

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

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Abstract

We present a 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.

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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

— 1 —

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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```

---

<sup>1</sup>Fully functional versions conforming to preceding 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  $\phi$  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  $\phi^{-1}$ :

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

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.

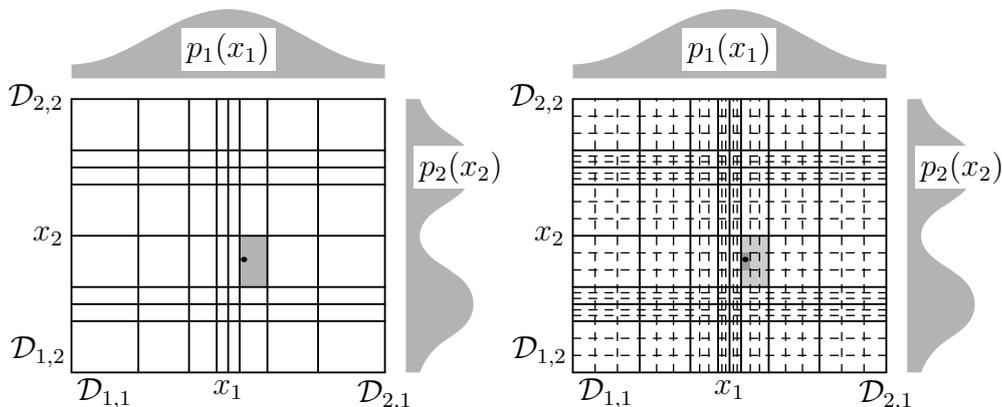


Figure 2.1: **vegas** grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions  $p_{1,2}$  are only in qualitative agreement.

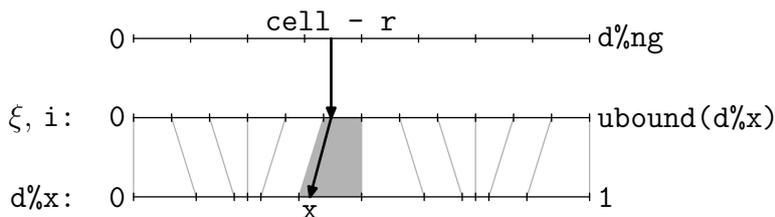


Figure 2.2: One-dimensional illustration of the **vegas** grid structure for pseudo stratified sampling, which is used in high dimensions.

## 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  $\pi$  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  $\mu_n$  may be used in the estimation of  $\mu'_n$ , 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  $\sigma$ .

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  $\phi$  is a forking operation and  $\iota$  is a joining operation, we are faced with the technical problem of a parallel random number source  $\rho$ . As made explicit in (2.18),  $S_0$  changes the state of the random number general  $\rho$ , demanding *identical* results therefore imposes a strict ordering on the operations and defeats parallelization. It is possible to devise implementations of  $S_0$  and  $\rho$  that circumvent this problem by distributing subsequences of  $\rho$  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 generator <sup>1</sup> Below, we will therefore use the notation  $x \approx y$  for “equal for an appropriate finite reordering of the  $\rho$  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  $\rho_i$  are statistically independent. This leaves us with  $G$  and  $a$  and we have to discuss importance sampling and stratified sampling separately.

---

<sup>1</sup>Arbitrary 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

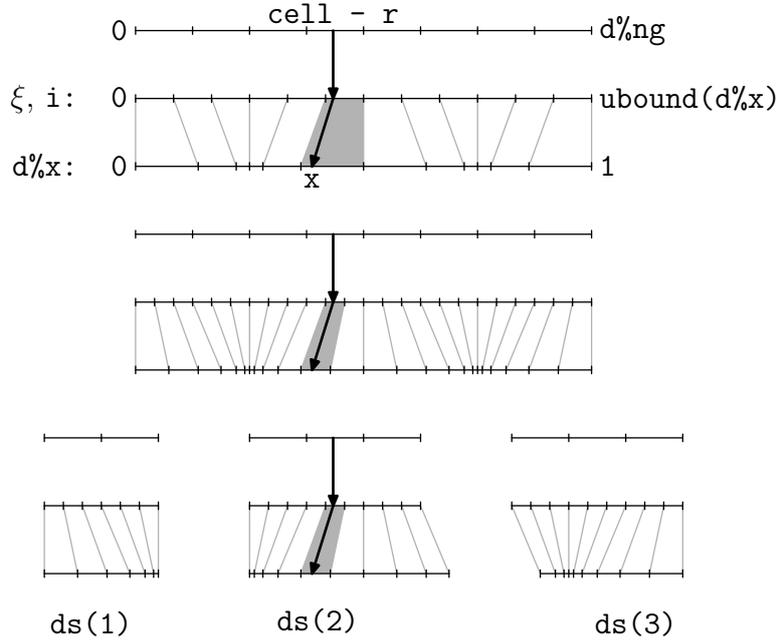


Figure 2.3: Forking one dimension  $d$  of a grid into three parts  $ds(1)$ ,  $ds(2)$ , and  $ds(3)$ . The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 2.2).

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,<sup>2</sup> 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-

<sup>2</sup>The coarsest grid covering the division of  $n_g$  bins into  $n_f$  forks has  $n_g / \text{gcd}(n_f, n_g) = \text{lcm}(n_f, n_g) / n_f$  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 <Serial implementation of $S_n = S_0(rS_0)^n$ 14>≡
 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
 <Interface declaration for func 22>
 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 *Parallel implementation of  $S_n = S_0(rS_0)^n$  (MPI) 17*≡

```

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
 Interface declaration for func 22
 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 86c 94d 104 113–15 120b 135d 137 139–42 170 176 182 183)

```
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
<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 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  $\chi^2$  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 χ^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 *<Interface declaration for phi 31a>*≡ (113-16 137 183a)

```
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 *<Interface declaration for ihp 31b>*≡ (113c)

```
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 *<Interface declaration for jacobian 31c>*≡ (113c 114a)

```
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,
 weightsl, 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 (... , [, ...])
```

## IMPLEMENTATION

### 5.1 *The Abstract Datatype `division`*

```

37a <divisions.f90 37a>≡
 ! divisions.f90 --
 <Copleft 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 61b>
 <Variables in divisions 46a>
 <Declaration of divisions types 37b>
 <Constants in divisions 65a>
 character(len=*), public, parameter :: DIVISIONS_RCS_ID = &
 "$Id: divisions.nw 314 2010-04-17 20:32:33Z ohl $"
 contains
 <Implementation of divisions procedures 38b>
 end module divisions

```



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

```

37b <Declaration of divisions types 37b>≡ (37a) 58a▷
 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  $0 < cell \cdot dxg < n_{div}$

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  $n_{\text{div}}$  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

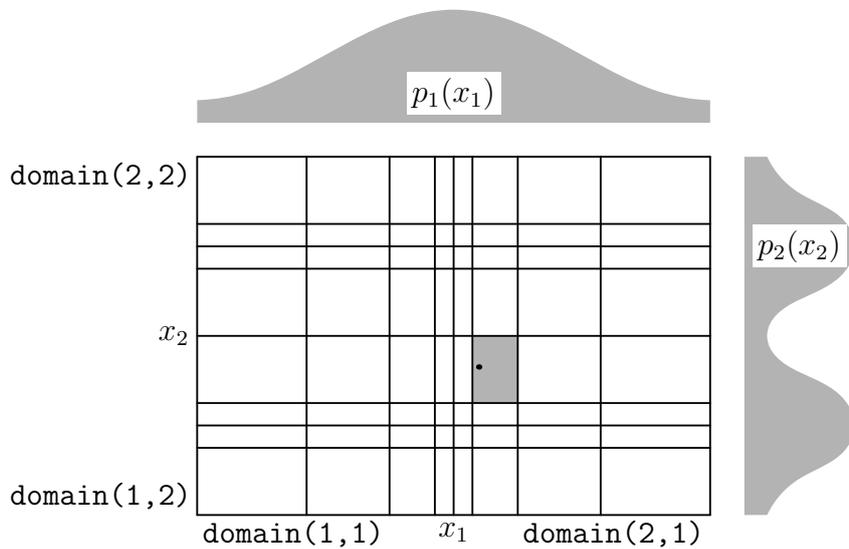


Figure 5.1: vegas grid structure for non-stratified sampling. N.B.: the grid and the weight functions  $p_{1,2}$  are only in qualitative agreement.

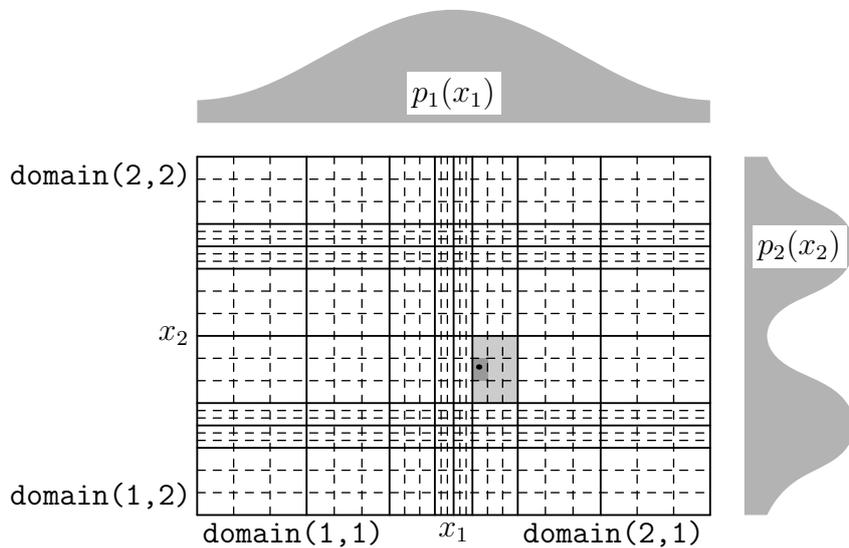


Figure 5.2: vegas grid structure for genuinely stratified sampling, which is used in low dimensions. N.B.: the grid and the weight functions  $p_{1,2}$  are only in qualitative agreement.

| $n_{\text{dim}}$ | $N_{\text{calls}}^{\text{max}}(n_g = 25)$ |
|------------------|-------------------------------------------|
| 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.

the contribution to the error is largest, but to use importance sampling, 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  $n_{\text{div}}$  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  $n_{\text{div}}$

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

```

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

```

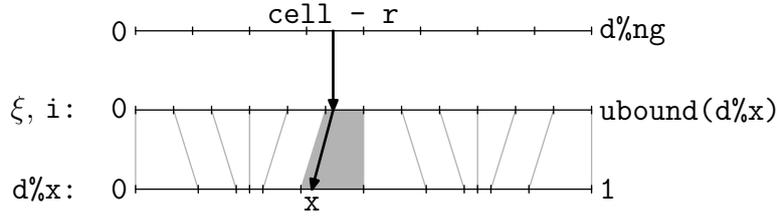


Figure 5.3: One-dimensional illustration of the vegas grid structure for pseudo stratified sampling, which is used in high dimensions.

```

 d%ng = equ_per_adap * num_div
 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  $N_{\text{calls}}$  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 <Set i, delta\_x, x, and wgt from xi 44a>≡ (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 <Implementation of divisions procedures 38b>+≡ (37a) <43b 44d>

```

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
 <Set i, delta_x, x, and wgt from xi 44a>
 idx = i
end subroutine inject_division_short

```

### 5.1.2 Grid Refinement

44c <Declaration of divisions procedures 38a>+≡ (37a) <43a 45d>

```

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

```

44d <Implementation of divisions procedures 38b>+≡ (37a) <44b 45a>

```

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

```

- 45a *<Implementation of divisions procedures 38b>+≡ (37a) <44d 45c>*  
 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
- 45b *<Implementation of divisions procedures (removed from WHIZARD) 45b>≡ 60d>*  
 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
- 45c *<Implementation of divisions procedures 38b>+≡ (37a) <45a 45e>*  
 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
- 45d *<Declaration of divisions procedures 38a>+≡ (37a) <44c 47a>*  
 public :: refine\_division
- 45e *<Implementation of divisions procedures 38b>+≡ (37a) <45c 46b>*  
 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`  $\geq 6$ , we know that `num_div`  $\geq 3$ .

46a *<Variables in divisions 46a>*  $\equiv$  (37a) 60a >  
`integer, private, parameter :: MIN_NUM_DIV = 3`

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

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

46b *<Implementation of divisions procedures 38b>*  $\equiv$  (37a) <45e 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`

---

<sup>1</sup>Some old timers call this a feature, however.

```

 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

```

47a  $\langle$ Declaration of divisions procedures 38a $\rangle + \equiv$  (37a)  $\langle$ 45d 48a $\rangle$   
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)  $\langle$ 46b 48e $\rangle$   
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  $\delta$  48b $\rangle$   
         $\langle$ Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c $\rangle$   
    end do  
    x\_new(num\_div) = 1.0  
end function rebin

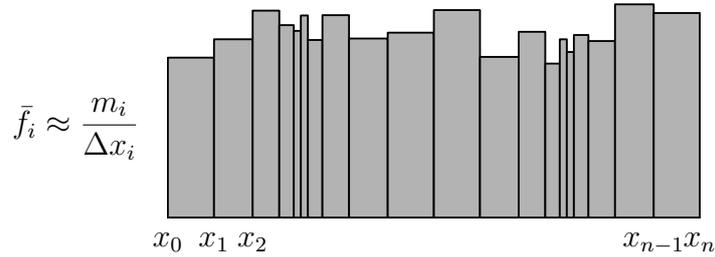


Figure 5.4: Typical weights used in the rebinning algorithm.

48a *<Declaration of divisions procedures 38a>+≡* (37a) *<47a 48d>*  
`private :: rebin`

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

48b *<Increment k until  $\sum m_k \geq \Delta$  and keep the surplus in  $\delta$  48b>≡* (47c)  
`do`  
`if (step <= delta) then`  
`exit`  
`end if`  
`k = k + 1`  
`delta = delta + m(k)`  
`end do`  
`delta = delta - step`

48c *<Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c>≡* (47c)  
`x_new(i) = x(k) - (x(k) - x(k-1)) * delta / m(k)`

### 5.1.3 Probability Density

48d *<Declaration of divisions procedures 38a>+≡* (37a) *<48a 49a>*  
`public :: probability`

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

and

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

48e *<Implementation of divisions procedures 38b>+≡* (37a) *<47c 49b>*  
`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) <48d 49c>*

```
public :: quadrupole_division
```

49b *<Implementation of divisions procedures 38b>+≡ (37a) <48e 50a>*

```

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 54c>*

```
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!

```
50a <Implementation of divisions procedures 38b>+≡ (37a) <49b 50b>
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 52b>
 else
 <Fork a pseudo stratified sampling division 54a>
 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
```

```
50b <Implementation of divisions procedures 38b>+≡ (37a) <50a 55a>
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 52c
 else
 Join pseudo stratified sampling divisions 54b
 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 *Join importance sampling divisions 51a*  $\equiv$  (50a)

```

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

```

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 90).

### *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.

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

```
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)
```

52b  $\langle$ Fork a pure stratified sampling division 52b $\rangle \equiv$  (50a)

```
 \langle Setup to fork a pure stratified sampling division 52a \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:

52c  $\langle$ Join pure stratified sampling divisions 52c $\rangle \equiv$  (50b)

```
 \langle Setup to fork a pure stratified sampling division 52a \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
```

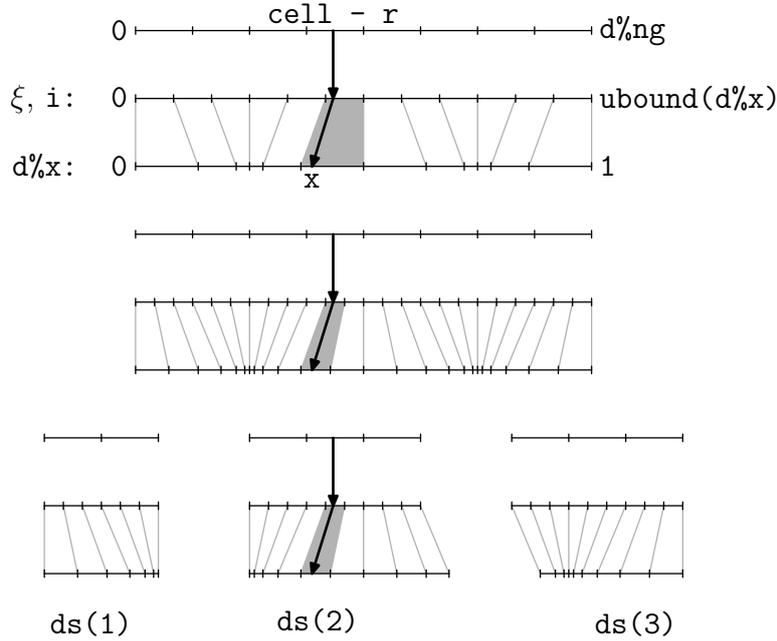


Figure 5.5: Forking one dimension  $d$  of a grid into three parts  $ds(1)$ ,  $ds(2)$ , and  $ds(3)$ . The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 5.3).

### *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.

53  $\langle$ Setup to fork a pseudo stratified sampling division 53 $\rangle \equiv$  (54)

```

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

```

```

54a <Fork a pseudo stratified sampling division 54a>≡ (50a)
 <Setup to fork a pseudo stratified sampling division 53>
 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)

54b <Join pseudo stratified sampling divisions 54b>≡ (50b)
 <Setup to fork a pseudo stratified sampling division 53>
 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)

54c <Declaration of divisions procedures 38a>+≡ (37a) <49c 56a>
 private :: subdivide
 private :: distribute

```

```
private :: collect
```

55a *<Implementation of divisions procedures 38b>+≡* (37a) *<50b 55b>*

```
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
```

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

```
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
```

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

```
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*

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

```
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

```

56a *<Declaration of divisions procedures 38a>*+≡ (37a) <54c 57a>

```

public :: debug_division
public :: dump_division

```

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

```

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

```

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

```

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:

- 57a *<Declaration of divisions procedures 38a>+≡ (37a) <56a 58b>*  
public :: **inside\_division**, **stratified\_division**  
public :: **volume\_division**, **rigid\_division**, **adaptive\_division**
- 57b *<Implementation of divisions procedures 38b>+≡ (37a) <56c 57c>*  
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**
- 57c *<Implementation of divisions procedures 38b>+≡ (37a) <57b 57d>*  
elemental function **stratified\_division** (d) result (yorn)  
type(**division\_t**), intent(in) :: d  
logical :: yorn  
yorn = d%**stratified**  
end function **stratified\_division**
- 57d *<Implementation of divisions procedures 38b>+≡ (37a) <57c 57e>*  
elemental function **volume\_division** (d) result (vol)  
type(**division\_t**), intent(in) :: d  
real(kind=default) :: vol  
vol = d%**dx**  
end function **volume\_division**
- 57e *<Implementation of divisions procedures 38b>+≡ (37a) <57d 57f>*  
elemental function **rigid\_division** (d) result (n)  
type(**division\_t**), intent(in) :: d  
integer :: n  
n = d%**ng**  
end function **rigid\_division**
- 57f *<Implementation of divisions procedures 38b>+≡ (37a) <57e 58c>*  
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

- 58a *<Declaration of divisions types 37b>+≡* (37a) <37b>  

```

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

```
- 58b *<Declaration of divisions procedures 38a>+≡* (37a) <57a 58d>  

```

public :: copy_history, summarize_division

```
- 58c *<Implementation of divisions procedures 38b>+≡* (37a) <57f 58e>  

```

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

```
- 58d *<Declaration of divisions procedures 38a>+≡* (37a) <58b 60b>  

```

private :: probabilities

```
- 58e *<Implementation of divisions procedures 38b>+≡* (37a) <58c 59a>  

```

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

```

59a *<Implementation of divisions procedures 38b>*+≡ (37a) <58e 59b>

```

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

```

59b *<Implementation of divisions procedures 38b>*+≡ (37a) <59a 61c>

```

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

```

60a *<Variables in divisions 46a>+≡* (37a) *<46a 62a>*  
integer, private, parameter :: BUFFER\_SIZE = 50

60b *<Declaration of divisions procedures 38a>+≡* (37a) *<58d 61a>*  
public :: print\_history, write\_history

60c *<Declaration of divisions procedures (removed from WHIZARD) 60c>≡*  
public :: division\_x, division\_integral  
public :: division\_variance, division\_efficiency

60d *<Implementation of divisions procedures (removed from WHIZARD) 45b>+≡* *<45b 60e>*  
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

60e *<Implementation of divisions procedures (removed from WHIZARD) 45b>+≡* *<60d 60f>*  
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

60f *<Implementation of divisions procedures (removed from WHIZARD) 45b>+≡* *<60e 60g>*  
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

60g *<Implementation of divisions procedures (removed from WHIZARD) 45b>+≡* *<60f>*  
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

61a *<Declaration of divisions procedures 38a>+≡* (37a) *<60b 66c>*

```

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

```

61b *<Interfaces of divisions procedures 61b>≡* (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.

61c *<Implementation of divisions procedures 38b>+≡* (37a) *<59b 62b>*

```

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
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) <60a

```

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) <61c 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  $\langle$ Insure that `ubound (d%x, dim=1) == num_div` 63a $\rangle \equiv$  (62b 65b 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 \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 62b 64a \rangle
- ```

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

```

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

```

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

```

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

```

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

```

```

65a <Constants in divisions 65a>≡ (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

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

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

66b <Implementation of divisions procedures 38b>+≡ (37a) <66a 66d>
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!

```

66c <Declaration of divisions procedures 38a>+≡ (37a) <61a 68a>
 public :: marshal_division_size, marshal_division, unmarshal_division

66d <Implementation of divisions procedures 38b>+≡ (37a) <66b 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
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) <66d 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 68b>

```

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

```

68a *<Declaration of divisions procedures 38a>+≡ (37a) <66c*  
public :: marshal\_div\_history\_size, marshal\_div\_history, unmarshal\_div\_history

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

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

68d *<Implementation of divisions procedures 38b>+≡ (37a) <68c 69>*  
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

69 *<Implementation of divisions procedures 38b>+≡ (37a) <68d 70a>*

```

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

```

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

```

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

```

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

```

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*

70c  $\langle$ vamp.f90 70c $\rangle \equiv$

71a $\rangle$

```
! 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.

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

 By WK for WHIZARD.

```
71b <vamp.f90 70c>+≡ <71a 75b>
 module vamp_equivalences
 use kinds
 use divisions
 use vamp_grid_type !NODEP!
 implicit none
 private
 <Declaration of vamp_equivalences procedures 72d>
 <Constants in vamp_equivalences 72b>
 <Declaration of vamp_equivalences types 71c>
 character(len=*), public, parameter :: VAMP_EQUIVALENCES_RCS_ID = &
 "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
 contains
 <Implementation of vamp_equivalences procedures 72c>
 end module vamp_equivalences
```

```
71c <Declaration of vamp_equivalences types 71c>≡ (71b) 72a>
 type, public :: vamp_equivalence_t
 integer :: left, right
 integer, dimension(:), allocatable :: permutation
 integer, dimension(:), allocatable :: mode
 end type vamp_equivalence_t
```

72a *<Declaration of vamp\_equivalences types 71c>+≡ (71b) <71c*

```

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

```

72b *<Constants in vamp\_equivalences 72b>≡ (71b)*

```

integer, parameter, public :: &
 VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3

```

72c *<Implementation of vamp\_equivalences procedures 72c>≡ (71b) 72e>*

```

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

```

72d *<Declaration of vamp\_equivalences procedures 72d>≡ (71b) 73b>*

```

public :: vamp_equivalences_init

```

72e *<Implementation of vamp\_equivalences procedures 72c>+≡ (71b) <72c 73a>*

```

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
73a <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <72e 73c>
 subroutine vamp_equivalence_final (eq)
 type(vamp_equivalence_t), intent(inout) :: eq
 deallocate (eq%permutation, eq%mode)
 end subroutine vamp_equivalence_final
73b <Declaration of vamp_equivalences procedures 72d>+≡ (71b) <72d 73e>
 public :: vamp_equivalences_final
73c <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <73a 73d>
 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
73d <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <73c 73f>
 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
73e <Declaration of vamp_equivalences procedures 72d>+≡ (71b) <73b 74a>
 public :: vamp_equivalences_write
73f <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <73d 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
else
 write (u, "(3x,A)") "[not allocated]"
end if
end subroutine vamp_equivalences_write

```

74a *<Declaration of vamp\_equivalences procedures 72d>+≡ (71b) <73e 74c>*  
public :: vamp\_equivalence\_set

74b *<Implementation of vamp\_equivalences procedures 72c>+≡ (71b) <73f 75a>*  
**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 72d>+≡ (71b) <74a>*  
public :: vamp\_equivalences\_complete

75a *<Implementation of vamp\_equivalences procedures 72c>+≡*

(71b) <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
```

75b *<vamp.f90 70c>+≡*

<71b 76a>

```
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 77a>
 <Interfaces of vamp procedures 96b>
 <Constants in vamp 153a>
 <Declaration of vamp types 77b>
 <Variables in vamp 79a>
character(len=*), public, parameter :: VAMP_RCS_ID = &
 "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
contains
 <Implementation of vamp procedures 78b>
end module vamp_rest

```

76a <vamp.f90 70c>+≡ ◁75b

```

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.

76b <Declaration of vamp\_grid\_type types 76b>≡ (71a)

```

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

```

77a  $\langle$ Declaration of vamp procedures 77a $\rangle \equiv$  (75b) 78a $\rangle$   
 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.

77b  $\langle$ Declaration of vamp types 77b $\rangle \equiv$  (75b) 77c $\rangle$   
 type, public :: vamp\_data\_t  
 end type vamp\_data\_t

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

77c  $\langle$ Declaration of vamp types 77b $\rangle + \equiv$  (75b)  $\langle$ 77b 106c $\rangle$   
 type(vamp\_data\_t), parameter, public :: NO\_DATA = vamp\_data\_t ()

## 5.2.2 Initialization

78a  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 77a 79b $\rangle$   
`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`.

78b  $\langle$ Implementation of `vamp` procedures 78b $\rangle \equiv$  (75b) 79c $\rangle$   
`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 `NUM_DIV_DEFAULT`  $\geq 6$ , but we will never go that low anyway.

79a  $\langle$ Variables in `vamp` 79a $\rangle \equiv$  (75b) 94c $\rangle$   
integer, private, parameter :: `NUM_DIV_DEFAULT` = 20

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

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

79b  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 78a 80b $\rangle$   
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:

79c  $\langle$ Implementation of `vamp` procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 78b 80a $\rangle$   
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

```

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

```

 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

```

80b *<Declaration of vamp procedures 77a>+≡ (75b) <79b 81a>*

```

 public :: vamp_discard_integral

```

Keep the current optimized grid, but drop the accumulated results for the integral (value and errors). If the second variable is given, it will be the new number of sampling points for the next call to `vamp_sample_grid`.

80c *<Implementation of vamp procedures 78b>+≡ (75b) <80a 81b>*

```

 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
81a <Declaration of vamp procedures 77a>+≡ (75b) <80b 83a>
 private :: set_grid_options
81b <Implementation of vamp procedures 78b>+≡ (75b) <80c 82>
 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`.

```
82 <Implementation of vamp procedures 78b>+≡ (75b) <81b 83b>
 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 84a>
 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.

```

83a <Declaration of vamp procedures 77a>+≡ (75b) <81a 84d>
 private :: vamp_reshape_grid_internal
 public :: vamp_reshape_grid

83b <Implementation of vamp procedures 78b>+≡ (75b) <82 84e>
 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:

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

```
84a <Adjust grid and other state for new num_calls 84a>≡ (82) 84b>
 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 = $\frac{\text{Volume}}{N_{\text{calls}}}$ (5.15)
```

and

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

```
84b <Adjust grid and other state for new num_calls 84a>+≡ (82) <84a 84c>
 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)
84c <Adjust grid and other state for new num_calls 84a>+≡ (82) <84b>
 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:

```
84d <Declaration of vamp procedures 77a>+≡ (75b) <83a 85a>
 public :: vamp_nullify_f_limits
84e <Implementation of vamp procedures 78b>+≡ (75b) <83b 85b>
 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
```

85a *<Declaration of vamp procedures 77a>+≡* (75b) <84d 86b>  
public :: vamp\_rigid\_divisions  
public :: vamp\_get\_covariance, vamp\_nullify\_covariance  
public :: vamp\_get\_variance, vamp\_nullify\_variance

85b *<Implementation of vamp procedures 78b>+≡* (75b) <84e 85c>  
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

85c *<Implementation of vamp procedures 78b>+≡* (75b) <85b 85d>  
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

85d *<Implementation of vamp procedures 78b>+≡* (75b) <85c 85e>  
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

85e *<Implementation of vamp procedures 78b>+≡* (75b) <85d 86a>  
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

```

86a *<Implementation of vamp procedures 78b>*+≡ (75b) <85e 86c>  
 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

86b *<Declaration of vamp procedures 77a>*+≡ (75b) <85a 92b>  
 public :: vamp\_sample\_grid  
 public :: vamp\_sample\_grid0  
 public :: vamp\_refine\_grid  
 public :: vamp\_refine\_grids

#### *Simple Non-Adaptive Sampling: $S_0$*

86c *<Implementation of vamp procedures 78b>*+≡ (75b) <86a 92c>  
 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 87c>*  
 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 92a>
 <Reset counters in vamp_sample_grid0 87b>
 loop_over_cells: do
 <Sample calls_per_cell points in the current cell 88b>
 <Collect integration and grid optimization data for current cell 90a>
 <Count up cell, exit if done 87a>
 end do loop_over_cells
 <Collect results of vamp_sample_grid0 90b>
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.

87a <Count up cell, exit if done 87a>≡ (86c)

```

 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

```

87b <Reset counters in vamp\_sample\_grid0 87b>≡ (86c)

```

 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

```

87c <Local variables in vamp\_sample\_grid0 87c>≡ (86c) 88a>

```

 real(kind=default), parameter :: &
 eps = tiny (1._default) / epsilon (1._default)
 character(len=6) :: buffer

```

88a *<Local variables in vamp\_sample\_grid0 87c>*+≡ (86c) *<87c 89c>*  
integer :: j, k  
integer, dimension(size(g%div)) :: cell

88b *<Sample calls\_per\_cell points in the current cell 88b>*≡ (86c)  
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 88c>*  
*<f = wgt \* func (x, weights, channel), iff x inside true\_domain 88d>*  
*<Collect integration and grid optimization data for x from f 89a>*  
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.

88c *<Get x in the current cell 88c>*≡ (88b)  
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.

88d *<f = wgt \* func (x, weights, channel), iff x inside true\_domain 88d>*≡ (88b 136a)  
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
89a <Collect integration and grid optimization data for x from f 89a>≡ (88b) 89b▷
 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
89b <Collect integration and grid optimization data for x from f 89a>+≡ (88b) <89a
 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
89c <Local variables in vamp_sample_grid0 87c>+≡ (86c) <88a
 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

```

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

90a *Collect integration and grid optimization data for current cell 90a* ≡ (86c)

```

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.

90b *Collect results of vamp\_sample\_grid0 90b* ≡ (86c) 91▷

```

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

```

91 <Collect results of vamp\_sample\_grid0 90b>+≡ (86c) <90b

```

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
 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

```

```

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

```

92a *<Check optional arguments in vamp\_sample\_grid0 92a>*≡ (86c)

```

if (present (channel) .neqv. present (weights)) then
 call raise_exception (exc, EXC_FATAL, FN, &
 "channel and weights required together")
return
end if

```

92b *<Declaration of vamp procedures 77a>*+≡ (75b) <86b 96a>

```

public :: vamp_probability

```

92c *<Implementation of vamp procedures 78b>*+≡ (75b) <86c 92d>

```

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

92d *<Implementation of vamp procedures 78b>*+≡ (75b) <92c 94a>

```

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

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

- 94a  $\langle$ Implementation of vamp procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 92d 94b $\rangle$
- ```

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

```
- 94b \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 94a 94d \rangle
- ```

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

```
- 94c  $\langle$ Variables in vamp 79a $\rangle + \equiv$  (75b)  $\langle$ 79a 110a $\rangle$
- ```

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

```

Adaptive Sampling: $S_n = S_0(rS_0)^n$

- 94d \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 94b 95 \rangle
- ```

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 107a>
 <Exit iterate if accuracy has been reached 97a>
 if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
<Copy results of vamp_sample_grid to dummy variables 96c>
end subroutine vamp_sample_grid

```

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

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

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

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

95 <Implementation of vamp procedures 78b>+≡ (75b) <94d 97d>  
 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

```

96a *<Declaration of vamp procedures 77a>*+≡ (75b) <92b 97b>

```

public :: vamp_average_iterations
private :: vamp_average_iterations_grid

```

96b *<Interfaces of vamp procedures 96b>*≡ (75b) 97c>

```

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.

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

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

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

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

96c *<Copy results of vamp\_sample\_grid to dummy variables 96c>*≡ (94d 104 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

```

97a *<Exit iterate if accuracy has been reached 97a>≡ (94d 104 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

97b *<Declaration of vamp procedures 77a>+≡ (75b) <96a 102b>*

```

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

```

97c *<Interfaces of vamp procedures 96b>+≡ (75b) <96b 107c>*

```

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.

97d *<Implementation of vamp procedures 78b>+≡ (75b) <95 100c>*

```

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 100b>
do j = 1, ndim
 if (j == d) then
 <call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 99c>
 else
 <call copy_division (gs%div(j), g%div(j)) 100a>
 end if
end do
if (d == 0) then
 <Handle g%calls_per_cell for d == 0 98a>
end if
<Copy the rest of g to the gs 98b>
end subroutine vamp_fork_grid_single

```

Divide the sampling points among identical grids

```

98a <Handle g%calls_per_cell for d == 0 98a>≡ (97d)
 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

```

```

98b <Copy the rest of g to the gs 98b>≡ (97d) 98c>
 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

```

98c <Copy the rest of g to the gs 98b>+≡ (97d) <98b 99a>
 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

```

99a *<Copy the rest of g to the gs 98b>+≡* (97d) *<98c 99b>*

```

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

```

99b *<Copy the rest of g to the gs 98b>+≡* (97d) *<99a*

```

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.

99c *<call fork\_division (g%div(j), gs%div(j), g%calls\_per\_cell, ...) 99c>≡* (97d)

```

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 99d>

```

99d *<Bail out if exception exc raised 99d>≡* (99c 100d 104 140c 142c)

```

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.

```
100a <call copy_division (gs%div(j), g%div(j)) 100a>≡ (97d)
 do i = 1, num_grids
 call copy_division (gs(i)%div(j), g%div(j))
 end do
```

```
100b <Allocate or resize the divisions 100b>≡ (97d)
 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
```

```
100c <Implementation of vamp procedures 78b>+≡ (75b) <97d 102a>
 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)) 100d>
 else
 <call sum_division (g%div(j), gs%div(j)) 101a>
 end if
 end do
 <Combine the rest of gs onto g 101b>
 end subroutine vamp_join_grid_single
```

```
100d <call join_division (g%div(j), gs%div(j)) 100d>≡ (100c)
 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 99d>
101a <call sum_division (g%div(j), gs%div(j)) 101a>≡ (100c)
 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)
101b <Combine the rest of gs onto g 101b>≡ (100c)
 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.

```

101c <Idioms 101c>≡ (250)
 type(vamp_grid), dimension(:), allocatable :: gx

```

---

<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.

```

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)

```

102a *Implementation of vamp procedures 78b*+≡ (75b) <100c 102c>

```

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)
 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

```

102b *Declaration of vamp procedures 77a*+≡ (75b) <97b 103b>

```

public :: vamp_fork_grid_joints

```

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

102c *Implementation of vamp procedures 78b*+≡ (75b) <102a 103a>

```

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

```

103a *<Implementation of vamp procedures 78b>*+≡ (75b) <102c 104>

```

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

103b *<Declaration of vamp procedures 77a>*+≡ (75b) <102b 107b>

```

public :: vamp_sample_grid_parallel
public :: vamp_distribute_work

```

HPF [10, 11, 15]:

```

104 <Implementation of vamp procedures 78b>+≡ (75b) <103a 105b>
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 105a>
 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 99d>
call vamp_average_iterations &
 (g, iteration, local_integral, local_std_dev, local_avg_chi2)
<Trace results of vamp_sample_grid 107a>
<Exit iterate if accuracy has been reached 97a>
if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
deallocate (d)
<Copy results of vamp_sample_grid to dummy variables 96c>
end subroutine vamp_sample_grid_parallel
105a <Gather exceptions in vamp_sample_grid_parallel 105a>≡ (104)
 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.

```

105b <Implementation of vamp procedures 78b>+≡ (75b) <104 107d>
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 106a>
end do try
end subroutine vamp_distribute_work
106a <Accept distribution among n workers 106a>≡ (105b) 106b>
 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
106b <Accept distribution among n workers 106a>+≡ (105b) <106a
 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

```

106c <Declaration of vamp types 77b>+≡ (75b) <77c 113a>
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

107a <Trace results of vamp_sample_grid 107a>≡ (94d 104)
 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

107b <Declaration of vamp procedures 77a>+≡ (75b) <103b 108c>
 public :: vamp_create_history, vamp_copy_history, vamp_delete_history
 public :: vamp_terminate_history
 public :: vamp_get_history, vamp_get_history_single

107c <Interfaces of vamp procedures 96b>+≡ (75b) <97c 108d>
 interface vamp_get_history
 module procedure vamp_get_history_single
 end interface

107d <Implementation of vamp procedures 78b>+≡ (75b) <105b 107e>
 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

107e <Implementation of vamp procedures 78b>+≡ (75b) <107d 108a>
 elemental subroutine vamp_terminate_history (h)
 type(vamp_history), intent(inout) :: h

```

```

 h%calls = 0.0
end subroutine vamp_terminate_history
108a <Implementation of vamp procedures 78b>+≡ (75b) <107e 109>
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 108b>
 call copy_history (h%div, summarize_division (g%div))
 end if
end subroutine vamp_get_history_single
108b <Adjust h%div iff necessary 108b>≡ (108a)
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
108c <Declaration of vamp procedures 77a>+≡ (75b) <107b 113b>
public :: vamp_print_history, vamp_write_history
private :: vamp_print_one_history, vamp_print_histories
! private :: vamp_write_one_history, vamp_write_histories
108d <Interfaces of vamp procedures 96b>+≡ (75b) <107c 124d>
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

```

109 *<Implementation of vamp procedures 78b>*+≡ (75b) <108a 110b>

```
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
 end do
 end if
 end if
end subroutine
```

```

 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

```

110a *<Variables in vamp 79a>*+≡ (75b) <94c 146a>  
 integer, private, parameter :: BUFFER\_SIZE = 50

110b *<Implementation of vamp procedures 78b>*+≡ (75b) <109 110c>

```

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

```



110c *<Implementation of vamp procedures 78b>*+≡ (75b) <110b 113c>

```

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
 end if
 end do
 end if
end if

```

```

 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  $\lambda$ :

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

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.

113a `<Declaration of vamp types 77b>+≡` (75b) <106c>

```

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

```

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

113b `<Declaration of vamp procedures 77a>+≡` (75b) <108c 114b>

```

public :: vamp_multi_channel, vamp_multi_channel0

```

113c `<Implementation of vamp procedures 78b>+≡` (75b) <110c 114a>

```

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

```

114a *<Implementation of vamp procedures 78b>*+≡ (75b) <113c 114c>

```

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

114b *<Declaration of vamp procedures 77a>*+≡ (75b) <113b 117a>

```

public :: vamp_jacobian, vamp_check_jacobian

```

114c *<Implementation of vamp procedures 78b>*+≡ (75b) <114a 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 78b>+≡*

(75b) *<114c 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))
 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 77a>*+≡ (75b) <114b 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 78b>*+≡ (75b) <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 78b>*+≡ (75b) <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 77a>*+≡ (75b) <117a 119a>

```

public :: vamp_discard_integrals

```

118c *<Implementation of vamp procedures 78b>*+≡ (75b) <118a 119b>

```

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

```

119a *<Declaration of vamp procedures 77a>+≡* (75b) <118b 119c>  
public :: vamp\_update\_weights

We must discard the accumulated integrals, because the weight function  $w = f / \sum_i \alpha_i g_i$  changes:

119b *<Implementation of vamp procedures 78b>+≡* (75b) <118c 119d>  
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

119c *<Declaration of vamp procedures 77a>+≡* (75b) <119a 120a>  
public :: vamp\_reshape\_grids

119d *<Implementation of vamp procedures 78b>+≡* (75b) <119b 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
 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 77a>+≡* (75b) *<119c 123a>*  
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 78b>+≡* (75b) *<119d 123b>*  
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) 122>
 else
 call vamp_nullify_variance (g%grids(ch))
 call vamp_nullify_covariance (g%grids(ch))
 end if
 end do
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 125a>
 <Exit iterate if accuracy has been reached 97a>
 end do iterate
 <Copy results of vamp_sample_grid to dummy variables 96c>
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`:

```

122 <Sample the grid g%grids(ch) 122>≡ (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

```

123a  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 120a 124a $\rangle$   
`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

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

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

123b  $\langle$ Implementation of `vamp` procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 120b 124b $\rangle$   
`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`

124a  $\langle$ Declaration of vamp procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 123a 124c $\rangle$   
public :: vamp\_refine\_weights

124b  $\langle$ Implementation of vamp procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 123b 124e $\rangle$   
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

124c  $\langle$ Declaration of vamp procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 124a 125b $\rangle$   
private :: vamp\_average\_iterations\_grids

124d  $\langle$ Interfaces of vamp procedures 96b $\rangle + \equiv$  (75b)  $\langle$ 108d 125c $\rangle$   
interface vamp\_average\_iterations  
module procedure vamp\_average\_iterations\_grids  
end interface

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

124e  $\langle$ Implementation of vamp procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 124b 125d $\rangle$   
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
125a <Trace results of vamp_sample_grids 125a>≡ (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
125b <Declaration of vamp procedures 77a>+≡ (75b) <124c 126a>
 private :: vamp_get_history_multi
125c <Interfaces of vamp procedures 96b>+≡ (75b) <124d 131b>
 interface vamp_get_history
 module procedure vamp_get_history_multi
 end interface
125d <Implementation of vamp procedures 78b>+≡ (75b) <124e 126b>
 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

```

 WK

126a  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 125b 127a $\rangle$   
`public :: vamp_sum_channels`

126b  $\langle$ Implementation of `vamp` procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 125d 127c $\rangle$   
`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`  
`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`, `evecs`), we have  $\text{evals}(j) = \lambda_j$  and  $\text{evecs}(:, j) = v_j$ . This is equivalent with  $\text{evecs}(i, j) = R_{ij}$ .

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.

127a *<Declaration of vamp procedures 77a>*+≡ (75b) <126a 128a>

```
public :: select_rotation_axis
public :: select_rotation_subspace
```

127b *<Set iv to the index of the optimal eigenvector 127b>*≡ (129d 130c)

```
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
```

127c *<Implementation of vamp procedures 78b>*+≡ (75b) <126b 129d>

```
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 77a $\rangle + \equiv$  (75b)  $\langle$ 127a 131c $\rangle$   
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  $|(v_j)_i|$ :<sup>3</sup>

128b  $\langle$ Set i(1), i(2) to the axes of the optimal plane 128b $\rangle \equiv$  (129d) 129a $\rangle$   
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))))

---

<sup>3</sup>The 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.



130a *<Handle optional pancake and cigar 130a>*≡ (129d 130c)

```

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:

130b *<Implementation of vamp procedures 78b>*+≡ (75b) <129d 130c>

```

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

```

130c *<Implementation of vamp procedures 78b>*+≡ (75b) <130b 131e>

```

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 130a>
 call diagonalize_real_symmetric (cov, evals, evecs)
 <Set iv to the index of the optimal eigenvector 127b>
 <Set subspace to the axes of the optimal plane 131a>

```

```

 call select_subspace_explicit (cov, r, subspace)
 end subroutine select_subspace_guess
131a <Set subspace to the axes of the optimal plane 131a>≡ (130c)
 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
131b <Interfaces of vamp procedures 96b>+≡ (75b) <125c 135b>
 interface select_rotation_subspace
 module procedure select_subspace_explicit, select_subspace_guess
 end interface
131c <Declaration of vamp procedures 77a>+≡ (75b) <128a 131d>
 private :: select_subspace_explicit
 private :: select_subspace_guess
131d <Declaration of vamp procedures 77a>+≡ (75b) <131c 132a>
 public :: vamp_print_covariance
131e <Implementation of vamp procedures 78b>+≡ (75b) <130c 133c>
 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(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  $n_{\text{dim}}$  eigenvalues into  $n_{\text{cl}} \ll n_{\text{dim}}$  clusters.

132a  $\langle$ Declaration of `vamp` procedures 77a $\rangle \equiv$  (75b)  $\langle$ 131d 134a $\rangle$

```

! 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!

132b  $\langle$ Initialize clusters 132b $\rangle \equiv$  (133c)

```

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.

```

133a <Join closest clusters 133a>≡ (133c) 133b>
 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)

133b <Join closest clusters 133a>+≡ (133c) <133a
 cl_pos(gap+1:cl_num-1) = cl_pos(gap+2:cl_num)
 cl(gap+1:cl_num-1,:) = cl(gap+2:cl_num,:)

133c <Implementation of vamp procedures 78b>+≡ (75b) <131e 134b>
 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 132b>
 do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
 <Join closest clusters 133a>
 print *, cl_num, ": action = ", condense_action (x, cl)
 end do
 end subroutine

```

```

end do
cluster_pos = cl_pos(1:cl_num)
clusters = cl(1:cl_num,:)
end subroutine condense

```

134a  $\langle$ Declaration of vamp procedures 77a $\rangle + \equiv$  (75b)  $\langle$ 132a 135a $\rangle$

```

! private :: condense_action
public :: condense_action

```

$$S = \sum_{c \in \text{clusters}} \text{var}^{\frac{\alpha}{2}}(c) \quad (5.38)$$

134b  $\langle$ Implementation of vamp procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 133c 135d $\rangle$

```

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

```

134c  $\langle$ ctest.f90 134c $\rangle \equiv$

```

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.

135a *<Declaration of vamp procedures 77a>+≡* (75b) *<134a 135c>*  
 public :: vamp\_next\_event

135b *<Interfaces of vamp procedures 96b>+≡* (75b) *<131b 140b>*  
 interface vamp\_next\_event  
 module procedure vamp\_next\_event\_single, vamp\_next\_event\_multi  
 end interface

135c *<Declaration of vamp procedures 77a>+≡* (75b) *<135a 139a>*  
 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.

135d *<Implementation of vamp procedures 78b>+≡* (75b) *<134b 137>*  
 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) 136a>
 if (present (weight)) then
 <Unconditionally accept weighted event 136b>
 else
 <Maybe accept unweighted event 136c>
 end if
end do rejection
end subroutine vamp_next_event_single

```

136a <Choose a x and calculate f(x) 136a>≡ (135d)

```

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 88d>
! call record_efficiency (g%div, ia, f/g%f_max)

```

136b <Unconditionally accept weighted event 136b>≡ (135d)

```

weight = f
exit rejection

```

136c <Maybe accept unweighted event 136c>≡ (135d)

```

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  $w(x)$ .

137  $\langle$ Implementation of vamp procedures 78b $\rangle + \equiv$  (75b)  $\langle$ 135d 139b $\rangle$

```

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
 \langle Interface declaration for func 22 \rangle
 \langle Interface declaration for phi 31a \rangle
 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
 \langle weights: $\alpha_i \rightarrow w_{\max,i} \alpha_i$ 138a \rangle
 rejection: do
 \langle Select channel from weights 138b \rangle
 call vamp_next_event_single &
 (xi, rng, g%grids(channel), func, data, wgt, &
 channel, g%weights, g%grids, exc)
 if (present (weight)) then
 \langle Unconditionally accept weighted multi channel event 138c \rangle
 else
 \langle Maybe accept unweighted multi channel event 138d \rangle
 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  $\alpha_i$  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.

138a  $\langle$ weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  138a $\rangle \equiv$  (137 138e)

```

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)

```

138b  $\langle$ Select channel from weights 138b $\rangle \equiv$  (137)

```

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 select_channel
channel = min (channel, size (g%weights)) ! for r = 1 and rounding errors

```

138c  $\langle$ Unconditionally accept weighted multi channel event 138c $\rangle \equiv$  (137)

```

weight = wgt * g%weights(channel) / weights(channel)
exit rejection

```

138d  $\langle$ Maybe accept unweighted multi channel event 138d $\rangle \equiv$  (137)

```

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

```

138e  $\langle$ Maybe accept unweighted multi channel event (old version) 138e $\rangle \equiv$

```

if (wgt > g%grids(channel)%f_max) then
 g%grids(channel)%f_max = wgt
 <weights: $\alpha_i \rightarrow w_{\max,i}\alpha_i$ 138a>
 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.

139a <Declaration of `vamp` procedures 77a>+≡ (75b) <135c 140a>  
 public :: `vamp_warmup_grid`, `vamp_warmup_grids`

139b <Implementation of `vamp` procedures 78b>+≡ (75b) <137 139c>  
 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!

139c <Implementation of `vamp` procedures 78b>+≡ (75b) <139b 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 77a>+≡ (75b) <139a 142a>  
public :: vamp\_integrate  
private :: vamp\_integrate\_grid, vamp\_integrate\_region
- 140b <Interfaces of vamp procedures 96b>+≡ (75b) <135b 142b>  
interface vamp\_integrate  
module procedure vamp\_integrate\_grid, vamp\_integrate\_region  
end interface
- 140c <Implementation of vamp procedures 78b>+≡ (75b) <139c 141>  
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 99d>
 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

```

141 <Implementation of **vamp** procedures 78b>+≡ (75b) <140c 142c>

```

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

```

142a *<Declaration of vamp procedures 77a>+≡* (75b) <140a 143>

```

public :: vamp_integratex
private :: vamp_integratex_region

```

142b *<Interfaces of vamp procedures 96b>+≡* (75b) <140b 144b>

```

interface vamp_integratex
 module procedure vamp_integratex_region
end interface

```

142c *<Implementation of vamp procedures 78b>+≡* (75b) <141 144d>

```

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 99d>
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 99d>
 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

```

143 <Declaration of vamp procedures 77a>+≡ (75b) <142a 144a>
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

```

144a *<Declaration of vamp procedures 77a>*+≡ (75b) <143 158a>

```

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

```

144b *<Interfaces of vamp procedures 96b>*+≡ (75b) <142b 144c>

```

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

```

144c *<Interfaces of vamp procedures 96b>*+≡ (75b) <144b>

```

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

```

144d *<Implementation of vamp procedures 78b>*+≡ (75b) <142c 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
end if

```

```

 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 79a>*+≡ (75b) <110a

```

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 78b>*+≡ (75b) <144d 149a>

```

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 153b 160b)

```

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 153b 160b)

```

if (associated (g%map)) then
 deallocate (g%map)
end if

```

148c <Insure that associated (g%mu\_x) == .false. 148c>≡ (146b 153b 160b)

```

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

```

149a *<Implementation of vamp procedures 78b>*+≡ (75b) <146b 149b>

```

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

```

149b *<Implementation of vamp procedures 78b>*+≡ (75b) <149a 149c>

```

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

```

149c *<Implementation of vamp procedures 78b>*+≡ (75b) <149b 150>

```

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

```

150 *<Implementation of vamp procedures 78b>+≡ (75b) <149c 151a>*

```

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

```

```

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

```

151a *<Implementation of vamp procedures 78b>+≡ (75b) <150 151b>*

```

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

```

151b *<Implementation of vamp procedures 78b>+≡ (75b) <151a 151c>*

```

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

```

151c *<Implementation of vamp procedures 78b>+≡ (75b) <151b 153b>*

```

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)
 end do
end if

```

```

 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

```

153a *<Constants in vamp 153a>*≡ (75b) 156b>

```

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

```

153b *<Implementation of vamp procedures 78b>*+≡ (75b) <151c 155a>

```

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
155a <Implementation of vamp procedures 78b>+≡ (75b) <153b 155b>
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
155b <Implementation of vamp procedures 78b>+≡ (75b) <155a 156a>
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

```

```

156a <Implementation of vamp procedures 78b>+≡ (75b) <155b 156c>
 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
 write (unit = unit) MAGIC_GRIDS_END
 end subroutine write_grids_raw_unit

156b <Constants in vamp 153a>+≡ (75b) <153a>
 integer, parameter, private :: MAGIC_GRIDS = 33333333
 integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1
 integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2

156c <Implementation of vamp procedures 78b>+≡ (75b) <156a 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 78b>*+≡ (75b) <156c 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 78b>*+≡ (75b) <157a 158b>

```

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)!

158a *<Declaration of vamp procedures 77a>*+≡ (75b) <144a 161>  
public :: vamp\_marshall\_grid\_size, vamp\_marshall\_grid, vamp\_unmarshal\_grid

158b *<Implementation of vamp procedures 78b>*+≡ (75b) <157b 160a>

```

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, idx, 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
160a <Implementation of vamp procedures 78b>+≡ (75b) <158b 160b>
 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
 iwords = iwords + 1
 if (associated (g%mu_x)) then
 dwords = dwords + 2 * (ndim + ndim**2)
 end if
 end subroutine vamp_marshall_grid_size
160b <Implementation of vamp procedures 78b>+≡ (75b) <160a 162a>
 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

```

161 <Declaration of vamp procedures 77a>+≡ (75b) <158a  
public :: vamp\_marshall\_history\_size, vamp\_marshall\_history

```

public :: vamp_unmarshal_history
162a <Implementation of vamp procedures 78b>+≡ (75b) <160b 162b>
pure subroutine vamp_marshall_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_marshall_history
162b <Implementation of vamp procedures 78b>+≡ (75b) <162a 163>
pure subroutine vamp_marshall_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

```

163 *<Implementation of vamp procedures 78b>*+≡ (75b) <162b 164>

```

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

164 *<Implementation of vamp procedures 78b>+≡* (75b) *<163 165a>*

```

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
 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

```

165a *<Implementation of vamp procedures 78b>*+≡ (75b) <164 165b>

```

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

```

165b *<Implementation of vamp procedures 78b>*+≡ (75b) <165a 166a>

```

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

```

166a  $\langle$ Implementation of vamp procedures 78b $\rangle$ + $\equiv$  (75b)  $\langle$ 165b 166b $\rangle$

```

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

```

166b  $\langle$ Implementation of vamp procedures 78b $\rangle$ + $\equiv$  (75b)  $\langle$ 166a 167a $\rangle$

```

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
end if

```

```

 end if
 call copy_history (lhs%div, rhs%div)
 end if
end subroutine vamp_copy_history

```

167a *<Implementation of vamp procedures 78b>+≡* (75b) <166b

```

 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:

167b *<vampi.f90 167b>≡* 167c>

```

! vampi.f90 --
<Copyleft notice 1>
module vamp_serial_mpi
 use vamp, &
 <vamp0_* => vamp_* 168c>
 VAMPO_RCS_ID => VAMP_RCS_ID
 public
end module vamp_serial_mpi

```

**vamp\_parallel\_mpi** contains the non trivial MPI code and will be discussed in detail below.

167c *<vampi.f90 167b>+≡* <167b 168a>

```

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 168b>
<Interfaces of vampi procedures 173a>
<Parameters in vampi 169b>
<Declaration of vampi types 173d>
character(len=*), public, parameter :: VAMPI_RCS_ID = &
 "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
contains
 <Implementation of vampi procedures 169a>
end module vamp_parallel_mpi

```

`vampi` is now a plug-in replacement for `vamp` and *must not* be used together with `vamp`:

```

168a <vampi.f90 167b>+≡ <167c
module vampi
 use vamp_serial_mpi !NODEP!
 use vamp_parallel_mpi !NODEP!
 public
end module vampi

```

### 5.3.1 Parallel Execution

#### Single Channel

```

168b <Declaration of vampi procedures 168b>≡ (167c) 172b>
 public :: vamp_create_grid
 public :: vamp_discard_integral
 public :: vamp_reshape_grid
 public :: vamp_sample_grid
 public :: vamp_delete_grid

168c <vamp0.* => vamp.* 168c>≡ (167b) 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, &
169a <Implementation of vampi procedures 169a>≡ (167c) 169c>
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
169b <Parameters in vampi 169b>≡ (167c) 177a>
integer, public, parameter :: VAMP_ROOT = 0
169c <Implementation of vampi procedures 169a>+≡ (167c) <169a 169d>
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
169d <Implementation of vampi procedures 169a>+≡ (167c) <169c 170>
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.

```

170 <Implementation of vampi procedures 169a>+≡ (167c) <169d 172a>
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
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
 end if
end if

```

```

 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
 if (present (avg_chi2)) then
 avg_chi2 = local_avg_chi2
 end if
end if
end subroutine vamp_sample_grid

```

172a *<Implementation of vampi procedures 169a>*+≡ (167c) <170 173b>

```

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 168b>*+≡ (167c) <168b 173f>

```

public :: vamp_print_history
private :: vamp_print_one_history, vamp_print_histories

```

172c *<vamp0.\* => vamp.\* 168c>*+≡ (167b) <168c 173e>

```

vamp0_print_history => vamp_print_history, &

```

- 173a *<Interfaces of vampi procedures 173a>*≡ (167c) 182c>  
 interface **vamp\_print\_history**  
 module procedure **vamp\_print\_one\_history**, **vamp\_print\_histories**  
 end interface
- 173b *<Implementation of vampi procedures 169a>*+≡ (167c) <172a 173c>  
**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**
- 173c *<Implementation of vampi procedures 169a>*+≡ (167c) <173b 174b>  
**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*

- 173d *<Declaration of vampi types 173d>*≡ (167c)  
 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**
- 173e *<vamp0.\* => vamp.\* 168c>*+≡ (167b) <172c 174a>  
**vamp0\_grids** => **vamp\_grids**, &  
 Partially duplicate the API of **vamp**:
- 173f *<Declaration of vampi procedures 168b>*+≡ (167c) <172b 179c>  
 public :: **vamp\_create\_grids**  
 public :: **vamp\_discard\_integrals**

```

public :: vamp_update_weights
public :: vamp_refine_weights
public :: vamp_delete_grids
public :: vamp_sample_grids

```

174a  $\langle$ vamp0.\* => vamp.\* 168c $\rangle$ + $\equiv$  (167b)  $\langle$ 173e 182b $\rangle$

```

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

174b  $\langle$ Implementation of vampi procedures 169a $\rangle$ + $\equiv$  (167c)  $\langle$ 173c 174c $\rangle$

```

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

```

174c  $\langle$ Implementation of vampi procedures 169a $\rangle$ + $\equiv$  (167c)  $\langle$ 174b 175a $\rangle$

```

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
175a <Implementation of vampi procedures 169a>+≡ (167c) <174c 175b>
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
175b <Implementation of vampi procedures 169a>+≡ (167c) <175a 175c>
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
175c <Implementation of vampi procedures 169a>+≡ (167c) <175b 176>
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`.

```
176 <Implementation of vampi procedures 169a>+≡ (167c) <175c 179d>
 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 177b>
 else
 <Distribute each grid among processes 181b>
 end if
 <Exit iterate if accuracy has been reached (MPI) 180a>
end do iterate
<Copy results of vamp_sample_grids to dummy variables 179f>
end subroutine vamp_sample_grids

```

Setting `VAMP_MAX_WASTE` to 1 disables the splitting of grids, which doesn't work yet.

```

177a <Parameters in vampi 169b>+≡ (167c) <169b 179e>
 real(kind=default), private, parameter :: VAMP_MAX_WASTE = 1.0
 ! real(kind=default), private, parameter :: VAMP_MAX_WASTE = 0.3

```

```

177b <Distribute complete grids among processes 177b>≡ (176) 177c>
 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) 177d>
 end if
 else
 call vamp_nullify_variance (g%g0%grids(ch))
 call vamp_nullify_covariance (g%g0%grids(ch))
 end if
 end do

```

Refine the grids after *all* grids have been sampled:

```

177c <Distribute complete grids among processes 177b>+≡ (176) <177b 178a>
 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 179a>
 end if
 end if
 end do

```

therefore we use `vamp_sample_grid0` instead of `vamp0_sample_grid`:

```

177d <Sample g%g0%grids(ch) 177d>≡ (177b)
 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

```

178a *<Distribute complete grids among processes 177b>+≡ (176) <177c*

```

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 179b>
 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:

178b *<Ship g%g0%grids from the root to the assigned processor 178b>≡*

```

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 do

```

```

 end if
 end if
end do
179a <Ship the result for channel #ch back to the root 179a>≡ (177c)
 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
179b <Receive the result for channel #ch at the root 179b>≡ (178a)
 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
179c <Declaration of vampi procedures 168b>+≡ (167c) <173f 180b>
 private :: object
179d <Implementation of vampi procedures 169a>+≡ (167c) <176 180c>
 pure function object (ch, obj) result (tag)
 integer, intent(in) :: ch, obj
 integer :: tag
 tag = 100 * ch + obj
 end function object
179e <Parameters in vampi 169b>+≡ (167c) <177a
 integer, public, parameter :: &
 TAG_INTEGRAL = 1, &
 TAG_STD_DEV = 2, &
 TAG_GRID = 3, &
 TAG_HISTORY = 6, &
 TAG_NEXT_FREE = 9
179f <Copy results of vamp_sample_grids to dummy variables 179f>≡ (176)
 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

```

180a *<Exit iterate if accuracy has been reached (MPI) 180a>*≡ (176)

```

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.

180b *<Declaration of vampi procedures 168b>*+≡ (167c) <179c 182a>  
 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.

180c *<Implementation of vampi procedures 169a>*+≡ (167c) <179d 182d>  
 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))
 end do

```

```

 fill(proc) = fill(proc) + sjobs(job)
 assign(idx(job)) = proc - 1
 end do
 <Estimate waste of processor time 181a>
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:

```

181a <Estimate waste of processor time 181a>≡ (180c)
 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!

```

181b <Distribute each grid among processes 181b>≡ (176)
 do ch = 1, size (g%g0%grids)
 if (g%active(ch)) then
 call vamp_discard_integral (g%g0%grids(ch))
 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

```

### 5.3.2 Event Generation

This is currently only a syntactical translation ...

- 182a *<Declaration of vampi procedures 168b>+≡* (167c) <180b 184a>  
 public :: vamp\_warmup\_grid  
 public :: vamp\_warmup\_grids  
 public :: vamp\_next\_event  
 private :: vamp\_next\_event\_single, vamp\_next\_event\_multi
- 182b *<vamp0\_\* => vamp\_\* 168c>+≡* (167b) <174a 184b>  
 vamp0\_warmup\_grid => vamp\_warmup\_grid, &  
 vamp0\_warmup\_grids => vamp\_warmup\_grids, &  
 vamp0\_next\_event => vamp\_next\_event, &
- 182c *<Interfaces of vampi procedures 173a>+≡* (167c) <173a 184c>  
 interface vamp\_next\_event  
 module procedure vamp\_next\_event\_single, vamp\_next\_event\_multi  
 end interface
- 182d *<Implementation of vampi procedures 169a>+≡* (167c) <180c 183a>  
 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
183a <Implementation of vampi procedures 169a>+≡ (167c) <182d 183b>
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
183b <Implementation of vampi procedures 169a>+≡ (167c) <183a 183c>
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
183c <Implementation of vampi procedures 169a>+≡ (167c) <183b 184d>
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

- 184a <Declaration of vampi procedures 168b>+≡ (167c) <182a 185c>  

```

public :: vamp_write_grid, vamp_read_grid
private :: write_grid_unit, write_grid_name
private :: read_grid_unit, read_grid_name

```
- 184b <vamp0.\* => vamp.\* 168c>+≡ (167b) <182b 185d>  

```

vamp0_write_grid => vamp_write_grid, &
vamp0_read_grid => vamp_read_grid, &

```
- 184c <Interfaces of vampi procedures 173a>+≡ (167c) <182c 185e>  

```

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

```
- 184d <Implementation of vampi procedures 169a>+≡ (167c) <183c 184e>  

```

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

```
- 184e <Implementation of vampi procedures 169a>+≡ (167c) <184d 185a>  

```

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
185a <Implementation of vampi procedures 169a>+≡ (167c) <184e 185b>
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
185b <Implementation of vampi procedures 169a>+≡ (167c) <185a 186a>
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
185c <Declaration of vampi procedures 168b>+≡ (167c) <184a 187a>
public :: vamp_write_grids, vamp_read_grids
private :: write_grids_unit, write_grids_name
private :: read_grids_unit, read_grids_name
185d <vamp0.* => vamp.* 168c>+≡ (167b) <184b>
vamp0_write_grids => vamp_write_grids, &
vamp0_read_grids => vamp_read_grids, &
185e <Interfaces of vampi procedures 173a>+≡ (167c) <184c 189a>
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

```

186a *<Implementation of vampi procedures 169a>*+≡ (167c) <185b 186b>

```

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

```

186b *<Implementation of vampi procedures 169a>*+≡ (167c) <186a 186c>

```

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

```

186c *<Implementation of vampi procedures 169a>*+≡ (167c) <186b 186d>

```

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

```

186d *<Implementation of vampi procedures 169a>*+≡ (167c) <186c 187b>

```

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

```
187a <Declaration of vampi procedures 168b>+≡ (167c) <185c 191a>
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`:

```
187b <Implementation of vampi procedures 169a>+≡ (167c) <186d 187c>
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
```

```
187c <Implementation of vampi procedures 169a>+≡ (167c) <187b 189b>
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`:

```

188a <Implementation of vampi procedures (doesn't work with MPICH yet) 188a>≡ 188b>
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 :: iwords, dwords
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call vamp_marshall_grid_size (g, iwords, dwords)
 allocate (ibuf(iwords), dbuf(dwords))
 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 ...

```

188b <Implementation of vampi procedures (doesn't work with MPICH yet) 188a>+≡ <188a
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.

```

189a <Interfaces of vampi procedures 173a>+≡ (167c) <185e
 interface vamp_broadcast_grid
 module procedure &
 vamp_broadcast_one_grid, vamp_broadcast_many_grids
 end interface

```

```

189b <Implementation of vampi procedures 169a>+≡ (167c) <187c 189c>
 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

```

```

189c <Implementation of vampi procedures 169a>+≡ (167c) <189b 190>

```

```

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

```

190 *<Implementation of vampi procedures 169a>*+≡ (167c) <189c 191b>

```

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

```

191a *<Declaration of vampi procedures 168b>+≡* (167c) <187a  
public :: vamp\_send\_history  
public :: vamp\_receive\_history

191b *<Implementation of vampi procedures 169a>+≡* (167c) <190 191c>  
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

191c *<Implementation of vampi procedures 169a>+≡* (167c) <191b  
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\_unmarshall\_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>≡ 200c▷
! vamp_test.f90 --
<Copleft notice 1>
<Module vamp_test_functions 192b>
<Module vamp_tests 196b>

192b <Module vamp_test_functions 192b>≡ (192a 202a)
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 *<Implementation of vamp\_test\_functions procedures 193a>*+≡ (192b) <193c 195a>

```

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  $\langle$ Implementation of `vamp_test_functions` procedures 193a $\rangle + \equiv$  (192b)  $\langle$ 194 195b $\rangle$

```

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  $\langle$ Implementation of `vamp_test_functions` procedures 193a $\rangle + \equiv$  (192b)  $\langle$ 195a 196a $\rangle$

```

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 *<Implementation of vamp\_test\_functions procedures 193a>*≡ (192b) <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 *<Module vamp\_tests 196b>*≡ (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
 <Declaration of procedures in vamp_tests 196c>
contains
 <Implementation of procedures in vamp_tests 197a>
end module vamp_tests

```

### Verification

196c *<Declaration of procedures in vamp\_tests 196c>*≡ (196b 202b) 198a>

```

! public :: check_jacobians, check_inverses, check_inverses3
public :: check_inverses, check_inverses3

```

196d *<Implementation of procedures in vamp\_tests (broken?) 196d>*≡

```

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 213a) 213b>*

```

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 divisions, only: DIVISIONS_RCS_ID
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"
print *, VAMP_RCS_ID
print *, DIVISIONS_RCS_ID
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 --`  
`<Copleyleft 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 divisions, only: DIVISIONS_RCS_ID
use vamp, only: VAMP_RCS_ID
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

```

```

 end if
 print *, VAMP_RCS_ID
 print *, VAMPI_RCS_ID
 print *, DIVISIONS_RCS_ID
 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* --  
*<Copyright notice 1>*  
*<Module vamp\_test0\_functions 205>*

### Single Channel

The functions to be integrated are shared by the serial and the parallel incarnation of the code.

```

205 <Module vamp_test0_functions 205>≡ (204b 220b)
 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 206a>
 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.

$$\begin{aligned}
N(x_{\min}, x_{\max}, x_0, \gamma) &= \sum_{p=1}^{n_p} \int_{x_{\min}}^{x_{\max}} dx \left| \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \\
&+ 2 \operatorname{Re} \sum_{p=1}^{n_p} \sum_{q=1}^{n_p} \int_{x_{\min}}^{x_{\max}} dx \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} \quad (6.6)
\end{aligned}$$

206a  $\langle$ Implementation of `vamp_test0_functions` procedures 206a $\rangle \equiv$  (205) 206b $\triangleright$

```

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 / cplx (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.

206b  $\langle$ Implementation of `vamp_test0_functions` procedures 206a $\rangle + \equiv$  (205)  $\langle$ 206a 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 (cplx (x_max - x0p, gp, kind=default) &
 / cplx (x_min - x0p, gp, kind=default)) &
 - log (cplx (x_max - x0q, -gq, kind=default) &
 / cplx (x_min - x0q, -gq, kind=default))) &
 / cplx (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 206a $\rangle + \equiv$  (205)  $\langle$ 206b 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 206a $\rangle + \equiv$  (205)  $\langle$ 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 206a $\rangle + \equiv$  (205)  $\langle$ 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 *<Implementation of vamp\_test0\_functions procedures 206a>+≡ (205) <207c 209a>*

```

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

$$\begin{aligned} \psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) = \\ \frac{x_{\max} \left( \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma} + \operatorname{atan} \frac{x - x_0}{\gamma} \right) + x_{\min} \left( \operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x}{\gamma} \right)}{\operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma}} \end{aligned} \quad (6.12)$$

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 *<Implementation of vamp\_test0\_functions procedures 206a>+≡ (205) <208 209c>*  

```

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 *<Decode channel into ch and p(:) 209b>≡ (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 *<Implementation of vamp\_test0\_functions procedures 206a>+≡ (205) <209a 210a>*  

```

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
 <Decode channel into ch and p(:) 209b>
 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
 end if

```

```

 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 206a $\rangle + \equiv$  (205)  $\langle$ 209c 210b $\rangle$

```

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 206a $\rangle + \equiv$  (205)  $\langle$ 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
 (Modules used by vamp_tests0 211b)
 use vamp
 implicit none
 private
 (Declaration of procedures in vamp_tests0 212a)
contains
 (Implementation of procedures in vamp_tests0 212b)
end module vamp_tests0

```

211b  $\langle$ Modules used by vamp\_tests0 211b $\rangle$  $\equiv$  (211a 220b)

```

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

```

```

 end do
end subroutine check_jacobians

```

### Integration

```

212a <Declaration of procedures in vamp_tests0 212a>≡ (211a 220b) 214a>
 public :: single_channel, multi_channel

212b <Implementation of procedures in vamp_tests0 212b>≡ (211a 220b) 213a>
 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

```

213a *<Implementation of procedures in vamp\_tests0 212b>+≡ (211a 220b) <212b 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**

213b *<Body of multi\_channel 199b>+≡ (199a 213a) <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 212a>+≡ (211a 220b) <212a*  
 public :: **single\_channel\_generator**, **multi\_channel\_generator**
- 214b *<Implementation of procedures in vamp\_tests0 212b>+≡ (211a 220b) <213a 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 212b>+≡ (211a 220b) <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 219d>
 implicit none
 <Variables in vamp_test0 219b>
 do_print = .true.
 print *, "Starting VAMP 1.0 self test..."
 print *, "serial code"
 print *, VAMP_RCS_ID
 print *, DIVISIONS_RCS_ID
 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
 end program

```

```

end if
call tao_random_seed (rng, ticks0)
<Set up integrand and region in vamp_test0 219f>
<Execute tests in vamp_test0 218a>
<Cleanup in vamp_test0 220a>
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 219a>

```

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"

```

```

219a <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"

219b <Variables in vamp_test0 219b>≡ (217 220c) 219e>
 logical :: do_print

219c <Execute command 219c>≡ (220c)

219d <Modules used by vamp_test0 219d>≡ (217 220c)
 use kinds
 use tao_random_numbers
 use divisions, only: DIVISIONS_RCS_ID
 use vamp, only: VAMP_RCS_ID
 use vamp_test0_functions !NODEP!
 use vamp_tests0 !NODEP!

219e <Variables in vamp_test0 219b>+≡ (217 220c) <219b
 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

219f <Set up integrand and region in vamp_test0 219f>≡ (217 220c)
 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

```

220a *<Cleanup in vamp\_test0 220a>*≡ (217 220c)  
 call `delete_sample` ()  
 deallocate (region)

## 6.2.2 Parallel Test

220b *<vampi\_test0.f90 220b>*≡ 220c>  
 ! vampi\_test0.f90 --  
*<Copyleft notice 1>*  
*<Module vamp\_test0\_functions 205>*  
 module `vamp_tests0`  
*<Modules used by vamp\_tests0 211b>*  
 use `vampi`  
 use `mpi90`  
 implicit none  
 private  
*<Declaration of procedures in vamp\_tests0 212a>*  
 contains  
*<Implementation of procedures in vamp\_tests0 212b>*  
 end module `vamp_tests0`

220c *<vampi\_test0.f90 220b>*+≡ <220b  
 program `vampi_test0`  
*<Modules used by vamp\_test0 219d>*  
 use `mpi90`  
 use `vampi`, only: `VAMPI_RCS_ID`  
 implicit none  
*<Variables in vamp\_test0 219b>*  
 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  
   print \*, `VAMP_RCS_ID`  
   print \*, `VAMPI_RCS_ID`  
   print \*, `DIVISIONS_RCS_ID`

```

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 219f>
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 219c>
 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 220a>
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>≡

## APPLICATION

### 7.1 Cross section

```
222a <application.f90 222a>≡ 239▷
! application.f90 --
<Copleft 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 *<XXX Variables in cross\_section 223a>*≡ 223b>

```
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 *<XXX Variables in cross\_section 223a>*+≡ <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 *<Variables in cross\_section 222b>*+≡ (222a) <222b 223f>

```
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 *<Declaration of cross\_section procedures 223d>*≡ (222a) 225a>

```
private :: cuts
```

223e *<XXX Implementation of cross\_section procedures 223e>*≡

```
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 *<Variables in cross\_section 222b>*+≡ (222a) <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} \to [(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

$$\begin{aligned}
& t_1^{\max/\min}(s_2) \\
& = m_a^2 + m_1^2 - \frac{(s + m_a^2 - m_b^2)(s - s_2 + m_1^2) \mp \sqrt{\lambda(s, m_a^2, m_b^2)\lambda(s, s_2, m_1^2)}}{2s}
\end{aligned}
\tag{7.2}$$

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)

```

$$J_\phi(x_1, \dots, x_5) = \begin{vmatrix} \frac{\partial s_2}{\partial x_1} & \frac{\partial t_1}{\partial x_1} \\ \frac{\partial s_2}{\partial x_2} & \frac{\partial t_1}{\partial x_2} \end{vmatrix} \cdot 8\pi^2 \quad (7.3)$$

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 *<Adjust Jacobian 226a>*≡ (226b 228b)

```
p%jacobian = p%jacobian &
 * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
```

226b *<Implementation of cross\_section procedures 224a>*+≡ (222a) <224b 227c>

```
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
 $m_a \leftrightarrow m_b, m_1 \leftrightarrow m_2$ for channel #1 226c)
 <Set (s2, t1, phi, cos theta3, phi3) from (x1, ..., x5) 225b)
 p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
 <Adjust Jacobian 226a)
 $p_1 \leftrightarrow p_2$ for channel #2 227a)
end function phase_space
```

226c *<math>m\_a \leftrightarrow m\_b, m\_1 \leftrightarrow m\_2</math> for channel #1 226c>*≡ (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 *<Declaration of cross\_section procedures 223d>+≡ (222a) <227b 228e>*  
 private :: phase\_space, phase\_space\_massless

228b *<Implementation of cross\_section procedures 224a>+≡ (222a) <227c 228f>*  
 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  
*<Set (s2, t1, φ, cos θ3, φ3) from (x1, ..., x5) (massless case) 225c>*  
 p = two\_to\_three (s, t1, s2, phi, cos\_theta3, phi3)  
*<Adjust Jacobian 226a>*  
*<p1 ↔ p2 for channel #2 227a>*  
 end function phase\_space\_massless

228c *<Types in cross\_section 228c>≡ (222a) 228d>*  
 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 *<Types in cross\_section 228c>+≡ (222a) <228c>*  
 type, public :: x5  
 ! private  
 real(kind=default), dimension(5) :: x  
 real(kind=default) :: jacobian  
 end type x5

228e *<Declaration of cross\_section procedures 223d>+≡ (222a) <228a 231a>*  
 private :: invariants\_from\_p, invariants\_to\_p  
 private :: invariants\_from\_x, invariants\_to\_x

228f *<Implementation of cross\_section procedures 224a>+≡ (222a) <228b 229a>*  
 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 *Implementation of cross-section procedures 224a*+≡ (222a) <228f 229b>

```

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 *Implementation of cross-section procedures 224a*+≡ (222a) <229a 230>

```

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)
 end if
end function sigma\_raw

```

else
 xs = 0.0
end if
end function sigma_raw

```

232a *Implementation of cross\_section procedures 224a*+≡ (222a) <231c 232c>

```

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

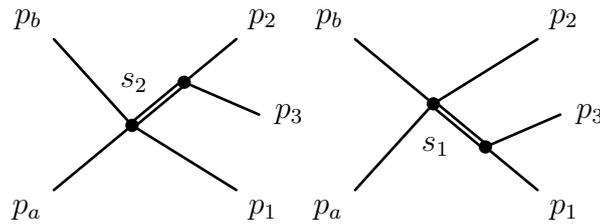
```

232b *Declaration of cross\_section procedures 223d*+≡ (222a) <231a 234a>

```

public :: w

```



232c *Implementation of cross\_section procedures 224a*+≡ (222a) <232a 233>

```

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 *<Implementation of cross-section procedures 224a>+≡ (222a) <232c 234c>*

```

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 *<Implementation of cross\_section procedures 224a>+≡ (222a) <235c 236b>*

```

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 *<Implementation of cross\_section procedures 224a>+≡ (222a) <236a 236c>*

```

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 *<Implementation of cross\_section procedures 224a>+≡ (222a) <236b 237a>*

```

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 case

```

```

 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
 character(len=*), public, parameter :: KINDS_RCS_ID = &
 "$Id: kinds.nw 314 2010-04-17 20:32:33Z ohl $"
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
 character(len=*), public, parameter :: CONSTANTS_RCS_ID = &
 "$Id: constants.nw 314 2010-04-17 20:32:33Z ohl $"
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 --
<Copleft 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>
 character(len=*), public, parameter :: EXCEPTIONS_RCS_ID = &
 "$Id: exceptions.nw 314 2010-04-17 20:32:33Z ohl $"
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 calling 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`

250 *<Idioms 101c>+≡*

*<101c*

```
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 *<API documentation 251>*+≡ <252h 253b>  
call `tao_random_destroy` (s)

Copy `tao_random_state` and `tao_random_raw_state` in all four combinations

253b *<API documentation 251>*+≡ <253a 253c>  
call `tao_random_copy` (lhs, rhs)  
lhs = rhs

253c *<API documentation 251>*+≡ <253b 253d>  
call `tao_random_flush` (s)

253d *<API documentation 251>*+≡ <253c 253e>  
call `tao_random_read` (s, unit)  
call `tao_random_write` (s, unit)

253e *<API documentation 251>*+≡ <253d 253f>  
call `tao_random_test` (name = name)

Here is a sample application of random number states:

253f *<API documentation 251>*+≡ <253e 253g>  
`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 *<API documentation 251>*+≡ <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

$$X_j = (X_{j-K} - X_{j-L}) \pmod{2^{30}} \quad (\text{C.1})$$

with lags  $K = 100$  and  $L = 37$ .

254a  $\langle$ Parameters in tao\_random\_numbers 254a $\rangle \equiv$  (273c 274a) 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 *Parameters in tao\_random\_numbers 254a*+≡ (273c 274a) <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 *Implementation of 30-bit tao\_random\_numbers 255a*≡ (273c) 256d>  
pure subroutine generate (a, state)  
integer(kind=tao\_i32), dimension(:), intent(inout) :: a, state  
integer :: j, n  
n = size (a)  
*Load a and refresh state 255c*  
end subroutine generate

255b *Declaration of tao\_random\_numbers 255b*≡ (273c 274a) 258g>  
private :: generate

`state(1:K)` is already set up properly:

255c *Load a and refresh state 255c*≡ (255a) 255d>  
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 *Load a and refresh state 255c*+≡ (255a) <255c 255e>  
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 *Load a and refresh state 255c*+≡ (255a) <255d>  
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 *Implementation of tao\_random\_numbers 255f*≡ (273c 274a) 256b>

```

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>+≡ (273c 274a) <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>+≡ (273c 274a) <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 $\rangle$   
integer, parameter :: DEFAULT\_SEED = 0

These must not be changed:

257b  $\langle$ Parameters local to tao\_random\_seed 257a $\rangle + \equiv$  (256d 259e)  $\langle$ 257a $\rangle$   
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 $\rangle$   
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)  $\langle$ 257d $\rangle$   
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  $\langle$  $p(z) \rightarrow p(z)^2$  (modulo  $z^K + z^L + 1$ ) 257g $\rangle \equiv$  (256d) 258a $\rangle$   
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 $\langle p(z) \rightarrow p(z)^2 \text{ (modulo } z^K + z^L + 1) \text{ 257g)} + \equiv$ (256d) \langle 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 $\langle p(z) \rightarrow zp(z) \text{ (modulo } z^K + z^L + 1) \text{ 258b)} \equiv$ (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 \langle Shift s or t and exit if t \leq 0 258c $\rangle \equiv$ (256d 259e)
 if (s /= 0) then
 s = s / 2
 else
 t = t - 1
 end if
 if (t <= 0) then
 exit
 end if

258d \langle Fill state from x 258d $\rangle \equiv$ (256d 259e)
 state(1:K-L) = x(L+1:K)
 state(K-L+1:K) = x(1:L)

258e \langle Warm up state 258e $\rangle \equiv$ (256d 259e)
 do j = 1, 10
 call generate (x, state)
 end do

258f \langle Interfaces of tao_random_numbers 258f $\rangle \equiv$ (273c 274a) 261e \rangle
 interface tao_random_seed
 module procedure \langle Specific procedures for tao_random_seed 258h \rangle
 end interface

258g \langle Declaration of tao_random_numbers 255b $\rangle + \equiv$ (273c 274a) \langle 255b 260a \rangle
 private :: \langle Specific procedures for tao_random_seed 258h \rangle

258h \langle Specific procedures for tao_random_seed 258h $\rangle \equiv$ (258)
 seed_static, seed_state, seed_raw_state

```

### C.2.3 Generation of 52-bit Random Numbers

$$X_j = (X_{j-K} + X_{j-L}) \pmod{1} \quad (\text{C.3})$$

259a *<Variables in 52-bit tao\_random\_numbers 259a>*≡ (274a) 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>*+≡ (274a) <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>*≡ (274a) 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>*+≡ (274a) <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>+≡ (273c 274a) <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 $\rangle \equiv$  (274a) 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 $\rangle + \equiv$ (274a) \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 $\rangle + \equiv$  (273c 274a)  $\triangleleft$ 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 $\rangle + \equiv$ (273c 274a) \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>*+≡ (273c 274a) <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>*+≡ (273c 274a) <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>*+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <261e 264a>
 interface tao_random_destroy
 module procedure destroy_state, destroy_raw_state
 end interface
263e <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <261f 264c>
 private :: destroy_state, destroy_raw_state
263f <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <263d 264b>*
- ```

interface tao_random_copy
    module procedure <Specific procedures for tao_random_copy 264d>
end interface

```
- 264b *<Interfaces of tao_random_numbers 258f>+≡ (273c 274a) <264a 265d>*
- ```

interface assignment(=)
 module procedure <Specific procedures for tao_random_copy 264d>
end interface

```
- 264c *<Declaration of tao\_random\_numbers 255b>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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>+≡ (273c 274a) <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 281a>
 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>+≡ (274a) <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>≡ (274a) 268c>
private :: write_state_array
268b <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <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>+≡ (274a) <268a 281e>
private :: read_state_array
268d <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <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>*≡ (273c 274a)  
integer, parameter, private :: MIN\_UNIT = 11, MAX\_UNIT = 99
- 269b *<Declaration of tao\_random\_numbers 255b>*+≡ (273c 274a) <266a 270b>  
private :: find\_free\_unit
- 269c *<Implementation of tao\_random\_numbers 255f>*+≡ (273c 274a) <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>*+≡ (273c 274a) <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>*+≡ (273c 274a) <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>*+≡ (273c 274a) <269e 281g>  
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 *<Interfaces of tao\_random\_numbers 258f>+≡ (273c 274a) <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 *<Declaration of tao_random_numbers 255b>+≡ (273c 274a) <269b 274b>*
- ```

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 *<Implementation of 30-bit tao\_random\_numbers 255a>+≡ (273c) <267d 271a>*
- ```

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 274c>
  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⟩*+≡ (274a) *◁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⟩*+≡ (274a) *◁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⟩*+≡ (274a) *◁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⟩*+≡ (274a) *◁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>+≡ (274a) <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>+≡ (274a) <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 280e>
    <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>
    character(len=*), public, parameter :: TAO_RANDOM_NUMBERS_RCS_ID = &
      "$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    <Implementation of tao_random_numbers 255f>
    <Implementation of 30-bit tao_random_numbers 255a>
  end module tao_random_numbers

```

```

274a <tao52_random_numbers.f90 274a>≡
! 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 281c>
  <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>
  character(len=*), public, parameter :: TAO52_RANDOM_NUMBERS_RCS_ID = &
    "$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of tao_random_numbers 255f>
  <Implementation of 52-bit tao_random_numbers 259c>
end module tao52_random_numbers

```

Ten functions are exported

```

274b <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <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 $0 \leq r < 2^{30} = 1073741824$:

```

274c <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) <274c 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>+≡ (274a) <273b 278a>

```

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>+≡ (274a) <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 277e>
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>≡ (276-78)
integer :: nu, done, todo, chunk
<Set nu to num or size(v) 277a>
<Prepare array buffer and done, todo, chunk 277b>
v(1:chunk) = NORM * buffer(last+1:last+chunk)
do
    <Update last, done and todo and set new chunk 277c>
    <Reload buffer or exit 277d>
    v(done+1:done+chunk) = NORM * buffer(1:chunk)
end do

```

277a *⟨Set nu to num or size(v) 277a⟩*≡ (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.

277b *⟨Prepare array buffer and done, todo, chunk 277b⟩*≡ (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.

277c *⟨Update last, done and todo and set new chunk 277c⟩*≡ (276c)

```

    last = last + chunk
    done = done + chunk
    todo = todo - chunk
    chunk = min (todo, buffer_end)

```

277d *⟨Reload buffer or exit 277d⟩*≡ (276c)

```

    if (chunk <= 0) then
        exit
    end if
    call generate (buffer, state)
    last = 0

```

277e *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) <276b 278b>

```

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 $v_i \in [0, 1)$.

```

278a <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <275e 278d>
  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:

```

278b <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <277e 278c>
  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

```

```

278c <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278b 278e>
  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 52-bit tao_random_numbers 259c>+≡ (274a) <278a 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

```

```

278e <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278c 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) <278e 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>*+≡ (274a) <278d 280a>

```

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 280b>

```

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 52-bit tao_random_numbers 259c⟩*+≡ (274a) *⟨279b 280d⟩*
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

280b *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) *⟨279e 280c⟩*
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

280c *⟨Implementation of 30-bit tao_random_numbers 255a⟩*+≡ (273c) *⟨280b 283b⟩*
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

280d *⟨Implementation of 52-bit tao_random_numbers 259c⟩*+≡ (274a) *⟨280a 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

280e *⟨Interfaces of 30-bit tao_random_numbers 280e⟩*≡ (273c)
interface tao_random_number
 module procedure *⟨Specific procedures for 30-bit tao_random_number 280f⟩*
end interface

280f *⟨Specific procedures for 30-bit tao_random_number 280f⟩*≡ (280e 281b)
integer_static, integer_state, &
integer_array_static, integer_array_state, &
real_static, real_state, real_array_static, real_array_state

These are not exported

- 281a *<Declaration of 30-bit tao_random_numbers 267c>*+≡ (273c) <267e 281b>
private :: &
 integer_stateless, integer_array_stateless, &
 real_stateless, real_array_stateless
- 281b *<Declaration of 30-bit tao_random_numbers 267c>*+≡ (273c) <281a
private :: *<Specific procedures for 30-bit tao_random_number 280f>*
- 281c *<Interfaces of 52-bit tao_random_numbers 281c>*≡ (274a)
interface tao_random_number
 module procedure *<Specific procedures for 52-bit tao_random_number 281d>*
end interface
- 281d *<Specific procedures for 52-bit tao_random_number 281d>*≡ (281)
real_static, real_state, real_array_static, real_array_state

These are not exported

- 281e *<Declaration of 52-bit tao_random_numbers 268a>*+≡ (274a) <268c 281f>
private :: real_stateless, real_array_stateless
- 281f *<Declaration of 52-bit tao_random_numbers 268a>*+≡ (274a) <281e
private :: *<Specific procedures for 52-bit tao_random_number 281d>*

C.4.6 Luxury

- 281g *<Implementation of tao_random_numbers 255f>*+≡ (273c 274a) <269f 281h>
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
- 281h *<Implementation of tao_random_numbers 255f>*+≡ (273c 274a) <281g 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 <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <281h 282b>
    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 <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <282a 282c>
    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 <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <282b 282d>
    subroutine luxury_static ()
        <Initialize a virginal random number generator 279c>
        call luxury_static_integer (size (s_buffer))
    end subroutine luxury_static

282d <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <282c 282e>
    subroutine luxury_static_integer (consumption)
        integer, intent(in) :: consumption
        <Initialize a virginal random number generator 279c>
        call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
    end subroutine luxury_static_integer

282e <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <282d
    subroutine luxury_static_real (consumption)
        real(kind=default), intent(in) :: consumption
        <Initialize a virginal random number generator 279c>
        call luxury_static_integer (int (consumption * size (s_buffer)))
    end subroutine luxury_static_real

282f <Interfaces of tao_random_numbers (unused luxury) 282f>≡
    interface tao_random_luxury
        module procedure <Specific procedures for tao_random_luxury 283a>
    end interface

282g <Declaration of tao_random_numbers (unused luxury) 282g>≡      282h>
    private :: luxury_stateless

282h <Declaration of tao_random_numbers (unused luxury) 282g>+≡      <282g
    private :: <Specific procedures for tao_random_luxury 283a>

```

283a \langle Specific procedures for `tao_random_luxury` 283a $\rangle \equiv$ (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

283b \langle Implementation of 30-bit `tao_random_numbers` 255a $\rangle + \equiv$ (273c) \triangleleft 280c
`subroutine tao_random_test (name)`
`character(len=*), optional, intent(in) :: name`
`character (len = *), parameter :: &`
`OK = "(1x,i10,' is ok. ')", &`
`NOT_OK = "(1x,i10,' is not ok, (expected ',i10,')!')"`
 \langle Parameters in `tao_random_test` 283c \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 *, TAO_RANDOM_NUMBERS_RCS_ID`
`print *, "testing the 30-bit tao_random_numbers ..."`
 \langle Perform simple tests of `tao_random_numbers` 283d \rangle
 \langle Perform more tests of `tao_random_numbers` 284c \rangle
`end subroutine tao_random_test`

283c \langle Parameters in `tao_random_test` 283c $\rangle \equiv$ (283b 285b)
`integer, parameter :: &`
`SEED = 310952, &`
`N = 2009, M = 1009, &`
`N_SHORT = 1984`

DEK's "official" test expects $a_{1009 \cdot 2009 + 1} = a_{2027082} = 995235265$:

283d \langle Perform simple tests of `tao_random_numbers` 283d $\rangle \equiv$ (283b 285b) 284b \triangleright
`! call tao_random_luxury ()`
`call tao_random_seed (SEED)`
`do i = 1, N+1`
`call tao_random_number (a, M)`
`end do`

⟨Test a(1) = A_2027082 284a⟩

```
284a ⟨Test a(1) = A_2027082 284a⟩≡ (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

```
284b ⟨Perform simple tests of tao_random_numbers 283d⟩+≡ (283b 285b) <283d
  call tao_random_seed (SEED)
  do i = 1, M+1
    call tao_random_number (a)
  end do
⟨Test a(1) = A_2027082 284a⟩
```

Now checkpoint the random number generator after $N_{\text{short}} \cdot M$ numbers

```
284c ⟨Perform more tests of tao_random_numbers 284c⟩≡ (283b 285b) 284d>
  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 284a⟩
```

and restart the saved generator

```
284d ⟨Perform more tests of tao_random_numbers 284c⟩+≡ (283b 285b) <284c 284e>
  do i = 1, N+1 - N_SHORT
    call tao_random_number (t, a, M)
  end do
⟨Test a(1) = A_2027082 284a⟩
```

The same story again, but this time saving the copy to a file

```
284e ⟨Perform more tests of tao_random_numbers 284c⟩+≡ (283b 285b) <284d 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 284a>
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 284a>
end if

```

And finally using marshaling/unmarshaling:

```

285a <Perform more tests of tao_random_numbers 284c>+≡ (283b 285b) <284e
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 284a>
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 284a>

```

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>+≡ (274a) <280d
subroutine tao_random_test (name)
character(len=*), optional, intent(in) :: name
character(len=*), parameter :: &
    OK = "(1x,f22.20,' is ok.')" , &
    NOT_OK = "(1x,f22.20,' is not ok, (A_2027082 ',f22.20,')!')'"
<Parameters in tao_random_test 283c>

```

```

real(kind=default), parameter :: &
    A_2027082 = 0.36410514377569680455_tao_r64
real(kind=default), 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 *, TAO52_RANDOM_NUMBERS_RCS_ID
print *, "testing the 52-bit tao_random_numbers ..."
  <Perform simple tests of tao_random_numbers 283d>
  <Perform more tests of tao_random_numbers 284c>
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>
  character(len=*), public, parameter :: SPECFUN_RCS_ID = &
    "$Id: specfun.nw 314 2010-04-17 20:32:33Z ohl $"
!WK:
  real(kind=default), public, parameter :: &
    PI = 3.1415926535897932384626433832795028841972_default
contains
  <Implementation of specfun procedures 288c>
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]:

$$\Gamma(u) = \begin{cases} (u-1)\Gamma(u-1) & \text{for } u > 4 \\ \frac{1}{u}\Gamma(u+1) & \text{for } u < 3 \end{cases} \quad (\text{D.2})$$

288a \langle Pull u into the interval $[3, 4]$ 288a $\rangle \equiv$ (288c)

```

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:

$$\begin{aligned}
 d_m &= d_{m+1} = 0 \\
 d_j &= 2xd_{j+1} - d_{j+2} + c_j \text{ for } 0 < j < m - 1 \\
 f(x) &= d_0 = xd_1 - d_2 + \frac{1}{2}c_0
 \end{aligned}
 \tag{D.3}$$

288b \langle Clenshaw's recurrence formula 288b $\rangle \equiv$ (288c)

```

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.

288c \langle Implementation of `specfun` procedures 288c $\rangle \equiv$ (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 =  $\langle c_0/2, c_1, c_2, \dots, c_{15}$  for  $\Gamma(x)$  289a  $\rangle$ 
  u = x
  if (u <= 0.0) then

```

```

    if (u == int (u)) then
        g = huge (g)
        return
    else
        u = 1 - u
    end if
endif
<Pull u into the intervall [3,4] 288a>
g = 2*u - 7
<Clenshaw's recurrence formula 288b>
if (x < 0) then
    g = PI / (sin (PI * x) * g)
end if
end function gamma

```

289a $\langle c_0/2, c_1, c_2, \dots, c_{15} \text{ for } \Gamma(x) \text{ 289a} \rangle \equiv$ (288c)

```

(/ 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, &
  0.0000000000002596_default, &
  0.0000000000000111_default, &
  0.0000000000000004_default /)

```

D.1 Test

289b $\langle \text{stest.f90 289b} \rangle \equiv$ (290c)

```

! stest.f90 --
<Copleft 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

292a `<vamp_stat.f90 292a>≡`
`! vamp_stat.f90 --`
`<Copyleft notice 1>`
`module vamp_stat`
`use kinds`
`implicit none`
`private`
`<Declaration of vamp_stat procedures 292b>`
`character(len=*), public, parameter :: VAMP_STAT_RCS_ID = &`
`"$Id: vamp_stat.nw 314 2010-04-17 20:32:33Z ohl $"`
`contains`
`<Implementation of vamp_stat procedures 292c>`
`end module vamp_stat`

292b `<Declaration of vamp_stat procedures 292b>≡` (292a) 293c>
`public :: average, standard_deviation, value_spread`

$$\text{avg}(X) = \frac{1}{|X|} \sum_{x \in X} x \quad (\text{E.1})$$

292c `<Implementation of vamp_stat procedures 292c>≡` (292a) 293a>
`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`

$$\text{stddev}(X) = \frac{1}{|X| - 1} \sum_{x \in X} (x - \text{avg}(X))^2 = \frac{1}{|X| - 1} \left(\frac{1}{|X|} \sum_{x \in X} x^2 - (\text{avg}(X))^2 \right) \quad (\text{E.2})$$

293a *<Implementation of vamp_stat procedures 292c>+≡ (292a) <292c 293b>*

```

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

```

$$\text{spread}(X) = \max_{x \in X}(x) - \min_{x \in X}(x) \quad (\text{E.3})$$

293b *<Implementation of vamp_stat procedures 292c>+≡ (292a) <293a 293d>*

```

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

```

293c *<Declaration of vamp_stat procedures 292b>+≡ (292a) <292b>*

```

public :: standard_deviation_percent, value_spread_percent

```

293d *<Implementation of vamp_stat procedures 292c>+≡ (292a) <293b 293e>*

```

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

```

293e *<Implementation of vamp_stat procedures 292c>+≡ (292a) <293d>*

```

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 un-descriptive 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.*

```
295a <histograms.f90 295a>≡
! histograms.f90 --
<Copyleft notice 1>
module histograms
  use kinds
  use utils, only: find_free_unit
  implicit none
  private
  <Declaration of histograms procedures 296b>
  <Interfaces of histograms procedures 296c>
  <Variables in histograms 296e>
  <Declaration of histograms types 295b>
  character(len=*), public, parameter :: HISTOGRAMS_RCS_ID = &
    "$Id: histograms.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of histograms procedures 296f>
end module histograms

295b <Declaration of histograms types 295b>≡ (295a) 296a>
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

```

296a *<Declaration of histograms types 295b>+≡* (295a) <295b

```

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

```

296b *<Declaration of histograms procedures 296b>≡* (295a) 296d>

```

public :: create_histogram
public :: fill_histogram
public :: delete_histogram
public :: write_histogram

```

296c *<Interfaces of histograms procedures 296c>≡* (295a) 301b>

```

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

```

296d *<Declaration of histograms procedures 296b>+≡* (295a) <296b 300a>

```

private :: create_histogram1, create_histogram2
private :: fill_histogram1, fill_histogram2s, fill_histogram2v
private :: delete_histogram1, delete_histogram2
private :: write_histogram1, write_histogram2

```

296e *<Variables in histograms 296e>≡* (295a)

```

integer, parameter, private :: N_BINS_DEFAULT = 10

```

296f *<Implementation of histograms procedures 296f>≡* (295a) 297a>

```

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

```

297a *<Implementation of histograms procedures 296f>+≡ (295a) <296f 297b>*

```

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

```

297b *<Implementation of histograms procedures 296f>+≡ (295a) <297a 298a>*

```

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

```

298a *<Implementation of histograms procedures 296f>+≡ (295a) <297b 298b>*
 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

298b *<Implementation of histograms procedures 296f>+≡ (295a) <298a 298c>*
 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

298c *<Implementation of histograms procedures 296f>+≡ (295a) <298b 299a>*
 elemental subroutine delete_histogram1 (h)
 type(histogram), intent(inout) :: h
 deallocate (h%bins, h%bins2)
 deallocate (h%bins3)
 end subroutine delete_histogram1

```

299a <Implementation of histograms procedures 296f>+≡ (295a) <298c 299b>
    elemental subroutine delete_histogram2 (h)
        type(histogram2), intent(inout) :: h
        deallocate (h%bins, h%bins2)
    end subroutine delete_histogram2

299b <Implementation of histograms procedures 296f>+≡ (295a) <299a 300b>
    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
        end if
    end subroutine write_histogram1

```

```

do i = 1, h%n_bins
  print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
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

```

300a *<Declaration of histograms procedures 296b>+≡ (295a) <296d 301a>*
 !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).

300b *<Implementation of histograms procedures 296f>+≡ (295a) <299b 301d>*

```

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

```

```

        end if
    end do
    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

```

- 301a *<Declaration of histograms procedures 296b>+≡* (295a) *<300a 301c>*
 private :: midpoint
- 301b *<Interfaces of histograms procedures 296c>+≡* (295a) *<296c*
 interface midpoint
 module procedure midpoint1, midpoint2
 end interface
- 301c *<Declaration of histograms procedures 296b>+≡* (295a) *<301a*
 private :: midpoint1, midpoint2
- 301d *<Implementation of histograms procedures 296f>+≡* (295a) *<300b 301e>*
 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
- 301e *<Implementation of histograms procedures 296f>+≡* (295a) *<301d 302>*
 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

```

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
    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
    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
    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

```
305a <utils.f90 305a>≡
! utils.f90 --
<Copleft notice 1>
module utils
  use kinds
  implicit none
  private
  <Declaration of utils procedures 305b>
  <Parameters in utils 312c>
  <Variables in utils 313b>
  <Interfaces of utils procedures 305c>
  character(len=*), public, parameter :: UTILS_RCS_ID = &
    "$Id: utils.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of utils procedures 306c>
end module utils
```

G.1 Memory Management

```
305b <Declaration of utils procedures 305b>≡ (305a) 307d>
  public :: create_array_pointer
  private :: create_integer_array_pointer
  private :: create_real_array_pointer
  private :: create_integer_array2_pointer
  private :: create_real_array2_pointer

305c <Interfaces of utils procedures 305c>≡ (305a) 307e>
  interface create_array_pointer
    module procedure &
      create_integer_array_pointer, &
      create_real_array_pointer, &
```

```

        create_integer_array2_pointer, &
        create_real_array2_pointer
    end interface
306a <Body of create_*_array_pointer 306a>≡ (306c 307a)
    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
306b <Body of create_*_array2_pointer 306b>≡ (307)
    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
306c <Implementation of utils procedures 306c>≡ (305a) 307a>
    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 306a>
end subroutine create_integer_array_pointer

```

307a <Implementation of utils procedures 306c>+≡ (305a) <306c 307b>

```

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 306a>
end subroutine create_real_array_pointer

```

307b <Implementation of utils procedures 306c>+≡ (305a) <307a 307c>

```

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 306b>
end subroutine create_integer_array2_pointer

```

307c <Implementation of utils procedures 306c>+≡ (305a) <307b 308a>

```

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 306b>
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.

307d <Declaration of utils procedures 305b>+≡ (305a) <305b 308e>

```

public :: copy_array_pointer
private :: copy_integer_array_pointer
private :: copy_real_array_pointer
private :: copy_integer_array2_pointer
private :: copy_real_array2_pointer

```

307e <Interfaces of utils procedures 305c>+≡ (305a) <305c 309a>

```

interface copy_array_pointer
  module procedure &
    copy_integer_array_pointer, &
    copy_real_array_pointer, &
    copy_integer_array2_pointer, &
    copy_real_array2_pointer

```

```

end interface

308a <Implementation of utils procedures 306c>+≡ (305a) <307c 308b>
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

308b <Implementation of utils procedures 306c>+≡ (305a) <308a 308c>
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

308c <Implementation of utils procedures 306c>+≡ (305a) <308b 308d>
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

308d <Implementation of utils procedures 306c>+≡ (305a) <308c 309b>
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

```

308e <Declaration of utils procedures 305b>+≡ (305a) <307d 310d>
public :: swap
private :: swap_integer, swap_real

```

309a *<Interfaces of utils procedures 305c>+≡* (305a) *<307e 311a>*
 interface **swap**
 module procedure **swap_integer**, **swap_real**
 end interface

309b *<Implementation of utils procedures 306c>+≡* (305a) *<308d 309c>*
 elemental **subroutine swap_integer** (a, b)
 integer, intent(inout) :: a, b
 integer :: tmp
 tmp = a
 a = b
 b = tmp
 end **subroutine swap_integer**

309c *<Implementation of utils procedures 306c>+≡* (305a) *<309b 309d>*
 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:

309d *<Implementation of utils procedures 306c>+≡* (305a) *<309c 310b>*
 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. 309e>
 do i = 1, size (key) - 1
 <Set j to minloc(key) 310a>
 if (j /= i) then
 call **swap** (key(i), key(j))
 end if
 end do
 end **subroutine sort_real**

309e *<Set rev to reverse or .false. 309e>≡* (309 310)
 if (present (reverse)) then
 rev = reverse
 else
 rev = .false.
 end if

```

310a  <Set j to minloc(key) 310a>≡ (309 310)
      if (rev) then
         j = sum (maxloc (key(i:))) + i - 1
      else
         j = sum (minloc (key(i:))) + i - 1
      end if

310b  <Implementation of utils procedures 306c>+≡ (305a) <309d 310c>
      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. 309e>
         do i = 1, size (key) - 1
            <Set j to minloc(key) 310a>
            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

310c  <Implementation of utils procedures 306c>+≡ (305a) <310b 311c>
      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. 309e>
         do i = 1, size (key) - 1
            <Set j to minloc(key) 310a>
            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

310d  <Declaration of utils procedures 305b>+≡ (305a) <308e 311b>
      public :: sort
      private :: sort_real, sort_real_and_real_array, sort_real_and_integer

```

311a *<Interfaces of utils procedures 305c>+≡* (305a) <309a>

```

interface sort
  module procedure &
    sort_real, sort_real_and_real_array, &
    sort_real_and_integer
end interface

```

G.3 Mathematics

311b *<Declaration of utils procedures 305b>+≡* (305a) <310d 311d>

```

public :: outer_product

```

Admittedly, one has to get used to this notation for the tensor product:

311c *<Implementation of utils procedures 306c>+≡* (305a) <310c 311e>

```

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

311d *<Declaration of utils procedures 305b>+≡* (305a) <311b 313a>

```

public :: factorize, gcd, lcm
private :: gcd_internal

```

For our purposes, a straightforward implementation of Euclid's algorithm suffices:

311e *<Implementation of utils procedures 306c>+≡* (305a) <311c 311f>

```

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:

311f *<Implementation of utils procedures 306c>+≡* (305a) <311e 312a>

```

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 $m*n$ does not overflow, we can use $\text{gcd}(m, n) \text{lcm}(m, n) = mn$:

312a *<Implementation of utils procedures 306c>+≡ (305a) <311f 312b>*

```

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.

312b *<Implementation of utils procedures 306c>+≡ (305a) <312a 313c>*

```

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

```

312c *<Parameters in utils 312c>≡ (305a)*

```

integer, dimension(13), parameter, private :: &
PRIMES = (/ 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41 /)

```

G.4 I/O

313a *<Declaration of utils procedures 305b>+≡* (305a) <311d
public :: **find_free_unit**

313b *<Variables in utils 313b>≡* (305a)
integer, parameter, private :: **MIN_UNIT** = 11, **MAX_UNIT** = 99

313c *<Implementation of utils procedures 306c>+≡* (305a) <312b
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

```

314a <linalg.f90 314a>≡
! linalg.f90 --
<Copleft notice 1>
module linalg
  use kinds
  use utils
  implicit none
  private
  <Declaration of linalg procedures 314b>
  character(len=*), public, parameter :: LINALG_RCS_ID = &
    "$Id: linalg.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of linalg procedures 315>
end module linalg

```

H.1 LU Decomposition

```

314b <Declaration of linalg procedures 314b>≡ (314a) 317a>
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

$$\begin{pmatrix} a_{11} & a_{1\cdot} \\ a_{\cdot 1} & A \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ l_{\cdot 1} & L \end{pmatrix} \begin{pmatrix} u_{11} & u_{1\cdot} \\ 0 & U \end{pmatrix} = \begin{pmatrix} u_{11} & u_{1\cdot} \\ l_{\cdot 1} u_{11} & l_{\cdot 1} \otimes u_{1\cdot} + LU \end{pmatrix} \quad (\text{H.2})$$

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.

```

315 <Implementation of linalg procedures 315>≡ (314a) 317b>
  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 316a>
    vv = maxval (abs (a), dim=2)
    if (any (vv == 0.0)) then
      a = 0.0
      <pivots = 0 and eps = 0 316c>
      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 316b>
        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 316d
end subroutine lu_decompose
316a eps = 1 316a≡ (315)
    if (present (eps)) then
        eps = 1.0
    end if
316b eps = - eps 316b≡ (315)
    if (present (eps)) then
        eps = - eps
    end if
316c pivots = 0 and eps = 0 316c≡ (315)
    if (present (pivots)) then
        pivots = 0
    end if
    if (present (eps)) then
        eps = 0
    end if
316d Return optional arguments in lu_decompose 316d≡ (315)
    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

```


results in

$$A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) = \begin{pmatrix} & A'_{1p} & & A'_{1q} & & & \\ & \vdots & & \vdots & & & \\ A'_{p1} & \cdots & A'_{pq} & \cdots & A'_{pq} & \cdots & A'_{pn} \\ & & \vdots & & \vdots & & \\ A'_{q1} & \cdots & A'_{qp} & \cdots & A'_{qq} & \cdots & A'_{qn} \\ & & \vdots & & \vdots & & \\ & & A'_{np} & & A'_{nq} & & \end{pmatrix} \quad (\text{H.5})$$

318a \langle Declaration of linalg procedures 314b $\rangle + \equiv$ (314a) \langle 317a 321c \rangle
public :: diagonalize_real_symmetric

318b \langle Implementation of linalg procedures 315 $\rangle + \equiv$ (314a) \langle 317b 321b \rangle
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)
 \langle Initialize num_rot 321e \rangle
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  $A'_{pq} = 0$  319⟩
        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

```

319 *⟨Perform the Jacobi rotation resulting in $A'_{pq} = 0$ 319⟩* ≡ (318b)

```

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  $A'_{pq} = 0$  320a⟩
    ⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  320c⟩
    ⟨ $V' = V \cdot P(\phi; p, q)$  321d⟩
    ⟨Update num_rot 321f⟩
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

$$t = \frac{1}{2 \cot 2\phi} = \frac{A_{pq}}{A_{pp} - A_{qq}} \quad (\text{H.11})$$

$$h = A_{qq} - A_{pp} \quad (\text{H.12})$$

320a \langle Determine ϕ for the Jacobi rotation $P(\phi; p, q)$ with $A'_{pq} = 0$ **320a** \equiv (319) **320b** \triangleright

```

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

$$\cos^2 \phi = \frac{\cos^2 \phi}{\cos^2 \phi + \sin^2 \phi} = \frac{1}{1 + \tan^2 \phi} \quad (\text{H.13a})$$

$$\sin \phi = \tan \phi \cos \phi \quad (\text{H.13b})$$

$$\tau \sin \phi = \frac{\sin^2}{1 + \cos \phi} = \frac{1 - \cos^2}{1 + \cos \phi} = 1 - \cos \phi \quad (\text{H.13c})$$

320b \langle Determine ϕ for the Jacobi rotation $P(\phi; p, q)$ with $A'_{pq} = 0$ **320a** \equiv (319) \triangleleft **320a**

```

c = 1.0 / sqrt (1.0 + t**2)
s = t * c
tau = s / (1.0 + c)

```

$$\begin{aligned} A'_{pp} &= c^2 A_{pp} + s^2 A_{qq} - 2scA_{pq} = A_{pp} - tA_{pq} \\ A'_{qq} &= s^2 A_{pp} + c^2 A_{qq} + 2scA_{pq} = A_{qq} + tA_{pq} \\ A'_{pq} &= (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) \end{aligned} \quad (\text{H.14})$$

320c $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$ **320c** \equiv (319) **321a** \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:

$$\begin{pmatrix} & a(1:p-1,p) & & a(1:p-1,q) & \\ \cdots & A_{pq} & a(p,p+1:q-1) & A_{pq} & a(p,q+1:\text{ndim}) \\ & \vdots & & a(p+1:q-1,q) & \\ \cdots & A_{qp} & \cdots & A_{qq} & a(q,q+1:\text{ndim}) \\ & \vdots & & \vdots & \end{pmatrix} \quad (\text{H.16})$$

321a $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) \text{ 320c} \rangle + \equiv \quad (319) \langle 320c \rangle$
`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:

$$\begin{aligned} V'_p &= cV_p - sV_q = V_p - s(V_q + \tau V_p) \\ V'_q &= sV_p + cV_q = V_q + s(V_p - \tau V_q) \end{aligned} \quad (\text{H.17})$$

321b $\langle \text{Implementation of linalg procedures 315} \rangle + \equiv \quad (314a) \langle 318b \text{ 322a} \rangle$
`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`

321c $\langle \text{Declaration of linalg procedures 314b} \rangle + \equiv \quad (314a) \langle 318a \text{ 322c} \rangle$
`private :: jacobi_rotation`

321d $\langle V' = V \cdot P(\phi; p, q) \text{ 321d} \rangle + \equiv \quad (319)$
`call jacobi_rotation (s, tau, evec(:,p), evec(:,q))`

321e $\langle \text{Initialize num_rot 321e} \rangle + \equiv \quad (318b)$
`if (present (num_rot)) then`
`num_rot = 0`
`end if`

321f $\langle \text{Update num_rot 321f} \rangle + \equiv \quad (319)$
`if (present (num_rot)) then`
`num_rot = num_rot + 1`
`end if`

322a *<Implementation of linalg procedures 315>*+≡ (314a) <321b 322b>

```
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
```

322b *<Implementation of linalg procedures 315>*+≡ (314a) <322a

```
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
```

322c *<Declaration of linalg procedures 314b>*+≡ (314a) <321c

```
public :: unit, diag
```

H.4 Test

322d *<la_sample.f90 322d>*≡

```
! la_sample.f90 --
<Copleft 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=1, 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

```
324 <products.f90 324>≡
! products.f90 --
<Copleft notice 1>
module products
  use kinds
  implicit none
  private
  public :: dot, sp, spc
  character(len=*), public, parameter :: PRODUCTS_RCS_ID = &
    "$Id: products.nw 314 2010-04-17 20:32:33Z ohl $"
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

```
325a <kinematics.f90 325a>≡ 330d>
! kinematics.f90 --
<Copleft notice 1>
module kinematics
  use kinds
  use constants
  use products, only: dot
  use specfun, only: gamma
  implicit none
  private
  <Declaration of kinematics procedures 325b>
  <Interfaces of kinematics procedures 325c>
  <Declaration of kinematics types 327g>
  character(len=*), public, parameter :: KINEMATICS_RCS_ID = &
    "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of kinematics procedures 326a>
end module kinematics
```

J.1 Lorentz Transformations

```
325b <Declaration of kinematics procedures 325b>≡ (325a) 327d>
  public :: boost_velocity
  private :: boost_one_velocity, boost_many_velocity
  public :: boost_momentum
  private :: boost_one_momentum, boost_many_momentum

325c <Interfaces of kinematics procedures 325c>≡ (325a) 327f>
  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 $\gamma = 1/\sqrt{1 - \beta^2}$, $\vec{p}_{\parallel} = \vec{\beta}(\vec{\beta} \vec{p})/\beta^2$ and $\vec{p}_{\perp} = \vec{p} - \vec{p}_{\parallel}$. Using $1/\beta^2 = \gamma^2/(\gamma + 1) \cdot 1/(\gamma - 1)$ and $\vec{b} = \gamma \vec{\beta}$ this can be rewritten as

$$p'_0 = \gamma p_0 - \vec{b} \vec{p} \quad (\text{J.2a})$$

$$\vec{p}' = \vec{p} + \left(\frac{\vec{b} \vec{p}}{\gamma + 1} - p_0 \right) \vec{b} \quad (\text{J.2b})$$

326a \langle Implementation of kinematics procedures **326a** $\rangle \equiv$ (325a) **326b** \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

```

326b \langle Implementation of kinematics procedures **326a** $\rangle + \equiv$ (325a) \langle **326a** **327a** \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 $\vec{\beta} = \vec{q}/|q_0|$:

327a \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 326b 327b \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**

327b \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 327a 327c \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

327c \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 327b 328a \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**

327d \langle Declaration of kinematics procedures 325b $\rangle + \equiv$ (325a) \langle 325b 327e \rangle
 public :: **lambda**

327e \langle Declaration of kinematics procedures 325b $\rangle + \equiv$ (325a) \langle 327d 329a \rangle
 public :: two_to_three
 private :: two_to_three_massive, **two_to_three_massless**

327f \langle Interfaces of kinematics procedures 325c $\rangle + \equiv$ (325a) \langle 325c 329b \rangle
 interface two_to_three
 module procedure two_to_three_massive, **two_to_three_massless**
 end interface

327g \langle Declaration of kinematics types 327g $\rangle \equiv$ (325a)
 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 .

328a \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 327c 328b \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:

328b \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 328a 329c \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

```

329a *<Declaration of kinematics procedures 325b>*+≡ (325a) <327e 330a>

```

public :: one_to_two
private :: one_to_two_massive, one_to_two_massless

```

329b *<Interfaces of kinematics procedures 325c>*+≡ (325a) <327f

```

interface one_to_two
  module procedure one_to_two_massive, one_to_two_massless
end interface

```

329c *<Implementation of kinematics procedures 326a>*+≡ (325a) <328b 329d>

```

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

```

329d *<Implementation of kinematics procedures 326a>*+≡ (325a) <329c 330b>

```

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
330a  $\langle$ Declaration of kinematics procedures 325b $\rangle + \equiv$  (325a)  $\langle$ 329a 333c $\rangle$ 
public :: polar_to_cartesian, on_shell
330b  $\langle$ Implementation of kinematics procedures 326a $\rangle + \equiv$  (325a)  $\langle$ 329d 330c $\rangle$ 
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
330c  $\langle$ Implementation of kinematics procedures 326a $\rangle + \equiv$  (325a)  $\langle$ 330b 333d $\rangle$ 
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

$$\begin{array}{ccccc}
U_1 & \xrightarrow{\xi_1} & P_1 & \xrightarrow{\phi_1} & M \\
\pi_U \downarrow & & \downarrow \pi_P & & \parallel \\
U_2 & \xrightarrow{\xi_2} & P_2 & \xrightarrow{\phi_2} & M
\end{array} \tag{J.6}$$

$$\begin{array}{ccccc}
U_1 & \xrightarrow{\xi} & P_1 & \xrightarrow{\phi} & M \\
\pi_U \downarrow & & \downarrow \pi_P & & \downarrow \pi \\
U_2 & \xrightarrow{\xi} & P_2 & \xrightarrow{\phi} & M
\end{array} \tag{J.7}$$

```

330d  $\langle$ kinematics.f90 325a $\rangle + \equiv$   $\langle$ 325a $\rangle$ 
module phase_space
use kinds
use constants
use kinematics !NODEP!
use tao_random_numbers
implicit none
private

```

```

    <Declaration of phase_space procedures 332b>
    <Interfaces of phase_space procedures 332c>
    <Declaration of phase_space types 331a>
    character(len=*), public, parameter :: PHASE_SPACE_RCS_ID = &
        "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
contains
    <Implementation of phase_space procedures 332d>
end module phase_space

                                LIPS3_unit : [0, 1]5                                (J.8)

331a <Declaration of phase_space types 331a>≡ (330d) 331b>
    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

331b <Declaration of phase_space types 331a>+≡ (330d) <331a 331c>
    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)

331c <Declaration of phase_space types 331a>+≡ (330d) <331b 331d>
    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

331d <Declaration of phase_space types 331a>+≡ (330d) <331c 331e>
    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)

331e <Declaration of phase_space types 331a>+≡ (330d) <331d 332a>

```

```

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
332a <Declaration of phase_space types 331a>+≡ (330d) <331e>
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
332b <Declaration of phase_space procedures 332b>≡ (330d) 332f>
public :: random_LIPS3
private :: random_LIPS3_unit, random_LIPS3_unit_massless
332c <Interfaces of phase_space procedures 332c>≡ (330d)
interface random_LIPS3
  module procedure random_LIPS3_unit, random_LIPS3_unit_massless
end interface
332d <Implementation of phase_space procedures 332d>≡ (330d) 332e>
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
332e <Implementation of phase_space procedures 332d>+≡ (330d) <332d 333a>
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
332f <Declaration of phase_space procedures 332b>+≡ (330d) <332b>
private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
332g <(Unused) Interfaces of phase_space procedures 332g>≡
interface assignment(=)
  module procedure &
    LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
end interface

```

```

333a <Implementation of phase_space procedures 332d>+≡ (330d) <332e 333b>
  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

333b <Implementation of phase_space procedures 332d>+≡ (330d) <333a>
  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

```

333c <Declaration of kinematics procedures 325b>+≡ (325a) <330a 334b>
  public :: massless_isotropic_decay

```

The massless RAMBO algorithm [26]:

```

333d <Implementation of kinematics procedures 326a>+≡ (325a) <330c 334c>
  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 333e>
    <Boost and rescale the vectors 334a>
  end function massless_isotropic_decay

```

Generate a xe^{-x} distribution for $q(\mathbf{k},0)$

```

333e <Generate isotropic null vectors 333e>≡ (333d)
  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).

334a \langle Boost and rescale the vectors 334a $\rangle \equiv$ (333d)

```

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

```

334b \langle Declaration of kinematics procedures 325b $\rangle + \equiv$ (325a) \langle 333c

```

public :: phase_space_volume

```

$$V_n(s) = \frac{1}{8\pi} \frac{n-1}{(\Gamma(n))^2} \left(\frac{s}{16\pi^2} \right)^{n-2} \quad (\text{J.11})$$

334c \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 333d

```

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

334d \langle ctest.f90 334d $\rangle \equiv$

```

program ctest
  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!

```

335 <Trivial ktest.f90 335>≡
  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

```

337 <coordinates.f90 337>≡
    ! coordinates.f90 --
    <Copyleft notice 1>
    module coordinates
    use kinds
    use constants, only: PI
    use specfun, only: gamma
    implicit none
    private
    <Declaration of coordinates procedures 338a>
contains
    <Implementation of coordinates procedures 338b>
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.

```

338a <Declaration of coordinates procedures 338a>≡ (337) 339c>
      public :: spherical_to_cartesian_2, &
                spherical_to_cartesian, spherical_to_cartesian_j

338b <Implementation of coordinates procedures 338b>≡ (337) 339a>
      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 ...

- 339a *<Implementation of coordinates procedures 338b>+≡ (337) <338b 339b>*
 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`
- 339b *<Implementation of coordinates procedures 338b>+≡ (337) <339a 339d>*
 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`
- 339c *<Declaration of coordinates procedures 338a>+≡ (337) <338a 341c>*
 public :: `cartesian_to_spherical_2`, &
`cartesian_to_spherical`, `cartesian_to_spherical_j`
- 339d *<Implementation of coordinates procedures 338b>+≡ (337) <339b 341a>*
 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
341a <Implementation of coordinates procedures 338b>+≡ (337) <339d 341b>
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
341b <Implementation of coordinates procedures 338b>+≡ (337) <341a 341d>
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

```

341c <Declaration of coordinates procedures 338a>+≡ (337) <339c 342c>
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

```

341d <Implementation of coordinates procedures 338b>+≡ (337) <341b 342a>
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
342a <Implementation of coordinates procedures 338b>+≡ (337) <341d 342b>
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
342b <Implementation of coordinates procedures 338b>+≡ (337) <342a 342d>
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
342c <Declaration of coordinates procedures 338a>+≡ (337) <341c 344b>
public :: cartesian_to_spherical_cos_2, &
    cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
342d <Implementation of coordinates procedures 338b>+≡ (337) <342b 343>
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

```

```

    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

```

343 *<Implementation of coordinates procedures 338b>+≡ (337) <342d 344a>*
 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

344a *Implementation of coordinates procedures 338b*+≡ (337) <343 344c>
 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

344b *Declaration of coordinates procedures 338a*+≡ (337) <342c>
 public :: `surface`

$$\int d\Omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)} = S_n \quad (\text{K.7})$$

344c *Implementation of coordinates procedures 338b*+≡ (337) <344a>
 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

```
345a <mpi90.f90 345a>≡
! mpi90.f90 --
<Copyleft notice 1>
module mpi90
  use kinds
  use mpi
  implicit none
  private
  <Declaration of mpi90 procedures 345b>
  <Interfaces of mpi90 procedures 348c>
  <Parameters in mpi90 (never defined)>
  <Variables in mpi90 (never defined)>
  <Declaration of mpi90 types 350b>
  character(len=*), public, parameter :: MPI90_RCS_ID = &
    "$Id: mpi90.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of mpi90 procedures 346a>
end module mpi90
```

L.1 Basics

```
345b <Declaration of mpi90 procedures 345b>≡ (345a) 348b▷
  public :: mpi90_init
  public :: mpi90_finalize
  public :: mpi90_abort
  public :: mpi90_print_error
  public :: mpi90_size
  public :: mpi90_rank
```

346a *<Implementation of mpi90 procedures 346a>*≡ (345a) 346d>

```

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) 346b>
end subroutine mpi90_init

```

346b *<Handle local_error (no mpi90_abort) 346b>*≡ (346)

```

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

```

346c *<Handle local_error 346c>*≡ (346-49 351c 353d 354b 356a)

```

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

```

346d *<Implementation of mpi90 procedures 346a>*+≡ (345a) <346a 346e>

```

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 346c>
end subroutine mpi90_finalize

```

346e *<Implementation of mpi90 procedures 346a>*+≡ (345a) <346d 347a>

```

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 347b>
call mpi_abort (local_domain, local_code, local_error)
<Handle local_error (no mpi90_abort) 346b>
end subroutine mpi90_abort

```

347a <Implementation of mpi90 procedures 346a>+≡ (345a) <346e 347c>

```

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

```

347b <Set default for domain 347b>≡ (346-50 356a) 354f>

```

if (present (domain)) then
    local_domain = domain
else
    local_domain = MPI_COMM_WORLD
end if

```

347c <Implementation of mpi90 procedures 346a>+≡ (345a) <347a 348a>

```

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 347b>
    call mpi_comm_size (local_domain, sz, local_error)
    <Handle local_error 346c>
end subroutine mpi90_size

```

348a <Implementation of mpi90 procedures 346a>+≡ (345a) <347c 348d>

```

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 347b>
  call mpi_comm_rank (local_domain, rank, local_error)
  <Handle local_error 346c>
end subroutine mpi90_rank

```

L.2 Point to Point

348b <Declaration of mpi90 procedures 345b>+≡ (345a) <345b 351d>

```

public :: mpi90_send
public :: mpi90_receive
public :: mpi90_receive_pointer

```

348c <Interfaces of mpi90 procedures 348c>≡ (345a) 350d>

```

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

```

348d <Implementation of mpi90 procedures 346a>+≡ (345a) <348a 348e>

```

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

```

348e <Implementation of mpi90 procedures 346a>+≡ (345a) <348d 349a>

```

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

```

349a *<Implementation of mpi90 procedures 346a>*+≡ (345a) <348e 349c>

```

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 349b>
end subroutine mpi90_send_integer_array

```

349b *<Body of mpi90_send.*_array 349b>*≡ (349)

```

integer :: local_domain, local_error
external mpi_send
<Set default for domain 347b>
call mpi_send (buffer, size (buffer), datatype, target, tag, &
               local_domain, local_error)
<Handle local_error 346c>

```

349c *<Implementation of mpi90 procedures 346a>*+≡ (345a) <349a 349d>

```

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 349b>
end subroutine mpi90_send_double_array

```

349d *<Implementation of mpi90 procedures 346a>*+≡ (345a) <349c 350a>

```

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
350a <Implementation of mpi90 procedures 346a>+≡ (345a) <349d 350c>
    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
350b <Declaration of mpi90 types 350b>≡ (345a)
    type, public :: mpi90_status
        integer :: count, source, tag, error
    end type mpi90_status
350c <Implementation of mpi90 procedures 346a>+≡ (345a) <350a 351a>
    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
350d <Interfaces of mpi90 procedures 348c>+≡ (345a) <348c 353a>
    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
350e <Set defaults for source, tag and domain 350e>≡ (351c 353c)
    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 347b>
351a <Implementation of mpi90 procedures 346a>+≡ (345a) <350c 351b>
    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
351b <Implementation of mpi90 procedures 346a>+≡ (345a) <351a 351e>
    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 351c>
    end subroutine mpi90_receive_integer_array
351c <Body of mpi90_receive.*_array 351c>≡ (351b 352a)
    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 350e>
    call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
        local_domain, local_status, local_error)
    <Handle local_error 346c>
    if (present (status)) then
        call decode_status (status, local_status, datatype)
    end if
351d <Declaration of mpi90 procedures 345b>+≡ (345a) <348b 354d>
    private :: decode_status

```

 Can we ignore ierror???

```

351e <Implementation of mpi90 procedures 346a>+≡ (345a) <351b 352a>
    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

```

352a *<Implementation of mpi90 procedures 346a>*+≡ (345a) <351e 352b>

```

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 351c>
end subroutine mpi90_receive_double_array

```

352b *<Implementation of mpi90 procedures 346a>*+≡ (345a) <352a 352c>

```

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

```

352c *<Implementation of mpi90 procedures 346a>*+≡ (345a) <352b 353b>

```

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

```

353a *<Interfaces of mpi90 procedures 348c>*+≡ (345a) <350d 354e>

```

interface mpi90_receive_pointer
    module procedure &
        mpi90_receive_integer_pointer, mpi90_receive_double_pointer
end interface

```

353b *<Implementation of mpi90 procedures 346a>*+≡ (345a) <352c 354c>

```

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 353c>
end subroutine mpi90_receive_integer_pointer

```

353c *<Body of mpi90_receive_*.pointer 353c>*≡ (353b 354c) 353d>

```

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 350e>

```

353d *<Body of mpi90_receive_*.pointer 353c>*+≡ (353b 354c) <353c 353e>

```

call mpi_probe (local_source, local_tag, local_domain, &
    local_status, local_error)
<Handle local_error 346c>

```

 Can we ignore ierror???

353e *<Body of mpi90_receive_*.pointer 353c>*+≡ (353b 354c) <353d 354a>

```

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

354a <Body of mpi90_receive_*_pointer 353c>+≡ (353b 354c) <353e 354b>
  call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
    local_domain, local_status, local_error)

354b <Body of mpi90_receive_*_pointer 353c>+≡ (353b 354c) <354a>
  <Handle local_error 346c>
  if (present (status)) then
    call decode_status (status, local_status, datatype)
  end if

354c <Implementation of mpi90 procedures 346a>+≡ (345a) <353b 355a>
  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 353c>
  end subroutine mpi90_receive_double_pointer

```

L.3 Collective Communication

```

354d <Declaration of mpi90 procedures 345b>+≡ (345a) <351d>
  public :: mpi90_broadcast

354e <Interfaces of mpi90 procedures 348c>+≡ (345a) <353a>
  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

354f <Set default for domain 347b>+≡ (346-50 356a) <347b>
  if (present (domain)) then
    local_domain = domain
  end if

```

```

else
    local_domain = MPI_COMM_WORLD
end if

355a <Implementation of mpi90 procedures 346a>+≡ (345a) <354c 355b>
    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

355b <Implementation of mpi90 procedures 346a>+≡ (345a) <355a 355c>
    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

355c <Implementation of mpi90 procedures 346a>+≡ (345a) <355b 355d>
    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

355d <Implementation of mpi90 procedures 346a>+≡ (345a) <355c 356b>
    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 356a>
end subroutine mpi90_broadcast_integer_array

356a <Body of mpi90_broadcast_*_array 356a>≡ (355 356)
integer :: local_domain, local_error
external mpi_bcast
<Set default for domain 347b>
call mpi_bcast (buffer, size (buffer), datatype, root, &
               local_domain, local_error)
<Handle local_error 346c>

356b <Implementation of mpi90 procedures 346a>+≡ (345a) <355d 356c>
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 356a>
end subroutine mpi90_broadcast_double_array

356c <Implementation of mpi90 procedures 346a>+≡ (345a) <356b 356d>
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 356a>
end subroutine mpi90_broadcast_logical_array

356d <Implementation of mpi90 procedures 346a>+≡ (345a) <356c 357a>
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

```

357a *<Implementation of mpi90 procedures 346a>+≡* (345a) <356d 357b>
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

357b *<Implementation of mpi90 procedures 346a>+≡* (345a) <357a 357c>
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

357c *<Implementation of mpi90 procedures 346a>+≡* (345a) <357b 357d>
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

357d *<Implementation of mpi90 procedures 346a>+≡* (345a) <357c 358>
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
358 <Implementation of mpi90 procedures 346a>+≡ (345a) <357d
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

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BIBLIOGRAPHY

- [1] G. P. Lepage, *J. Comp. Phys.* **27**, 192 (1978).
- [2] G. P. Lepage, *VEGAS – An Adaptive Multi-dimensional Integration Program*, Cornell preprint, CLNS-80/447, March 1980.
- [3] T. Ohl, *Vegas Revisited: Adaptive Monte Carlo Integration Beyond Factorization*, hep-ph/9806432, Preprint IKDA 98/15, Darmstadt University of Technology, 1998.
- [4] D. E. Knuth, *Literate Programming*, Vol. 27 of *CSLI Lecture Notes* (Center for the Study of Language and Information, Leland Stanford Junior University, Stanford, CA, 1991).
- [5] N. Ramsey, *IEEE Software* **11**, 97 (1994).
- [6] American National Standards Institute, *American National Standard Programming Languages FORTRAN, ANSI X3.9-1978*, New York, 1978.
- [7] International Standards Organization, *ISO/IEC 1539:1991, Information technology — Programming Languages — Fortran*, Geneva, 1991.
- [8] International Standards Organization, *ISO/IEC 1539-1:2004, Information technology — Programming Languages — Fortran*, Geneva, 2004.
- [9] International Standards Organization, *ISO/IEC 1539:1997, Information technology — Programming Languages — Fortran*, Geneva, 1997.
- [10] High Performance Fortran Forum, *High Performance Fortran Language Specification, Version 1.1*, Rice University, Houston, Texas, 1994.
- [11] High Performance Fortran Forum, *High Performance Fortran Language Specification, Version 2.0*, Rice University, Houston, Texas, 1997.
- [12] Message Passing Interface Forum, *MPI: A Message Passing Interface Standard*, Technical Report CS-94230, University of Tennessee, Knoxville, Tennessee, 1994.

- [13] J. C. Adams, W. S. Brainerd, J. T. Martin, B. T. Smith, and J. L. Wagner, *Fortran 95 Handbook*, The MIT Press, Cambridge, MA, 1997.
- [14] Michael Metcalf and John Reid, *The F Programming Language*, (Oxford University Press, 1996).
- [15] C. H. Koelbel, D. B. Loveman, R. S. Schreiber, G. L. Steele Jr., and M. E. Zosel, *The High Performance Fortran Handbook*, The MIT Press, Cambridge, MA, 1994.
- [16] D. E. Knuth, *Seminumerical Algorithms* (third edition), Vol. 2 of *The Art of Computer Programming*, (Addison-Wesley, 1997).
- [17] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing*, 2nd edition, (Cambridge University Press, 1992)
- [18] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in Fortran77: The Art of Scientific Computing*, Volume 1 of *Fortran Numerical Recipes*, 2nd edition, (Cambridge University Press, 1992)
- [19] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in Fortran90: The Art of Parallel Scientific Computing*, Volume 2 of *Fortran Numerical Recipes*, (Cambridge University Press, 1992)
- [20] S. Kawabata, *Comp. Phys. Comm.* **41**, 127 (1986).
- [21] MINAMI-TATEYA Group, *GRACE Manual*, KEK Report 92-19.
- [22] S. Veseli, *Comp. Phys. Comm.* **108**, 9 (1998).
- [23] R. Kleiss, R. Pittau, *Weight Optimization in Multichannel Monte Carlo*, *Comp. Phys. Comm.* **83**, 141 (1994).
- [24] George Marsaglia, *The Marsaglia Random Number CD-ROM*, FSU, Dept. of Statistics and SCRI, 1996.
- [25] Y. L. Luke, *Mathematical Functions and their Approximations*, Academic Press, New York, 1975.
- [26] R. Kleiss, W. J. Stirling, S. D. Ellis, *A New Monte Carlo Treatment of Multiparticle Phase Space at High Energies*, *Comp. Phys. Comm.* **40**, 359 (1986).