots & & \mathbf{a(p+1:q-1,q)} & \\ \cdots & A_{qp} & \cdots & A_{qq} & \mathbf{a(q,q+1:ndim)} \\ & \vdots & & \vdots & \end{pmatrix} \quad (\text{H.16})$$

319c $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) \text{ } \mathbf{319b} \rangle + \equiv \quad (\mathbf{318a}) \triangleleft \mathbf{319b}$

```

call jacobi_rotation (s, tau, aa(1:p-1,p), aa(1:p-1,q))
call jacobi_rotation (s, tau, aa(p,p+1:q-1), aa(p+1:q-1,q))
call jacobi_rotation (s, tau, aa(p,q+1:ndim), aa(q,q+1:ndim))

```


Using (H.13c), we can write the rotation as a perturbation:

$$\begin{aligned} V'_p &= cV_p - sV_q = V_p - s(V_q + \tau V_p) \\ V'_q &= sV_p + cV_q = V_q + s(V_p - \tau V_q) \end{aligned} \quad (\text{H.17})$$

```

320a  <Implementation of linalg procedures 314>+≡ (313a) <317b 320f>
      pure subroutine jacobi_rotation (s, tau, vp, vq)
        real(kind=default), intent(in) :: s, tau
        real(kind=default), dimension(:), intent(inout) :: vp, vq
        real(kind=default), dimension(size(vp)) :: vp_tmp
        vp_tmp = vp
        vp = vp - s * (vq      + tau * vp)
        vq = vq + s * (vp_tmp - tau * vq)
      end subroutine jacobi_rotation

320b  <Declaration of linalg procedures 313b>+≡ (313a) <317a 321a>
      private :: jacobi_rotation

320c  <V' = V · P(φ; p, q) 320c>≡ (318a)
      call jacobi_rotation (s, tau, evec(:,p), evec(:,q))

320d  <Initialize num_rot 320d>≡ (317b)
      if (present (num_rot)) then
        num_rot = 0
      end if

320e  <Update num_rot 320e>≡ (318a)
      if (present (num_rot)) then
        num_rot = num_rot + 1
      end if

320f  <Implementation of linalg procedures 314>+≡ (313a) <320a 320g>
      pure subroutine unit (u)
        real(kind=default), dimension(:, :), intent(out) :: u
        integer :: i
        u = 0.0
        do i = 1, min (size (u, dim = 1), size (u, dim = 2))
          u(i,i) = 1.0
        end do
      end subroutine unit

320g  <Implementation of linalg procedures 314>+≡ (313a) <320f>
      pure function diag (a) result (d)
        real(kind=default), dimension(:, :), intent(in) :: a
        real(kind=default), dimension(min(size(a,dim=1),size(a,dim=2))) :: d
        integer :: i
        do i = 1, min (size (a, dim = 1), size (a, dim = 2))

```

```

        d(i) = a(i,i)
    end do
end function diag
321a  ⟨Declaration of linalg procedures 313b⟩+≡ (313a) <320b
      public :: unit, diag

```

H.4 Test

```

321b  ⟨la_sample.f90 321b⟩≡
      ! la_sample.f90 --
      ⟨Copyleft notice 1⟩
      program la_sample
      use kinds
      use utils
      use tao_random_numbers
      use linalg
      implicit none
      integer, parameter :: N = 200
      real(kind=default), dimension(N,N) :: a, evec, a0, l, u, NAG_bug
      real(kind=default), dimension(N) :: b, eval
      real(kind=default) :: d
      integer :: i
      call system_clock (i)
      call tao_random_seed (i)
      print *, i
      do i = 1, N
          call tao_random_number (a(:,i))
      end do
      NAG_bug = (a + transpose (a)) / 2
      a = NAG_bug
      a0 = a
      call lu_decompose (a, l=l, u=u)
      a = matmul (l, u)
      print *, maxval (abs(a-a0))
      call determinant (a, d)
      print *, d
      call diagonalize_real_symmetric (a, eval, evec)
      print *, product (eval)
      stop
      call sort (eval, evec)
      do i = 1, N
          b = matmul (a, evec(:,i)) - eval(i) * evec(:,i)

```

```

        write (unit = *, fmt = "(A,I3, 2(A,E11.4))") &
            "eval #", i, " = ", eval(i), ", |(A-lambda)V|_infty = ", &
            maxval (abs(b)) / maxval (abs(evec(:,i)))
    end do
end program la_sample

```

—I—

PRODUCTS

```
323 <products.f90 323>≡
! products.f90 --
<Copyleft notice 1>
module products
  use kinds
  implicit none
  private
  public :: dot, sp, spc
contains
  pure function dot (p, q) result (pq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    real(kind=default) :: pq
    pq = p(0)*q(0) - dot_product (p(1:), q(1:))
  end function dot
  pure function sp (p, q) result (sppq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: sppq
    sppq = cmplx (p(2), p(3), kind=default) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
      - cmplx (q(2), q(3), kind=default) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
  end function sp
  pure function spc (p, q) result (spcpq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: spcpq
    spcpq = conjg (sp (p, q))
  end function spc
end module products
```

—J—

KINEMATICS

```

324a  <kinematics.f90 324a>≡                                     329d>
      ! kinematics.f90 --
      <Copyleft notice 1>
      module kinematics
        use kinds
        use constants
        use products, only: dot
        use specfun, only: gamma
        implicit none
        private
        <Declaration of kinematics procedures 324b>
        <Interfaces of kinematics procedures 324c>
        <Declaration of kinematics types 326f>
        contains
        <Implementation of kinematics procedures 325a>
      end module kinematics

```

J.1 Lorentz Transformations

```

324b  <Declaration of kinematics procedures 324b>≡                 (324a) 326c>
      public :: boost_velocity
      private :: boost_one_velocity, boost_many_velocity
      public :: boost_momentum
      private :: boost_one_momentum, boost_many_momentum

324c  <Interfaces of kinematics procedures 324c>≡                 (324a) 326e>
      interface boost_velocity
        module procedure boost_one_velocity, boost_many_velocity
      end interface
      interface boost_momentum
        module procedure boost_one_momentum, boost_many_momentum

```

end interface

Boost a four vector p to the inertial frame moving with the velocity β :

$$p'_0 = \gamma (p_0 - \vec{\beta} \vec{p}) \quad (\text{J.1a})$$

$$\vec{p}' = \gamma (\vec{p}_{\parallel} - \vec{\beta} p_0) + \vec{p}_{\perp} \quad (\text{J.1b})$$

with $\gamma = 1/\sqrt{1 - \vec{\beta}^2}$, $\vec{p}_{\parallel} = \vec{\beta}(\vec{\beta} \vec{p})/\vec{\beta}^2$ and $\vec{p}_{\perp} = \vec{p} - \vec{p}_{\parallel}$. Using $1/\vec{\beta}^2 = \gamma^2/(\gamma + 1) \cdot 1/(\gamma - 1)$ and $\vec{b} = \gamma \vec{\beta}$ this can be rewritten as

$$p'_0 = \gamma p_0 - \vec{b} \vec{p} \quad (\text{J.2a})$$

$$\vec{p}' = \vec{p} + \left(\frac{\vec{b} \vec{p}}{\gamma + 1} - p_0 \right) \vec{b} \quad (\text{J.2b})$$

325a \langle Implementation of kinematics procedures 325a $\rangle \equiv$ (324a) 325b \rangle

```
pure function boost_one_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(0:3) :: p_prime
  real(kind=default), dimension(1:3) :: b
  real(kind=default) :: gamma, b_dot_p
  gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
  b = gamma * beta
  b_dot_p = dot_product (b, p(1:3))
  p_prime(0) = gamma * p(0) - b_dot_p
  p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
end function boost_one_velocity
```

325b \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 325a 325c \rangle

```
pure function boost_many_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  integer :: i
  do i = 1, size (p, dim=1)
    p_prime(i,:) = boost_one_velocity (p(i,:), beta)
  end do
end function boost_many_velocity
```

Boost a four vector p to the rest frame of the four vector q . The velocity is $\vec{\beta} = \vec{q}/|q_0|$:

325c \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 325b 326a \rangle

```

pure function boost_one_momentum (p, q) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p, q
  real(kind=default), dimension(0:3) :: p_prime
  p_prime = boost_velocity (p, q(1:3) / abs (q(0)))
end function boost_one_momentum

```

326a \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 325c 326b \rangle

```

pure function boost_many_momentum (p, q) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(0:), intent(in) :: q
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  p_prime = boost_many_velocity (p, q(1:3) / abs (q(0)))
end function boost_many_momentum

```

J.2 Massive Phase Space

$$\lambda(a, b, c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca = (a - b - c)^2 - 4bc \quad (\text{J.3})$$

and permutations

326b \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 326a 327a \rangle

```

pure function lambda (a, b, c) result (lam)
  real(kind=default), intent(in) :: a, b, c
  real(kind=default) :: lam
  lam = a**2 + b**2 + c**2 - 2*(a*b + b*c + c*a)
end function lambda

```

326c \langle Declaration of kinematics procedures 324b $\rangle + \equiv$ (324a) \langle 324b 326d \rangle

```

public :: lambda

```

326d \langle Declaration of kinematics procedures 324b $\rangle + \equiv$ (324a) \langle 326c 328a \rangle

```

public :: two_to_three
private :: two_to_three_massive, two_to_three_massless

```

326e \langle Interfaces of kinematics procedures 324c $\rangle + \equiv$ (324a) \langle 324c 328b \rangle

```

interface two_to_three
  module procedure two_to_three_massive, two_to_three_massless
end interface

```

326f \langle Declaration of kinematics types 326f $\rangle \equiv$ (324a)

```

type, public :: LIPS3
  real(kind=default), dimension(3,0:3) :: p
  real(kind=default) :: jacobian
end type LIPS3

```

$$dLIPS_3 = \int \frac{d^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{d^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{d^3\vec{p}_3}{(2\pi)^3 2E_3} (2\pi)^4 \delta^4(p_1 + p_2 + p_3 - p_a - p_b) \quad (J.4)$$

The jacobian is given by

$$dLIPS_3 = \frac{1}{(2\pi)^5} \int d\phi dt_1 ds_2 d\Omega_3^{[23]} \frac{1}{32\sqrt{ss_2}} \frac{|p_3^{[23]}|}{|p_a^{[ab]}|} \quad (J.5)$$

where $\vec{p}_i^{[jk]}$ denotes the momentum of particle i in the center of mass system of particles j and k .

327a \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 326b 327b \rangle

```

pure function two_to_three_massive &
  (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
    s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
    1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive

```

A specialized version for massless particles can be faster, because the kinematics is simpler:

327b \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \langle 327a 328c \rangle

```

pure function two_to_three_massless (s, t1, s2, phi, cos_theta3, phi3) &
  result (p)
  real(kind=default), intent(in) :: s, t1, s2, phi, cos_theta3, phi3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: pa_abs, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (s) / 2
  p1_abs = (s - s2) / (2 * sqrt (s))

```



```

    p3_abs = sqrt (s2) / 2
    p%jacobian = 1.0 / ((2*PI)**5 * 32 * s)
    cos_theta = 1 + t1 / (2*pa_abs*p1_abs)
    p%p(1,0) = p1_abs
    p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p23(1:3) = - p%p(1,1:3)
    p23(0) = on_shell (p23, sqrt (s2))
    p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3)
end function two_to_three_massless

328a <Declaration of kinematics procedures 324b>+≡ (324a) <326d 329a>
    public :: one_to_two
    private :: one_to_two_massive, one_to_two_massless

328b <Interfaces of kinematics procedures 324c>+≡ (324a) <326e
    interface one_to_two
        module procedure one_to_two_massive, one_to_two_massless
    end interface

328c <Implementation of kinematics procedures 325a>+≡ (324a) <327b 328d>
    pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi, m1, m2
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: s, p1_abs
        s = dot (p12, p12)
        p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,1:3) = - p(1,1:3)
        p(1,0) = on_shell (p(1,:), m1)
        p(2,0) = on_shell (p(2,:), m2)
        p = boost_momentum (p, - p12)
    end function one_to_two_massive

328d <Implementation of kinematics procedures 325a>+≡ (324a) <328c 329b>
    pure function one_to_two_massless (p12, cos_theta, phi) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: p1_abs
        p1_abs = sqrt (dot (p12, p12)) / 2
        p(1,0) = p1_abs
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,0) = p1_abs
        p(2,1:3) = - p(1,1:3)
        p = boost_momentum (p, - p12)

```

```

end function one_to_two_massless

329a <Declaration of kinematics procedures 324b>+≡ (324a) <328a 332c>
public :: polar_to_cartesian, on_shell

329b <Implementation of kinematics procedures 325a>+≡ (324a) <328d 329c>
pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
  real(kind=default), intent(in) :: v_abs, cos_theta, phi
  real(kind=default), dimension(3) :: v
  real(kind=default) :: sin_phi, cos_phi, sin_theta
  sin_theta = sqrt (1.0 - cos_theta**2)
  cos_phi = cos (phi)
  sin_phi = sin (phi)
  v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
end function polar_to_cartesian

329c <Implementation of kinematics procedures 325a>+≡ (324a) <329b 332d>
pure function on_shell (p, m) result (E)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), intent(in) :: m
  real(kind=default) :: E
  E = sqrt (m**2 + dot_product (p(1:3), p(1:3)))
end function on_shell

```

J.3 Massive 3-Particle Phase Space Revisited

$$\begin{array}{ccccc}
U_1 & \xrightarrow{\xi_1} & P_1 & \xrightarrow{\phi_1} & M \\
\pi_U \downarrow & & \downarrow \pi_P & & \parallel \\
U_2 & \xrightarrow{\xi_2} & P_2 & \xrightarrow{\phi_2} & M
\end{array} \tag{J.6}$$

$$\begin{array}{ccccc}
U_1 & \xrightarrow{\xi} & P_1 & \xrightarrow{\phi} & M \\
\pi_U \downarrow & & \downarrow \pi_P & & \downarrow \pi \\
U_2 & \xrightarrow{\xi} & P_2 & \xrightarrow{\phi} & M
\end{array} \tag{J.7}$$

```

329d <kinematics.f90 324a>+≡ <324a>
module phase_space
  use kinds
  use constants
  use kinematics !NODEP!
  use tao_random_numbers
  implicit none
  private

```

```

    <Declaration of phase_space procedures 331b>
    <Interfaces of phase_space procedures 331c>
    <Declaration of phase_space types 330a>
contains
    <Implementation of phase_space procedures 331d>
end module phase_space

                                LIPS3_unit : [0, 1]5                                (J.8)

330a <Declaration of phase_space types 330a>≡                                (329d) 330b>
    type, public :: LIPS3_unit
        real(kind=default), dimension(5) :: x
        real(kind=default) :: s
        real(kind=default), dimension(2) :: mass_in
        real(kind=default), dimension(3) :: mass_out
        real(kind=default) :: jacobian
    end type LIPS3_unit

330b <Declaration of phase_space types 330a>+≡                                (329d) <330a 330c>
    type, public :: LIPS3_unit_massless
        real(kind=default), dimension(5) :: x
        real(kind=default) :: s
        real(kind=default) :: jacobian
    end type LIPS3_unit_massless

                                LIPS3_s2_t1_angles : (s2, t1, ϕ, cos θ3, ϕ3)                                (J.9)

330c <Declaration of phase_space types 330a>+≡                                (329d) <330b 330d>
    type, public :: LIPS3_s2_t1_angles
        real(kind=default) :: s2, t1, phi, cos_theta3, phi3
        real(kind=default) :: s
        real(kind=default), dimension(2) :: mass_in
        real(kind=default), dimension(3) :: mass_out
        real(kind=default) :: jacobian
    end type LIPS3_s2_t1_angles

330d <Declaration of phase_space types 330a>+≡                                (329d) <330c 330e>
    type, public :: LIPS3_s2_t1_angles_massless
        real(kind=default) :: s2, t1, phi, cos_theta3, phi3
        real(kind=default) :: s
        real(kind=default) :: jacobian
    end type LIPS3_s2_t1_angles_massless

                                LIPS3_momenta : (p1, p2, p3)                                (J.10)

330e <Declaration of phase_space types 330a>+≡                                (329d) <330d 331a>
    type, public :: LIPS3_momenta
        real(kind=default), dimension(0:3,3) :: p

```

```

    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_momenta

331a <Declaration of phase_space types 330a>+≡ (329d) <330e>
type, public :: LIPS3_momenta_massless
    real(kind=default), dimension(0:3,3) :: p
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_momenta_massless

331b <Declaration of phase_space procedures 331b>≡ (329d) 331f>
public :: random_LIPS3
private :: random_LIPS3_unit, random_LIPS3_unit_massless

331c <Interfaces of phase_space procedures 331c>≡ (329d)
interface random_LIPS3
    module procedure random_LIPS3_unit, random_LIPS3_unit_massless
end interface

331d <Implementation of phase_space procedures 331d>≡ (329d) 331e>
pure subroutine random_LIPS3_unit (rng, lips)
    type(tao_random_state), intent(inout) :: rng
    type(LIPS3_unit), intent(inout) :: lips
    call tao_random_number (rng, lips%x)
    lips%jacobian = 1
end subroutine random_LIPS3_unit

331e <Implementation of phase_space procedures 331d>+≡ (329d) <331d 332a>
pure subroutine random_LIPS3_unit_massless (rng, lips)
    type(tao_random_state), intent(inout) :: rng
    type(LIPS3_unit_massless), intent(inout) :: lips
    call tao_random_number (rng, lips%x)
    lips%jacobian = 1
end subroutine random_LIPS3_unit_massless

331f <Declaration of phase_space procedures 331b>+≡ (329d) <331b>
private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0

331g <(Unused) Interfaces of phase_space procedures 331g>≡
interface assignment(=)
    module procedure &
        LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
end interface

```

332a *<Implementation of phase_space procedures 331d>+≡ (329d) <331e 332b>*
 pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
 type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
 type(LIPS3_unit), intent(in) :: unit
 end subroutine LIPS3_unit_to_s2_t1_angles

332b *<Implementation of phase_space procedures 331d>+≡ (329d) <332a*
 pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
 type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
 type(LIPS3_unit_massless), intent(in) :: unit
 end subroutine LIPS3_unit_to_s2_t1_angles_m0

J.4 Massless n -Particle Phase Space: RAMBO

332c *<Declaration of kinematics procedures 324b>+≡ (324a) <329a 333b>*
 public :: massless_isotropic_decay

The massless RAMBO algorithm [26]:

332d *<Implementation of kinematics procedures 325a>+≡ (324a) <329c 333c>*
 pure function massless_isotropic_decay (roots, ran) result (p)
 real (kind=default), intent(in) :: roots
 real (kind=default), dimension(:, :), intent(in) :: ran
 real (kind=default), dimension(size(ran,dim=1),0:3) :: p
 real (kind=default), dimension(size(ran,dim=1),0:3) :: q
 real (kind=default), dimension(0:3) :: qsum
 real (kind=default) :: cos_theta, sin_theta, phi, qabs, x, r, z
 integer :: k
 <Generate isotropic null vectors 332e>
 <Boost and rescale the vectors 333a>
 end function massless_isotropic_decay

Generate a xe^{-x} distribution for $q(\mathbf{k}, 0)$

332e *<Generate isotropic null vectors 332e>≡ (332d)*
 do k = 1, size (p, dim = 1)
 q(k,0) = - log (ran(k,1) * ran(k,2))
 cos_theta = 2 * ran(k,3) - 1
 sin_theta = sqrt (1 - cos_theta**2)
 phi = 2 * PI * ran(k,4)
 q(k,1) = q(k,0) * sin_theta * cos (phi)
 q(k,2) = q(k,0) * sin_theta * sin (phi)
 q(k,3) = q(k,0) * cos_theta
 enddo

The proof that the Jacobian of the transformation vanishes can be found in [26]. The transformation is really a Lorentz boost (as can be seen easily).

333a \langle Boost and rescale the vectors 333a $\rangle \equiv$ (332d)

```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
  r = dot (q(k,:), qsum) / qabs
  z = (q(k,0) + r) / (qsum(0) + qabs)
  p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
  p(k,0) = x * r
enddo
```

333b \langle Declaration of kinematics procedures 324b $\rangle + \equiv$ (324a) \triangleleft 332c

```
public :: phase_space_volume
```

$$V_n(s) = \frac{1}{8\pi} \frac{n-1}{(\Gamma(n))^2} \left(\frac{s}{16\pi^2} \right)^{n-2} \quad (\text{J.11})$$

333c \langle Implementation of kinematics procedures 325a $\rangle + \equiv$ (324a) \triangleleft 332d

```
pure function phase_space_volume (n, roots) result (volume)
  integer, intent(in) :: n
  real (kind=default), intent(in) :: roots
  real (kind=default) :: volume
  real (kind=default) :: nd
  nd = n
  volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

J.5 Tests

333d \langle ktest.f90 333d $\rangle \equiv$

```
program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default) :: &
    ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: t1_min, t1_max
  real(kind=default), dimension(5) :: r
  type(LIPS3) :: p
```

```

integer :: i
character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
ma = 1.0
mb = 1.0
m1 = 10.0
m2 = 20.0
m3 = 30.0
s = 100.0 ** 2
do i = 1, 10
  call tao_random_number (r)
  s2 = (r(1) * (sqrt (s) - m1) + (1 - r(1)) * (m2 + m3)) ** 2
  t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1 = r(2) * t1_max + (1 - r(2)) * t1_min
  phi = 2*PI * r(3)
  cos_theta3 = 2 * r(4) - 1
  phi3 = 2*PI * r(5)
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
  print fmt, "p1      = ", p%p(1,:)
  print fmt, "p2      = ", p%p(2,:)
  print fmt, "p3      = ", p%p(3,:)
  print fmt, "p1,2,3^2 = ", dot (p%p(1,:), p%p(1,)), &
    dot (p%p(2,:), p%p(2,)), dot (p%p(3,:), p%p(3,))
  print fmt, "sum(p)   = ", p%p(1,:) + p%p(2,:) + p%p(3,:)
  print fmt, "|J|     = ", p%jacobian
end do
end program ktest

```



Trivial check for typos, should be removed from the finalized program!

334 \langle Trivial ktest.f90 334 $\rangle \equiv$

```

program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default), dimension(0:3) :: p, q, p_prime, p0
  real(kind=default) :: m
  character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
  integer :: i

```

```

do i = 1, 5
  if (i == 1) then
    p = (/ 1.0_double, 0.0_double, 0.0_double, 0.0_double /)
    m = 1.0
  else
    call tao_random_number (p)
    m = sqrt (PI)
  end if
  call tao_random_number (q(1:3))
  q(0) = sqrt (m**2 + dot_product (q(1:3), q(1:3)))
  p_prime = boost_momentum (p, q)
  print fmt, "p    = ", p
  print fmt, "q    = ", q
  print fmt, "p'   = ", p_prime
  print fmt, "p^2  = ", dot (p, p)
  print fmt, "p'^2 = ", dot (p_prime, p_prime)
  if (dot (p, p) > 0.0) then
    p0 = boost_momentum (p, p)
    print fmt, "p0   = ", p0
    print fmt, "p0^2 = ", dot (p0, p0)
  end if
end do
end program ktest

```


—K—

COORDINATES

```

336  <coordinates.f90 336>≡
      ! coordinates.f90 --
      <Copyleft notice 1>
      module coordinates
        use kinds
        use constants, only: PI
        use specfun, only: gamma
        implicit none
        private
        <Declaration of coordinates procedures 337a>
      contains
        <Implementation of coordinates procedures 337b>
      end module coordinates

```

K.1 Angular Spherical Coordinates

$$\begin{aligned}
 x_n &= r \cos \theta_{n-2} \\
 x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
 &\dots \\
 x_3 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \cos \theta_1 \\
 x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \cos \phi \\
 x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \sin \phi
 \end{aligned} \tag{K.1}$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} (\sin \theta_i)^i \tag{K.2}$$

We can minimize the number of multiplications by computing the products

$$P_j = \prod_{i=j}^{n-2} \sin \theta_i \quad (\text{K.3})$$

Then

$$\begin{aligned} x_n &= r \cos \theta_{n-2} \\ x_{n-1} &= r P_{n-2} \cos \theta_{n-3} \\ &\dots \\ x_3 &= r P_2 \cos \theta_1 \\ x_2 &= r P_1 \cos \phi \\ x_1 &= r P_1 \sin \phi \end{aligned} \quad (\text{K.4})$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} P_i \quad (\text{K.5})$$

Note that $\theta_i \in [0, \pi]$ and $\phi \in [0, 2\pi]$ or $\phi \in [-\pi, \pi]$. Therefore $\sin \theta_i \geq 0$ and

$$\sin \theta_i = \sqrt{1 - \cos^2 \theta_i} \quad (\text{K.6})$$

which is not true for ϕ . Since `sqrt` is typically much faster than `sin` and `cos`, we use (K.6) where ever possible.

```

337a <Declaration of coordinates procedures 337a>≡ (336) 338c>
      public :: spherical_to_cartesian_2, &
               spherical_to_cartesian, spherical_to_cartesian_j

337b <Implementation of coordinates procedures 337b>≡ (336) 338a>
      pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(theta)) :: cos_theta
        real(kind=default), dimension(size(theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (theta) + 2
        cos_theta = cos (theta)
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
          product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do

```

```

if (present (x)) then
  x(1) = r * product_sin_theta(1) * sin (phi)
  x(2) = r * product_sin_theta(1) * cos (phi)
  x(3:) = r * product_sin_theta(2:n-1) * cos_theta
end if
if (present (jacobian)) then
  jacobian = r**(n-1) * product (product_sin_theta)
end if
end subroutine spherical_to_cartesian_2

```



Note that call inside of a function breaks F-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where `theta` could not be assumed shape ...

- 338a *<Implementation of coordinates procedures 337b>+≡ (336) <337b 338b>*
 pure function `spherical_to_cartesian` (r, phi, theta) result (x)
 real(kind=default), intent(in) :: r, phi
 real(kind=default), dimension(:), intent(in) :: theta
 real(kind=default), dimension(size(theta)+2) :: x
 call `spherical_to_cartesian_2` (r, phi, theta, x = x)
 end function `spherical_to_cartesian`
- 338b *<Implementation of coordinates procedures 337b>+≡ (336) <338a 338d>*
 pure function `spherical_to_cartesian_j` (r, phi, theta) &
 result (jacobian)
 real(kind=default), intent(in) :: r, phi
 real(kind=default), dimension(:), intent(in) :: theta
 real(kind=default) :: jacobian
 call `spherical_to_cartesian_2` (r, phi, theta, jacobian = jacobian)
 end function `spherical_to_cartesian_j`
- 338c *<Declaration of coordinates procedures 337a>+≡ (336) <337a 340c>*
 public :: `cartesian_to_spherical_2`, &
 `cartesian_to_spherical`, `cartesian_to_spherical_j`
- 338d *<Implementation of coordinates procedures 337b>+≡ (336) <338b 340a>*
 pure subroutine `cartesian_to_spherical_2` (x, r, phi, theta, jacobian)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), intent(out), optional :: r, phi
 real(kind=default), dimension(:), intent(out), optional :: theta
 real(kind=default), intent(out), optional :: jacobian
 real(kind=default) :: local_r
 real(kind=default), dimension(size(x)-2) :: cos_theta
 real(kind=default), dimension(size(x)-1) :: product_sin_theta

```

integer :: n, i
n = size (x)
local_r = sqrt (dot_product (x, x))
if (local_r == 0) then
  if (present (r)) then
    r = 0
  end if
  if (present (phi)) then
    phi = 0
  end if
  if (present (theta)) then
    theta = 0
  end if
  if (present (jacobian)) then
    jacobian = 1
  end if
else
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
    if (product_sin_theta(i-1) == 0) then
      cos_theta(i-2) = 0
    else
      cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    end if
    product_sin_theta(i-2) = &
      product_sin_theta(i-1) * sqrt (1 - cos_theta(i-2)**2)
  end do
  if (present (r)) then
    r = local_r
  end if
  if (present (phi)) then
    ! Set phi = 0 for vanishing vector
    if (x(1) == 0 .and. x(2)==0) then
      phi = 0
    else
      phi = atan2 (x(1), x(2))
    end if
  end if
  if (present (theta)) then
    theta = acos (cos_theta)
  end if
  if (present (jacobian)) then
    jacobian = local_r**(1-n) / product (product_sin_theta)
  end if
end if

```

```

        end if
    end if
end subroutine cartesian_to_spherical_2
340a  <Implementation of coordinates procedures 337b>+≡ (336) <338d 340b>
pure subroutine cartesian_to_spherical (x, r, phi, theta)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(out) :: r, phi
    real(kind=default), dimension(:), intent(out) :: theta
    call cartesian_to_spherical_2 (x, r, phi, theta)
end subroutine cartesian_to_spherical
340b  <Implementation of coordinates procedures 337b>+≡ (336) <340a 340d>
pure function cartesian_to_spherical_j (x) result (jacobian)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default) :: jacobian
    call cartesian_to_spherical_2 (x, jacobian = jacobian)
end function cartesian_to_spherical_j

```

K.2 Trigonometric Spherical Coordinates

```

340c  <Declaration of coordinates procedures 337a>+≡ (336) <338c 341c>
public :: spherical_cos_to_cartesian_2, &
        spherical_cos_to_cartesian, spherical_cos_to_cartesian_j

```

Using the cosine, we have to drop P_1 from the Jacobian

```

340d  <Implementation of coordinates procedures 337b>+≡ (336) <340b 341a>
pure subroutine spherical_cos_to_cartesian_2 (r, phi, cos_theta, x, jacobian)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: cos_theta
    real(kind=default), dimension(:), intent(out), optional :: x
    real(kind=default), intent(out), optional :: jacobian
    real(kind=default), dimension(size(cos_theta)+1) :: product_sin_theta
    integer :: n, i
    n = size (cos_theta) + 2
    product_sin_theta(n-1) = 1.0_default
    do i = n - 2, 1, -1
        product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
    end do
    if (present (x)) then
        x(1) = r * product_sin_theta(1) * sin (phi)
        x(2) = r * product_sin_theta(1) * cos (phi)
        x(3:) = r * product_sin_theta(2:n-1) * cos_theta
    end if
end subroutine spherical_cos_to_cartesian_2

```

```

        end if
        if (present (jacobian)) then
            jacobian = r**(n-1) * product (product_sin_theta(2:))
        end if
    end subroutine spherical_cos_to_cartesian_2
341a  <Implementation of coordinates procedures 337b>+≡ (336) <340d 341b>
    pure function spherical_cos_to_cartesian (r, phi, theta) result (x)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(size(theta)+2) :: x
        call spherical_cos_to_cartesian_2 (r, phi, theta, x = x)
    end function spherical_cos_to_cartesian
341b  <Implementation of coordinates procedures 337b>+≡ (336) <341a 341d>
    pure function spherical_cos_to_cartesian_j (r, phi, theta) &
        result (jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default) :: jacobian
        call spherical_cos_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
    end function spherical_cos_to_cartesian_j
341c  <Declaration of coordinates procedures 337a>+≡ (336) <340c 343b>
    public :: cartesian_to_spherical_cos_2, &
        cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
341d  <Implementation of coordinates procedures 337b>+≡ (336) <341b 342>
    pure subroutine cartesian_to_spherical_cos_2 (x, r, phi, cos_theta, jacobian)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out), optional :: r, phi
        real(kind=default), dimension(:), intent(out), optional :: cos_theta
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default) :: local_r
        real(kind=default), dimension(size(x)-2) :: local_cos_theta
        real(kind=default), dimension(size(x)-1) :: product_sin_theta
        integer :: n, i
        n = size (x)
        local_r = sqrt (dot_product (x, x))
        if (local_r == 0) then
            if (present (r)) then
                r = 0
            end if
            if (present (phi)) then
                phi = 0
            end if
        end if
    end subroutine

```

```

    if (present (cos_theta)) then
        cos_theta = 0
    end if
    if (present (jacobian)) then
        jacobian = 1
    end if
else
    product_sin_theta(n-1) = 1
    do i = n, 3, -1
        if (product_sin_theta(i-1) == 0) then
            local_cos_theta(i-2) = 0
        else
            local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
        end if
        product_sin_theta(i-2) = &
            product_sin_theta(i-1) * sqrt (1 - local_cos_theta(i-2)**2)
    end do
    if (present (r)) then
        r = local_r
    end if
    if (present (phi)) then
        ! Set phi = 0 for vanishing vector
        if (x(1) == 0 .and. x(2)==0) then
            phi = 0
        else
            phi = atan2 (x(1), x(2))
        end if
    end if
    if (present (cos_theta)) then
        cos_theta = local_cos_theta
    end if
    if (present (jacobian)) then
        jacobian = local_r**(1-n) / product (product_sin_theta(2:))
    end if
end if
end subroutine cartesian_to_spherical_cos_2
342  <Implementation of coordinates procedures 337b>+≡ (336) <341d 343a>
    pure subroutine cartesian_to_spherical_cos (x, r, phi, cos_theta)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out) :: r, phi
        real(kind=default), dimension(:), intent(out), optional :: cos_theta
        call cartesian_to_spherical_cos_2 (x, r, phi, cos_theta)
    end subroutine cartesian_to_spherical_cos

```

343a \langle Implementation of coordinates procedures 337b $\rangle + \equiv$ (336) \triangleleft 342 343c \triangleright

```

pure function cartesian_to_spherical_cos_j (x) result (jacobian)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: jacobian
  call cartesian_to_spherical_cos_2 (x, jacobian = jacobian)
end function cartesian_to_spherical_cos_j

```

K.3 Surface of a Sphere

343b \langle Declaration of coordinates procedures 337a $\rangle + \equiv$ (336) \triangleleft 341c

```

public :: surface

```

$$\int d\Omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)} = S_n \quad (\text{K.7})$$

343c \langle Implementation of coordinates procedures 337b $\rangle + \equiv$ (336) \triangleleft 343a

```

pure function surface (n) result (vol)
  integer, intent(in) :: n
  real(kind=default) :: vol
  real(kind=default) :: n_by_2
  n_by_2 = 0.5_default * n
  vol = 2 * PI**n_by_2 / gamma (n_by_2)
end function surface

```


—L—

IDIOMATIC FORTRAN90 INTERFACE FOR MPI

```

344a  <mpi90.f90 344a>≡
      ! mpi90.f90 --
      <Copyleft notice 1>
      module mpi90
        use kinds
        use mpi
        implicit none
        private
        <Declaration of mpi90 procedures 344b>
        <Interfaces of mpi90 procedures 347c>
        <Parameters in mpi90 (never defined)>
        <Variables in mpi90 (never defined)>
        <Declaration of mpi90 types 349b>
      contains
        <Implementation of mpi90 procedures 344c>
      end module mpi90

```

L.1 Basics

```

344b  <Declaration of mpi90 procedures 344b>≡                                     (344a) 347b▷
      public :: mpi90_init
      public :: mpi90_finalize
      public :: mpi90_abort
      public :: mpi90_print_error
      public :: mpi90_size
      public :: mpi90_rank

344c  <Implementation of mpi90 procedures 344c>≡                               (344a) 345c▷
      subroutine mpi90_init (error)

```

```

integer, intent(out), optional :: error
integer :: local_error
character(len=*), parameter :: FN = "mpi90_init"
external mpi_init
call mpi_init (local_error)
<Handle local_error (no mpi90_abort) 345a>
end subroutine mpi90_init

345a <Handle local_error (no mpi90_abort) 345a>≡ (344c 345d)
    if (present (error)) then
        error = local_error
    else
        if (local_error /= MPI_SUCCESS) then
            call mpi90_print_error (local_error, FN)
            stop
        end if
    end if

345b <Handle local_error 345b>≡ (345-48 350c 352d 353b 355a)
    if (present (error)) then
        error = local_error
    else
        if (local_error /= MPI_SUCCESS) then
            call mpi90_print_error (local_error, FN)
            call mpi90_abort (local_error)
            stop
        end if
    end if

345c <Implementation of mpi90 procedures 344c>+≡ (344a) <344c 345d>
    subroutine mpi90_finalize (error)
        integer, intent(out), optional :: error
        integer :: local_error
        character(len=*), parameter :: FN = "mpi90_finalize"
        external mpi_finalize
        call mpi_finalize (local_error)
        <Handle local_error 345b>
    end subroutine mpi90_finalize

345d <Implementation of mpi90 procedures 344c>+≡ (344a) <345c 346a>
    subroutine mpi90_abort (code, domain, error)
        integer, intent(in), optional :: code, domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_abort"
        integer :: local_domain, local_code, local_error
        external mpi_abort

```

```

    if (present (code)) then
        local_code = code
    else
        local_code = MPI_ERR_UNKNOWN
    end if
    <Set default for domain 346b>
    call mpi_abort (local_domain, local_code, local_error)
    <Handle local_error (no mpi90_abort) 345a>
end subroutine mpi90_abort

346a <Implementation of mpi90 procedures 344c>+≡ (344a) <345d 346c>
subroutine mpi90_print_error (error, msg)
    integer, intent(in) :: error
    character(len=*), optional :: msg
    character(len=*), parameter :: FN = "mpi90_print_error"
    integer :: msg_len, local_error
    external mpi_error_string
    call mpi_error_string (error, msg, msg_len, local_error)
    if (local_error /= MPI_SUCCESS) then
        print *, "PANIC: even MPI_ERROR_STRING() failed!!!"
        call mpi90_abort (local_error)
    else if (present (msg)) then
        print *, trim (msg), ": ", trim (msg(msg_len+1:))
    else
        print *, "mpi90: ", trim (msg(msg_len+1:))
    end if
end subroutine mpi90_print_error

346b <Set default for domain 346b>≡ (345-49 355a) 353f>
    if (present (domain)) then
        local_domain = domain
    else
        local_domain = MPI_COMM_WORLD
    end if

346c <Implementation of mpi90 procedures 344c>+≡ (344a) <346a 347a>
subroutine mpi90_size (sz, domain, error)
    integer, intent(out) :: sz
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_size"
    integer :: local_domain, local_error
    external mpi_comm_size
    <Set default for domain 346b>
    call mpi_comm_size (local_domain, sz, local_error)

```

```

    <Handle local_error 345b>
end subroutine mpi90_size
347a <Implementation of mpi90 procedures 344c>+≡ (344a) <346c 347d>
    subroutine mpi90_rank (rank, domain, error)
        integer, intent(out) :: rank
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_rank"
        integer :: local_domain, local_error
        external mpi_comm_rank
        <Set default for domain 346b>
        call mpi_comm_rank (local_domain, rank, local_error)
        <Handle local_error 345b>
    end subroutine mpi90_rank

```

L.2 Point to Point

```

347b <Declaration of mpi90 procedures 344b>+≡ (344a) <344b 350d>
    public :: mpi90_send
    public :: mpi90_receive
    public :: mpi90_receive_pointer
347c <Interfaces of mpi90 procedures 347c>≡ (344a) 349d>
    interface mpi90_send
        module procedure &
            mpi90_send_integer, mpi90_send_double, &
            mpi90_send_integer_array, mpi90_send_double_array, &
            mpi90_send_integer_array2, mpi90_send_double_array2
    end interface
347d <Implementation of mpi90 procedures 344c>+≡ (344a) <347a 347e>
    subroutine mpi90_send_integer (value, target, tag, domain, error)
        integer, intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        call mpi90_send_integer_array ((/ value /), target, tag, domain, error)
    end subroutine mpi90_send_integer
347e <Implementation of mpi90 procedures 344c>+≡ (344a) <347d 348a>
    subroutine mpi90_send_double (value, target, tag, domain, error)
        real(kind=default), intent(in) :: value
        integer, intent(in) :: target, tag

```

```

integer, intent(in), optional :: domain
integer, intent(out), optional :: error
call mpi90_send_double_array (/ value /), target, tag, domain, error)
end subroutine mpi90_send_double

348a <Implementation of mpi90 procedures 344c>+≡ (344a) <347e 348c>
subroutine mpi90_send_integer_array (buffer, target, tag, domain, error)
integer, dimension(:), intent(in) :: buffer
integer, intent(in) :: target, tag
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_send_integer_array"
integer, parameter :: datatype = MPI_INTEGER
<Body of mpi90_send.*_array 348b>
end subroutine mpi90_send_integer_array

348b <Body of mpi90_send.*_array 348b>≡ (348)
integer :: local_domain, local_error
external mpi_send
<Set default for domain 346b>
call mpi_send (buffer, size (buffer), datatype, target, tag, &
               local_domain, local_error)
<Handle local_error 345b>

348c <Implementation of mpi90 procedures 344c>+≡ (344a) <348a 348d>
subroutine mpi90_send_double_array (buffer, target, tag, domain, error)
real(kind=default), dimension(:), intent(in) :: buffer
integer, intent(in) :: target, tag
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_send_double_array"
integer, parameter :: datatype = MPI_DOUBLE_PRECISION
<Body of mpi90_send.*_array 348b>
end subroutine mpi90_send_double_array

348d <Implementation of mpi90 procedures 344c>+≡ (344a) <348c 349a>
subroutine mpi90_send_integer_array2 (value, target, tag, domain, error)
integer, dimension(:, :), intent(in) :: value
integer, intent(in) :: target, tag
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
integer, dimension(size(value)) :: buffer
buffer = reshape (value, shape(buffer))
call mpi90_send_integer_array (buffer, target, tag, domain, error)
end subroutine mpi90_send_integer_array2

```

349a *<Implementation of mpi90 procedures 344c>+≡* (344a) *<348d 349c>*
`subroutine mpi90_send_double_array2 (value, target, tag, domain, error)`
`real(kind=default), dimension(:,,:), intent(in) :: value`
`integer, intent(in) :: target, tag`
`integer, intent(in), optional :: domain`
`integer, intent(out), optional :: error`
`real(kind=default), dimension(size(value)) :: buffer`
`buffer = reshape (value, shape(buffer))`
`call mpi90_send_double_array (buffer, target, tag, domain, error)`
`end subroutine mpi90_send_double_array2`

349b *<Declaration of mpi90 types 349b>≡* (344a)
`type, public :: mpi90_status`
`integer :: count, source, tag, error`
`end type mpi90_status`

349c *<Implementation of mpi90 procedures 344c>+≡* (344a) *<349a 350a>*
`subroutine mpi90_receive_integer (value, source, tag, domain, status, error)`
`integer, intent(out) :: value`
`integer, intent(in), optional :: source, tag, domain`
`type(mpi90_status), intent(out), optional :: status`
`integer, intent(out), optional :: error`
`integer, dimension(1) :: buffer`
`call mpi90_receive_integer_array (buffer, source, tag, domain, status, error)`
`value = buffer(1)`
`end subroutine mpi90_receive_integer`

349d *<Interfaces of mpi90 procedures 347c>+≡* (344a) *<347c 352a>*
`interface mpi90_receive`
`module procedure &`
`mpi90_receive_integer, mpi90_receive_double, &`
`mpi90_receive_integer_array, mpi90_receive_double_array, &`
`mpi90_receive_integer_array2, mpi90_receive_double_array2`
`end interface`

349e *<Set defaults for source, tag and domain 349e>≡* (350c 352c)
`if (present (source)) then`
`local_source = source`
`else`
`local_source = MPI_ANY_SOURCE`
`end if`
`if (present (tag)) then`
`local_tag = tag`
`else`
`local_tag = MPI_ANY_TAG`
`end if`

<Set default for domain 346b>

- 350a *<Implementation of mpi90 procedures 344c>+≡* (344a) *<349c 350b>*
 subroutine mpi90_receive_double (value, source, tag, domain, status, error)
 real(kind=default), intent(out) :: value
 integer, intent(in), optional :: source, tag, domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 real(kind=default), dimension(1) :: buffer
 call mpi90_receive_double_array (buffer, source, tag, domain, status, error)
 value = buffer(1)
 end subroutine mpi90_receive_double
- 350b *<Implementation of mpi90 procedures 344c>+≡* (344a) *<350a 350e>*
 subroutine mpi90_receive_integer_array &
 (buffer, source, tag, domain, status, error)
 integer, dimension(:), intent(out) :: buffer
 integer, intent(in), optional :: source, tag, domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 character(len=*), parameter :: FN = "mpi90_receive_integer_array"
 integer, parameter :: datatype = MPI_INTEGER
 <Body of mpi90_receive_.array 350c>*
 end subroutine mpi90_receive_integer_array
- 350c *<Body of mpi90_receive_*.array 350c>≡* (350b 351a)
 integer :: local_source, local_tag, local_domain, local_error
 integer, dimension(MPI_STATUS_SIZE) :: local_status
 external mpi_receive, mpi_get_count
 <Set defaults for source, tag and domain 349e>
 call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
 local_domain, local_status, local_error)
 <Handle local_error 345b>
 if (present (status)) then
 call **decode_status** (status, local_status, datatype)
 end if
- 350d *<Declaration of mpi90 procedures 344b>+≡* (344a) *<347b 353d>*
 private :: **decode_status**



Can we ignore ierror???

- 350e *<Implementation of mpi90 procedures 344c>+≡* (344a) *<350b 351a>*
 subroutine decode_status (status, mpi_status, datatype)
 type(mpi90_status), intent(out) :: status
 integer, dimension(:), intent(in) :: mpi_status

```

integer, intent(in), optional :: datatype
integer :: ierror
if (present (datatype)) then
    call mpi_get_count (mpi_status, datatype, status%count, ierror)
else
    status%count = 0
end if
status%source = mpi_status(MPI_SOURCE)
status%tag = mpi_status(MPI_TAG)
status%error = mpi_status(MPI_ERROR)
end subroutine decode_status

```

351a *<Implementation of mpi90 procedures 344c>+≡* (344a) *<350e 351b>*

```

subroutine mpi90_receive_double_array &
    (buffer, source, tag, domain, status, error)
real(kind=default), dimension(:), intent(out) :: buffer
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_receive_double_array"
integer, parameter :: datatype = MPI_DOUBLE_PRECISION
<Body of mpi90_receive.*_array 350c>
end subroutine mpi90_receive_double_array

```

351b *<Implementation of mpi90 procedures 344c>+≡* (344a) *<351a 351c>*

```

subroutine mpi90_receive_integer_array2 &
    (value, source, tag, domain, status, error)
integer, dimension(:, :), intent(out) :: value
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
integer, dimension(size(value)) :: buffer
call mpi90_receive_integer_array &
    (buffer, source, tag, domain, status, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_receive_integer_array2

```

351c *<Implementation of mpi90 procedures 344c>+≡* (344a) *<351b 352b>*

```

subroutine mpi90_receive_double_array2 &
    (value, source, tag, domain, status, error)
real(kind=default), dimension(:, :), intent(out) :: value
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
real(kind=default), dimension(size(value)) :: buffer


```



```

        call mpi90_receive_double_array &
            (buffer, source, tag, domain, status, error)
        value = reshape (buffer, shape(value))
    end subroutine mpi90_receive_double_array2
352a  <Interfaces of mpi90 procedures 347c>+≡ (344a) <349d 353e>
        interface mpi90_receive_pointer
            module procedure &
                mpi90_receive_integer_pointer, mpi90_receive_double_pointer
        end interface
352b  <Implementation of mpi90 procedures 344c>+≡ (344a) <351c 353c>
        subroutine mpi90_receive_integer_pointer &
            (buffer, source, tag, domain, status, error)
            integer, dimension(:), pointer :: buffer
            integer, intent(in), optional :: source, tag, domain
            type(mpi90_status), intent(out), optional :: status
            integer, intent(out), optional :: error
            character(len=*), parameter :: FN = "mpi90_receive_integer_pointer"
            integer, parameter :: datatype = MPI_INTEGER
            <Body of mpi90_receive_*.pointer 352c>
        end subroutine mpi90_receive_integer_pointer
352c  <Body of mpi90_receive_*.pointer 352c>≡ (352b 353c) 352d>
        integer :: local_source, local_tag, local_domain, local_error, buffer_size
        integer, dimension(MPI_STATUS_SIZE) :: local_status
        integer :: ierror
        external mpi_receive, mpi_get_count
        <Set defaults for source, tag and domain 349e>
352d  <Body of mpi90_receive_*.pointer 352c>+≡ (352b 353c) <352c 352e>
        call mpi_probe (local_source, local_tag, local_domain, &
            local_status, local_error)
        <Handle local_error 345b>

```

 Can we ignore ierror???

```

352e  <Body of mpi90_receive_*.pointer 352c>+≡ (352b 353c) <352d 353a>
        call mpi_get_count (local_status, datatype, buffer_size, ierror)
        if (associated (buffer)) then
            if (size (buffer) /= buffer_size) then
                deallocate (buffer)
                allocate (buffer(buffer_size))
            end if
        else
            allocate (buffer(buffer_size))
        end if

```

353a *<Body of mpi90_receive_*_pointer 352c>+≡* (352b 353c) *<352e 353b>*
 call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
 local_domain, local_status, local_error)

353b *<Body of mpi90_receive_*_pointer 352c>+≡* (352b 353c) *<353a*
 <Handle local_error 345b>
 if (present (status)) then
 call decode_status (status, local_status, datatype)
 end if

353c *<Implementation of mpi90 procedures 344c>+≡* (344a) *<352b 354a>*
 subroutine mpi90_receive_double_pointer &
 (buffer, source, tag, domain, status, error)
 real(kind=default), dimension(:), pointer :: buffer
 integer, intent(in), optional :: source, tag, domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 character(len=*), parameter :: FN = "mpi90_receive_double_pointer"
 integer, parameter :: datatype = MPI_DOUBLE_PRECISION
 *<Body of mpi90_receive_*_pointer 352c>*
 end subroutine mpi90_receive_double_pointer

L.3 Collective Communication

353d *<Declaration of mpi90 procedures 344b>+≡* (344a) *<350d*
 public :: mpi90_broadcast

353e *<Interfaces of mpi90 procedures 347c>+≡* (344a) *<352a*
 interface mpi90_broadcast
 module procedure &
 mpi90_broadcast_integer, mpi90_broadcast_integer_array, &
 mpi90_broadcast_integer_array2, mpi90_broadcast_integer_array3, &
 mpi90_broadcast_double, mpi90_broadcast_double_array, &
 mpi90_broadcast_double_array2, mpi90_broadcast_double_array3, &
 mpi90_broadcast_logical, mpi90_broadcast_logical_array, &
 mpi90_broadcast_logical_array2, mpi90_broadcast_logical_array3
 end interface

353f *<Set default for domain 346b>+≡* (345–49 355a) *<346b*
 if (present (domain)) then
 local_domain = domain
 else
 local_domain = MPI_COMM_WORLD
 end if

```

354a  <Implementation of mpi90 procedures 344c>+≡ (344a) <353c 354b>
      subroutine mpi90_broadcast_integer (value, root, domain, error)
        integer, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_integer_array (buffer, root, domain, error)
        value = buffer(1)
      end subroutine mpi90_broadcast_integer

354b  <Implementation of mpi90 procedures 344c>+≡ (344a) <354a 354c>
      subroutine mpi90_broadcast_double (value, root, domain, error)
        real(kind=default), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_double_array (buffer, root, domain, error)
        value = buffer(1)
      end subroutine mpi90_broadcast_double

354c  <Implementation of mpi90 procedures 344c>+≡ (344a) <354b 354d>
      subroutine mpi90_broadcast_logical (value, root, domain, error)
        logical, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        logical, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_logical_array (buffer, root, domain, error)
        value = buffer(1)
      end subroutine mpi90_broadcast_logical

354d  <Implementation of mpi90 procedures 344c>+≡ (344a) <354c 355b>
      subroutine mpi90_broadcast_integer_array (buffer, root, domain, error)
        integer, dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_broadcast_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_broadcast.*_array 355a>

```

```

        end subroutine mpi90_broadcast_integer_array

355a  <Body of mpi90_broadcast_*.array 355a>≡ (354 355)
        integer :: local_domain, local_error
        external mpi_bcast
        <Set default for domain 346b>
        call mpi_bcast (buffer, size (buffer), datatype, root, &
                        local_domain, local_error)
        <Handle local_error 345b>

355b  <Implementation of mpi90 procedures 344c>+≡ (344a) <354d 355c>
        subroutine mpi90_broadcast_double_array (buffer, root, domain, error)
            real(kind=default), dimension(:), intent(inout) :: buffer
            integer, intent(in) :: root
            integer, intent(in), optional :: domain
            integer, intent(out), optional :: error
            integer, parameter :: datatype = MPI_DOUBLE_PRECISION
            character(len=*), parameter :: FN = "mpi90_broadcast_double_array"
            <Body of mpi90_broadcast_*.array 355a>
        end subroutine mpi90_broadcast_double_array

355c  <Implementation of mpi90 procedures 344c>+≡ (344a) <355b 355d>
        subroutine mpi90_broadcast_logical_array (buffer, root, domain, error)
            logical, dimension(:), intent(inout) :: buffer
            integer, intent(in) :: root
            integer, intent(in), optional :: domain
            integer, intent(out), optional :: error
            integer, parameter :: datatype = MPI_LOGICAL
            character(len=*), parameter :: FN = "mpi90_broadcast_logical_array"
            <Body of mpi90_broadcast_*.array 355a>
        end subroutine mpi90_broadcast_logical_array

355d  <Implementation of mpi90 procedures 344c>+≡ (344a) <355c 355e>
        subroutine mpi90_broadcast_integer_array2 (value, root, domain, error)
            integer, dimension(:, :), intent(inout) :: value
            integer, intent(in) :: root
            integer, intent(in), optional :: domain
            integer, intent(out), optional :: error
            integer, dimension(size(value)) :: buffer
            buffer = reshape (value, shape(buffer))
            call mpi90_broadcast_integer_array (buffer, root, domain, error)
            value = reshape (buffer, shape(value))
        end subroutine mpi90_broadcast_integer_array2

355e  <Implementation of mpi90 procedures 344c>+≡ (344a) <355d 356a>
        subroutine mpi90_broadcast_double_array2 (value, root, domain, error)

```

```

real(kind=default), dimension(:,:), intent(inout) :: value
integer, intent(in) :: root
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
real(kind=default), dimension(size(value)) :: buffer
buffer = reshape (value, shape(buffer))
call mpi90_broadcast_double_array (buffer, root, domain, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_double_array2
356a <Implementation of mpi90 procedures 344c>+≡ (344a) <355e 356b>
subroutine mpi90_broadcast_logical_array2 (value, root, domain, error)
logical, dimension(:,:), intent(inout) :: value
integer, intent(in) :: root
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
logical, dimension(size(value)) :: buffer
buffer = reshape (value, shape(buffer))
call mpi90_broadcast_logical_array (buffer, root, domain, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_logical_array2
356b <Implementation of mpi90 procedures 344c>+≡ (344a) <356a 356c>
subroutine mpi90_broadcast_integer_array3 (value, root, domain, error)
integer, dimension(:,:,:), intent(inout) :: value
integer, intent(in) :: root
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
integer, dimension(size(value)) :: buffer
buffer = reshape (value, shape(buffer))
call mpi90_broadcast_integer_array (buffer, root, domain, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_integer_array3
356c <Implementation of mpi90 procedures 344c>+≡ (344a) <356b 357>
subroutine mpi90_broadcast_double_array3 (value, root, domain, error)
real(kind=default), dimension(:,:,:), intent(inout) :: value
integer, intent(in) :: root
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
real(kind=default), dimension(size(value)) :: buffer
buffer = reshape (value, shape(buffer))
call mpi90_broadcast_double_array (buffer, root, domain, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_double_array3

```

357 *⟨Implementation of mpi90 procedures 344c⟩+≡* (344a) *◁356c*

```

subroutine mpi90_broadcast_logical_array3 (value, root, domain, error)
  logical, dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  logical, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_logical_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_logical_array3

```

—M— IDEAS

M.1 Toolbox for Interactive Optimization

Idea: Provide a OpenGL interface to visualize the grid optimization.

Motivation: Would help multi channel developers.

Implementation: Coding is straightforward, but interface design is hard.

M.2 Partially Non-Factorized Importance Sampling

Idea: Allow non-factorized grid optimization in two- or three-dimensional subspaces.

Motivation: Handle nastiest subspaces. Non-factorized approaches are impossible in higher than three dimensions (and probably only realistic in two dimensions), but there are cases that are best handled by including non-factorized optimization in two dimensions.

Implementation: The problem is that the present `vamp_sample_grid0` can't accomodate this, because other auxiliary information has to be collected, but a generalization is straightforward. Work has to start from an extended `divisions` module.

M.3 Correlated Importance Sampling (?)

Idea: Is it possible to include *some* correlations in a mainly factorized context?

Motivation: Would be nice ...

Implementation: First, I have to think about the maths ...

M.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region)

Idea: Solve **vegas**' nastiest problem by finding the direction(s) along which singularities are aligned.

Motivation: Automatically choose proper coordinate system in generator generators and separate wild and smooth directions.

Implementation: Diagonalize the covariance matrix $\text{cov}(x_i x_j)$ to find better axes. Caveats:

- damp rotations (rotate only if eigenvalues are spread out sufficiently).
- be careful about blow up of the integration volume, which is $V' = V d^{d/2}$ in the worst case for hypercubes and can be even worse for stretched cubes. (An adaptive grid can help, since we will have more smooth directions!)

Maybe try non-linear transformations as well.

M.5 Automagic Multi Channel

Idea: Find and extract one singularity after the other.

Motivation: Obvious.

Implementation: Either use multiple of **vegas**' $p(x)$ for importance sampling. Or find hot region(s) and split the integration region (à la signal/background).

—N—

CROSS REFERENCES

N.1 Identifiers

abs_evec: [128b](#), [128c](#), [128d](#), [129a](#), [130a](#), [130b](#)
 accuracy: [94c](#), [96b](#), [103b](#), [120b](#), [140c](#), [141a](#), [142b](#), [169d](#), [175c](#), [179d](#)
 adaptive_division: [56b](#), [57d](#)
 average: [108c](#), [110](#), [134a](#), [291b](#), [291c](#), [292a](#), [292d](#), [292e](#)
 avg_chi2: [94c](#), [95a](#), [96a](#), [103b](#), [106a](#), [107b](#), [108c](#), [110](#), [120b](#), [123b](#), [125a](#),
[140c](#), [141a](#), [142b](#), [161b](#), [162b](#), [166a](#), [169d](#), [175c](#), [179c](#)
 boost_many_momentum: [324b](#), [324c](#), [326a](#)
 boost_many_velocity: [324b](#), [324c](#), [325b](#), [326a](#)
 boost_momentum: [228f](#), [324b](#), [324c](#), [328c](#), [328d](#), [334](#)
 boost_one_momentum: [324b](#), [324c](#), [325c](#)
 boost_one_velocity: [324b](#), [324c](#), [325a](#), [325b](#)
 boost_velocity: [324b](#), [324c](#), [325c](#)
 buffer_end: [261b](#), [261d](#), [262b](#), [262d](#), [264e](#), [266b](#), [266c](#), [270c](#), [271b](#), [272a](#),
[272c](#), [274b](#), [275c](#), [275d](#), [275e](#), [276a](#), [276b](#), [277a](#), [277b](#), [277d](#), [277e](#), [278a](#),
[278b](#), [278c](#), [278d](#), [279a](#), [279b](#), [281f](#), [282a](#)
 BUFFER_SIZE: [58d](#), [59a](#), [108c](#), [109a](#), [109b](#), [110](#), [266b](#)
 calls: [24d](#), [76a](#), [83](#), [84a](#), [88b](#), [98c](#), [100c](#), [106a](#), [106e](#), [107a](#), [107b](#), [108c](#), [110](#),
[125a](#), [135d](#), [140c](#), [141a](#), [142b](#), [144b](#), [146b](#), [151b](#), [153](#), [157d](#), [160](#), [161b](#),
[162b](#), [163](#), [166a](#), [239](#), [242a](#), [242b](#), [243](#), [244](#)
 calls_per_cell: [76a](#), [83](#), [84a](#), [87d](#), [89b](#), [97b](#), [98c](#), [98d](#), [144b](#), [146b](#), [151b](#),
[153](#), [157d](#), [160](#), [163](#)
 cartesian_to_spherical: [338c](#), [340a](#)
 cartesian_to_spherical_2: [338c](#), [338d](#), [340a](#), [340b](#)
 cartesian_to_spherical_cos: [195a](#), [341c](#), [342](#)
 cartesian_to_spherical_cos_2: [197b](#), [341c](#), [341d](#), [342](#), [343a](#)
 cartesian_to_spherical_cos_j: [195b](#), [341c](#), [343a](#)
 cartesian_to_spherical_j: [338c](#), [340b](#)

cell: [43b](#), [86b](#), [87a](#), [87c](#), [87e](#)
 check_inverses: [196c](#), [197a](#), [200c](#)
 check_inverses3: [196c](#), [197b](#), [200c](#)
 check_jacobians: [196c](#), [196d](#), [200c](#), [211c](#), [211d](#), [218e](#)
 check_kinematics: [234b](#), [234c](#), [239](#)
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