

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

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## **Abstract**

We present an new implementation of the classic Vegas algorithm for adaptive multi-dimensional Monte Carlo integration in Fortran95. This implementation improves the performance for a large class of integrands, supporting stratified sampling in higher dimensions through automatic identification of the directions of largest variation. This implementation also supports multi channel sampling with individual adaptive grids. Sampling can be performed in parallel on workstation clusters and other parallel hardware.

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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:** Fortran95 [8] (Fortran90 [7] and F [13] versions available as well)
- **Number of program lines in distributed program, including test data, etc.:**  $\approx 4300$  (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 [8, 12]<sup>1</sup>. 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 it paves the road for a more parallelizable implementation.

The variable names are more in line with [1] than with [2] or with [16, 17, 18], 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) [9, 10, 14], and to the Fortran90 subset F [13] 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, 19]). 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.

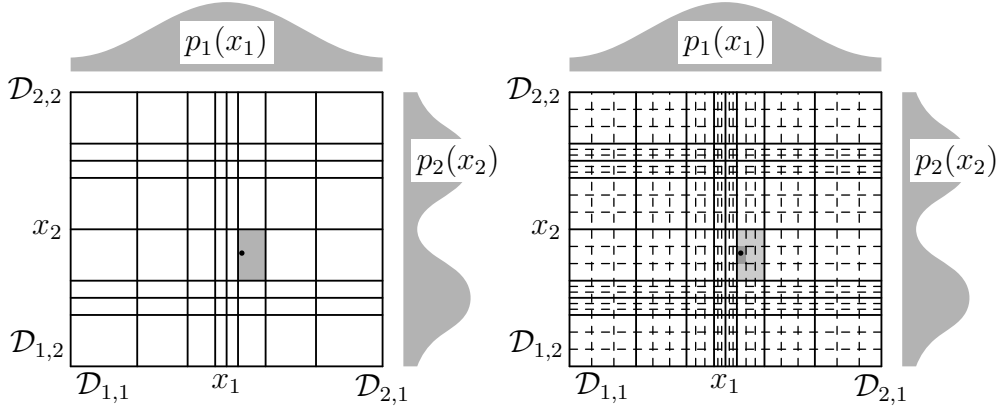


Figure 2.1: **vegas** grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions  $p_{1,2}$  are only in qualitative agreement.



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** [19], where one set of “wild” variables is separated from “smooth” variables [20].

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 [21].

### 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 [21], 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 [11]. 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 [11] takes advantage of the ability of Knuth's generator [15] to generate statistically independent subse-

<sup>2</sup>The coarsest grid covering the division of  $n_g$  bins into  $n_f$  forks has  $n_g / \gcd(n_f, n_g) = \text{lcm}(n_f, n_g) / n_f$  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 [9, 10, 14] and MPI [11], respectively. From these examples, it should be obvious how to adapt VAMP to other parallel computing paradigms.

#### Serial

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

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

#### HPF

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

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

Instead of one random number generator state `rng`, it takes an array consisting of one state per processor. These `rng(:)` are assumed to be initialized, such that the resulting sequences are statistically independent. For this purpose, Knuth's random number generator [15] 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  $\langle$ Parallel implementation of  $S_n = S_0(rS_0)^n$  (HPF) 15 $\rangle \equiv$

```

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 vamp_sample_grid_hpf

```



```

        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 [15] 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*  $\equiv$

```

subroutine vamp_sample_grid_mpi (rng, g, iterations, func)
  type(tao_random_state), dimension(:), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: iterations
  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 [8] 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, 8] 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⟩*≡

```
interface
  pure function func (xi, prc_index, weights, channel, grids) result (f)
    use kinds
    use vamp_grid_type !NODEP!
    real(kind=default), dimension(:), intent(in) :: xi
    integer, intent(in) :: prc_index
    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

```

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

```

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

```



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

```
24a <basic.f90 23a>+≡
    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>+≡
    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>+≡
    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  $\chi^2$ ).

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

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

```

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

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

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

subroutine vamp_copy_grid (lhs, rhs)

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

subroutine vamp_delete_grid (g)

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

```

#### 4.2.4 *Inout/Output and Marshling*

```

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

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

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

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

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

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

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

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

pure subroutine vamp_marshall_grid (g, integer_buffer,
    double_buffer)

```

```

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

```

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



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

```

pure subroutine vamp_marshall_grid_size (g, integer_size,
    double_size)

```

```

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

```

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

```

pure subroutine vamp_unmarshal_grid (g, integer_buffer,
    double_buffer)

```

```

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

```

Marshaling and unmarshaling need to use two separate buffers for integers and floating point numbers. In a homogeneous network, the intrinsic procedure `transfer` could be used to store the floating point numbers in the integer array. In a heterogeneous 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 [11]

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*  $\equiv$

```
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*  $\equiv$

```
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*  $\equiv$

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

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

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



```

integer, intent(in) :: channel
type(vamp_grid), dimension(:), intent(in) ::
    grids

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

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

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

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

```

Verify that

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

```

subroutine vamp_copy_grids (lhs, rhs)

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

subroutine vamp_delete_grids (g)

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

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

```

```

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

subroutine vamp_create_empty_grids (g)

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

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

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

subroutine vamp_refine_weights (g [, power)

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

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

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

subroutine vamp_reshape_grids (g, num_calls [, stratified])

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

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

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

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

```

```

    type(vamp_grids), intent(inout) :: g
    func
    integer, intent(in) :: iterations
function vamp_sum_channels (x, weights, func)

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

```

#### *4.2.6 Event Generation*

```

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

    type(vamp_grid), intent(inout) :: g
    func
    integer, intent(in) :: iterations
subroutine vamp_warmup_grids (g, [, ...])

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

```

#### *4.2.7 Parallelization*

```

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

    type(vamp_grid), intent(inout) :: g
subroutine vamp_join_grid (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_fork_grid_joints (g, [, ...])

```

```

    type(vamp_grid), intent(inout) :: g
subroutine vamp_sample_grid_parallel (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_distribute_work (g, [, ...])

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

```

#### 4.2.8 *Diagnostics*

```

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

    type(vamp_grid), intent(inout) :: g
subroutine vamp_copy_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_delete_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_terminate_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_get_history (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_get_history_single (g, [, ...])

    type(vamp_grid), intent(inout) :: g
subroutine vamp_print_history (g, [, ...])

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

```



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

#### *4.2.9 Other Procedures*

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

#### *4.2.10 (Currently) Undocumented Procedures*


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

# —5—

## IMPLEMENTATION

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

```
37a <divisions.f90 37a>≡
! divisions.f90 --
<Copyleft notice 1>
module divisions
  use kinds
  use exceptions
  use vamp_stat
  use utils
  use iso_fortran_env
  implicit none
  private
  <Declaration of divisions procedures 38a>
  <Interfaces of divisions procedures 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>≡
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>*≡

```

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

```

**38b** *<Implementation of divisions procedures 38b>*≡

```

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⟩*+≡  
 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⟩*+≡  
 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⟩*+≡  
 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>*≡

```

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>*≡

```

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⟩*≡  
 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>+≡
      public :: inject_division, inject_division_short

43b  <Implementation of divisions procedures 38b>+≡
      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>≡
    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>+≡
    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>+≡
    public :: record_integral, record_variance, clear_integral_and_variance
    ! public :: record_efficiency

```

```

44d <Implementation of divisions procedures 38b>+≡
    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>+≡*  
 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>≡*  
 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>+≡*  
 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>+≡*  
 public :: refine\_division

45e *<Implementation of divisions procedures 38b>+≡*  
 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*  $\equiv$   
`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*  $\equiv$   

```

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 *<Declaration of divisions procedures 38a>+≡*  
 private :: rebinning\_weights



The NaN test is probably not portable:

47b *<Bail out if any (d == NaN) 47b>≡*  
 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 *<Implementation of divisions procedures 38b>+≡*  
 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  
*<Increment k until  $\sum m_k \geq \Delta$  and keep the surplus in  $\delta$  48b>*  
*<Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c>*  
 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>+≡
      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>≡
      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>≡
      x_new(i) = x(k) - (x(k) - x(k-1)) * delta / m(k)

```

### 5.1.3 Probability Density

```

48d  <Declaration of divisions procedures 38a>+≡
      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>+≡
      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>+≡*  
 public :: quadrupole\_division
- 49b *<Implementation of divisions procedures 38b>+≡*  
 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>+≡*  
 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⟩+≡*

```
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⟩+≡*

```
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 Fork an importance sampling division 51a≡
  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≡
  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 88).

### *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 *⟨Setup to fork a pure stratified sampling division 52a⟩*≡

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

52b *⟨Fork a pure stratified sampling division 52b⟩*≡

```
⟨Setup to fork a pure stratified sampling division 52a⟩
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 *⟨Join pure stratified sampling divisions 52c⟩*≡

```
⟨Setup to fork a pure stratified sampling division 52a⟩
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** *<Setup to fork a pseudo stratified sampling division 53>*  $\equiv$   
`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>≡
      <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>≡
      <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>+≡
      private :: subdivide
      private :: distribute

```

```
private :: collect
```

55a *⟨Implementation of divisions procedures 38b⟩+≡*

```
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⟩+≡*

```
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⟩+≡*

```
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⟩+≡*

```
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>+≡*

```

public :: debug_division
public :: dump_division

```

56b *<Implementation of divisions procedures 38b>+≡*

```

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>+≡*

```

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>+≡*  
public :: inside\_division, stratified\_division  
public :: volume\_division, rigid\_division, adaptive\_division
- 57b *<Implementation of divisions procedures 38b>+≡*  
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>+≡*  
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>+≡*  
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>+≡*  
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>+≡*  
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>+≡*  
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>+≡*  
public :: copy\_history, summarize\_division
- 58c *<Implementation of divisions procedures 38b>+≡*  
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>+≡*  
private :: probabilities
- 58e *<Implementation of divisions procedures 38b>+≡*  
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>+≡*

```

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>+≡*

```

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(E10.3,A4,E10.3,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(E10.3,A4,E10.3,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 = "*"
    end if
  end do
end subroutine write_history

```

```

        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>+≡
    integer, private, parameter :: BUFFER_SIZE = 50

60b  <Declaration of divisions procedures 38a>+≡
    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>+≡
    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>+≡
    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>+≡
    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>+≡
    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>+≡*

```

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>≡*

```

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>+≡*

```

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>+≡*

```

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>+≡*

```

subroutine read_division_unit (d, unit, read_integrals)
  type(division_t), intent(inout) :: d
  integer, intent(in) :: unit
  logical, intent(in), optional :: read_integrals
  logical :: read_integrals0
  integer :: i, idum, num_div
  character(len=80) :: chdum
  read_integrals0 = .false.
  if (present(read_integrals)) read_integrals0 = read_integrals
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = integer_fmt) chdum, num_div
  <Insure that ubound (d%x, dim=1) == num_div 63a>
  read (unit = unit, fmt = integer_fmt) chdum, d%ng
  read (unit = unit, fmt = logical_fmt) chdum, d%stratified
  read (unit = unit, fmt = double_fmt) chdum, d%dx
  read (unit = unit, fmt = double_fmt) chdum, d%dxg
  read (unit = unit, fmt = double_fmt) chdum, d%x_min

```

```

read (unit = unit, fmt = double_fmt) chdum, d%x_max
read (unit = unit, fmt = double_fmt) chdum, d%x_min_true
read (unit = unit, fmt = double_fmt) chdum, d%x_max_true
read (unit = unit, fmt = descr_fmt) chdum
do i = 0, ubound (d%x, dim=1)
  if (read_integrals0 .and. i/=0) then
    read (unit = unit, fmt = double_array_fmt) &
      & idum, d%x(i), d%integral(i), d%variance(i)
  else
    read (unit = unit, fmt = double_array_fmt) idum, d%x(i)
  end if
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
if (.not.read_integrals0) then
  d%integral = 0.0
  d%variance = 0.0
!   d%efficiency = 0.0
end if
end subroutine read_division_unit

```



What happened to d%efficiency?

**63a** *<Insure that ubound (d%x, dim=1) == num\_div 63a>≡*

```

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

```

**63b** *<Implementation of divisions procedures 38b>+≡*

```

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⟩+≡*

```

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⟩+≡*

```

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>≡
      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>+≡
      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>+≡
    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>+≡
    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>+≡
    public :: marshal_division_size, marshal_division, unmarshal_division

66d  <Implementation of divisions procedures 38b>+≡
    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⟩*+≡

```

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⟩*+≡

```

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>+≡
    public :: marshal_div_history_size, marshal_div_history, unmarshal_div_history

68b <Implementation of divisions procedures 38b>+≡
    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>+≡
    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>+≡
    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>+≡*

```

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 $\rangle + \equiv$

```

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 $\rangle + \equiv$

```

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 $\rangle \equiv$

```
! 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>+≡
    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>+≡
    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>≡
    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>+≡
      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>≡
      integer, parameter, public :: &
         VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3

72c  <Implementation of vamp_equivalences procedures 72c>≡
      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>≡
      public :: vamp_equivalences_init

72e  <Implementation of vamp_equivalences procedures 72c>+≡
      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>+≡
      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>+≡
      public :: vamp_equivalences_final

73c  <Implementation of vamp_equivalences procedures 72c>+≡
      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>+≡
      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, "(1x,A,2(1x,I4))") "Equivalent channels:", eq%left, eq%right
        write (u, "(1x,A,25(1x,I2))") " Permutation:", eq%permutation
        write (u, "(1x,A,25(1x,I2))") " Mode:          ", eq%mode
      end subroutine vamp_equivalence_write

73e  <Declaration of vamp_equivalences procedures 72d>+≡
      public :: vamp_equivalences_write

73f  <Implementation of vamp_equivalences procedures 72c>+≡
      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, *) "Inequivalent channels:"
do ch=1, eq%n_ch
  if (eq%independent(ch)) then
    write (u, *) "  Channel", ch, ":", &
      & "    Mult. =", eq%multiplicity(ch), &
      & "    Symm. =", eq%symmetry(ch), &
      & "    Invar.:", eq%div_is_invariant(ch,:)
  end if
end do
write (u, *) "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, *) "[not allocated]"
end if
end subroutine vamp_equivalences_write

```

74a *<Declaration of vamp\_equivalences procedures 72d>+≡*  
public :: vamp\_equivalence\_set

74b *<Implementation of vamp\_equivalences procedures 72c>+≡*  
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>+≡*  
public :: vamp\_equivalences\_complete

74d *<Implementation of vamp\_equivalences procedures 72c>+≡*  
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

```

75 <vamp.f90 70c>+≡

```

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 94b>
<Constants in vamp 150a>
<Declaration of vamp types 104c>
<Variables in vamp 78a>
character(len=*), public, parameter :: VAMP_RCS_ID = &
    "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
contains
    <Implementation of vamp procedures 77c>
end module vamp_rest

```

76a <vamp.f90 70c>+≡

```

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.

76b <Declaration of vamp\_grid\_type types 76b>≡

```

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) :: 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** $\rangle \equiv$   

```

public :: vamp_copy_grid, vamp_delete_grid

```

### 5.2.1 Initialization

**77b**  $\langle$ Declaration of vamp procedures **77a** $\rangle + \equiv$   

```

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`.

**77c**  $\langle$ Implementation of vamp procedures **77c** $\rangle \equiv$   

```

pure subroutine vamp_create_grid &
    (g, domain, num_calls, num_div, &
     stratified, quadrupole, covariance, map, exc)
type(vamp_grid), intent(inout) :: g
real(kind=default), dimension(:, :), intent(in) :: domain
integer, intent(in) :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
real(kind=default), dimension(:, :), intent(in), optional :: map
type(exception), intent(inout), optional :: exc
character(len=*), parameter :: FN = "vamp_create_grid"
real(kind=default), dimension(size(domain, dim=2)) :: &
    x_min, x_max, x_min_true, x_max_true
integer :: ndim
ndim = size (domain, dim=2)
allocate (g%div(ndim), g%num_div(ndim))
x_min = domain(1, :)
x_max = domain(2, :)
if (present (map)) then
    allocate (g%map(ndim, ndim))

```

```

    g%map = map
    x_min_true = x_min
    x_max_true = x_max
    call map_domain (g%map, x_min_true, x_max_true, x_min, x_max)
    call create_division (g%div, x_min, x_max, x_min_true, x_max_true)
else
    nullify (g%map)
    call create_division (g%div, x_min, x_max)
end if
g%num_calls = num_calls
if (present (num_div)) then
    g%num_div = num_div
else
    g%num_div = NUM_DIV_DEFAULT
end if
g%stratified = .true.
g%quadrupole = .false.
g%independent = .true.
g%equivalent_to_ch = 0
g%multiplicity = 1
nullify (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
call vamp_discard_integral &
    (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
end subroutine vamp_create_grid

```

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

**78a**  $\langle \text{Variables in vamp 78a} \rangle \equiv$

integer, private, parameter :: NUM\_DIV\_DEFAULT = 20

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

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

**78b**  $\langle \text{Declaration of vamp procedures 77a} \rangle + \equiv$

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:

**78c**  $\langle \text{Implementation of vamp procedures 77c} \rangle + \equiv$

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

```

79a *⟨Implementation of vamp procedures 77c⟩*+≡  
 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

79b *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_discard\_integral

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

79c *⟨Implementation of vamp procedures 77c⟩*+≡  
 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\_gi = 0.0  
 g%sum\_integral = 0.0  
 g%sum\_weights = 0.0



```

g%sum_chi2 = 0.0
g%sum_mu_gi = 0.0
if (associated (g%sum_mu_x)) then
  g%sum_mu_x = 0.0
  g%sum_mu_xx = 0.0
end if
call set_grid_options (g, num_calls, num_div, stratified, quadrupole, &
  independent, equivalent_to_ch, multiplicity)
if ((present (num_calls)) &
  .or. (present (num_div)) &
  .or. (present (stratified)) &
  .or. (present (quadrupole)) &
  .or. (present (covariance))) then
  call vamp_reshape_grid &
    (g, g%num_calls, g%num_div, &
    g%stratified, g%quadrupole, covariance, exc)
end if
end subroutine vamp_discard_integral

```

80a *<Declaration of vamp procedures 77a>+≡*  
 private :: set\_grid\_options

80b *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine set\_grid\_options &  
 (g, num\_calls, num\_div, stratified, quadrupole, &  
 independent, equivalent\_to\_ch, multiplicity)  
 type(vamp\_grid), intent(inout) :: g  
 integer, intent(in), optional :: num\_calls  
 integer, dimension(:), intent(in), optional :: num\_div  
 logical, intent(in), optional :: stratified, quadrupole  
 logical, intent(in), optional :: independent  
 integer, intent(in), optional :: equivalent\_to\_ch, multiplicity  
 if (present (num\_calls)) then  
 g%num\_calls = num\_calls  
 end if  
 if (present (num\_div)) then  
 g%num\_div = num\_div  
 end if  
 if (present (stratified)) then  
 g%stratified = stratified  
 end if  
 if (present (quadrupole)) then  
 g%quadrupole = quadrupole  
 end if  
 if (present (independent)) then

```

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

```

### *Setting Up the Initial Grid*

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

81 *<Implementation of vamp procedures 77c>+≡*

```

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 83a>
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
    end if
end if

```

```

        g%sum_mu_xx = 0.0
    else if ((.not. covariance) .and. (associated (g%mu_x))) then
        deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
    end if
end if
end subroutine vamp_reshape_grid_internal

```

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

82a *<Declaration of vamp procedures 77a>+≡*

```

private :: vamp_reshape_grid_internal
public :: vamp_reshape_grid

```

82b *<Implementation of vamp procedures 77c>+≡*

```

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:

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

**83a** *<Adjust grid and other state for new num\_calls 83a>*≡  
 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

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

**83b** *<Adjust grid and other state for new num\_calls 83a>*+≡  
 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)  
**83c** *<Adjust grid and other state for new num\_calls 83a>*+≡  
 g%f\_min = 1.0  
 g%f\_max = 0.0

```

84a  <Declaration of vamp procedures 77a>+≡
      public :: vamp_rigid_divisions
      public :: vamp_get_covariance, vamp_nullify_covariance
      public :: vamp_get_variance, vamp_nullify_variance

84b  <Implementation of vamp procedures 77c>+≡
      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

84c  <Implementation of vamp procedures 77c>+≡
      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

84d  <Implementation of vamp procedures 77c>+≡
      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

84e  <Implementation of vamp procedures 77c>+≡
      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

```

85a *⟨Implementation of vamp procedures 77c⟩*+≡  
 elemental subroutine vamp\_nullify\_variance (g)  
 type(vamp\_grid), intent(inout) :: g  
 g%sum\_mu\_gi = 0  
end subroutine vamp\_nullify\_variance

### 5.2.2 Sampling

85b *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_sample\_grid  
 public :: vamp\_sample\_grid0  
 public :: vamp\_refine\_grid  
 public :: vamp\_refine\_grids

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

85c *⟨Implementation of vamp procedures 77c⟩*+≡  
 pure subroutine vamp\_sample\_grid0 &  
 (rng, g, func, prc\_index, channel, weights, grids, exc, &  
 negative\_weights)  
 type(tao\_random\_state), intent(inout) :: rng  
 type(vamp\_grid), intent(inout) :: g  
 integer, intent(in) :: prc\_index  
 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 86c⟩*  
 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 90a>
<Reset counters in vamp_sample_grid0 86b>
loop_over_cells: do
    <Sample calls_per_cell points in the current cell 87a>
    <Collect integration and grid optimization data for current cell 88d>
    <Count up cell, exit if done 86a>
end do loop_over_cells
<Collect results of vamp_sample_grid0 89a>
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.

```

86a <Count up cell, exit if done 86a>≡
    do j = ndim, 1, -1
        cell(j) = modulo (cell(j), rigid_division (g%div(j))) + 1
        if (cell(j) /= 1) then
            cycle loop_over_cells
        end if
    end do
    exit loop_over_cells

86b <Reset counters in vamp_sample_grid0 86b>≡
    g%mu = 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

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

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

```

```

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

```

87b  <Get x in the current cell 87b>≡
      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.

```

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

```



```

end if

88a  <Collect integration and grid optimization data for x from f 88a>≡
    if (g%f_min > g%f_max) then
        g%f_min = f * g%calls
        g%f_max = f * g%calls
    else if (f * g%calls < g%f_min) then
        g%f_min = f * g%calls
    else if (f * g%calls > g%f_max) then
        g%f_max = f * g%calls
    end if

88b  <Collect integration and grid optimization data for x from f 88a>+≡
    f2 = f * f
    sum_f = sum_f + f
    sum_f2 = sum_f2 + f2
    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

88c  <Local variables in vamp_sample_grid0 86c>+≡
    real(kind=default) :: wgt, f, f2, sum_f, sum_f2, var_f
    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


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


88d  <Collect integration and grid optimization data for current cell 88d>≡
    var_f = sum_f2 * g%calls_per_cell - sum_f**2
    if (var_f <= 0.0) then
        var_f = tiny (1.0_default)
    end if
    g%mu = g%mu + (/ sum_f, var_f /)
    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
    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.

89a  $\langle \text{Collect results of vamp\_sample\_grid0 89a} \rangle \equiv$

```

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

```

89b  $\langle \text{Collect results of vamp\_sample\_grid0 89a} \rangle + \equiv$

```

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
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

```

90a *⟨Check optional arguments in vamp\_sample\_grid0 90a⟩*≡  
 if (present (channel) .neqv. present (weights)) then  
     call raise\_exception (exc, EXC\_FATAL, FN, &  
         "channel and weights required together")  
 return  
end if

90b *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_probability

90c *⟨Implementation of vamp procedures 77c⟩*+≡  
 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

90d *⟨Implementation of vamp procedures 77c⟩*+≡  
 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

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

92a *⟨Implementation of vamp procedures 77c⟩+≡*

```

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)
  end if
end subroutine vamp_refine_grid

```

92b *⟨Implementation of vamp procedures 77c⟩+≡*

```

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)
  end do
end subroutine vamp_refine_grids

```

92c *⟨Variables in vamp 78a⟩+≡*

```

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

```

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

92d *⟨Implementation of vamp procedures 77c⟩+≡*

```

pure subroutine vamp_sample_grid &
  (rng, g, func, prc_index, 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) :: prc_index
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, prc_index, channel, weights, grids, exc)
  call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
  <Trace results of vamp_sample_grid 104d>
  <Exit iterate if accuracy has been reached 95a>
  if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
<Copy results of vamp_sample_grid to dummy variables 94c>
end subroutine vamp_sample_grid

```

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

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

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

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

93 <Implementation of vamp procedures 77c>+≡

```

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

```

94a *⟨Declaration of vamp procedures 77a⟩*  $\equiv$   
 public :: vamp\_average\_iterations  
 private :: vamp\_average\_iterations\_grid

94b *⟨Interfaces of vamp procedures 94b⟩*  $\equiv$   
 interface vamp\_average\_iterations  
 module procedure vamp\_average\_iterations\_grid  
 end interface

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

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

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

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

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

94c *⟨Copy results of vamp\_sample\_grid to dummy variables 94c⟩*  $\equiv$   
 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

```

95a *<Exit iterate if accuracy has been reached 95a>≡*

```

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

```

### 5.2.3 Forking and Joining

95b *<Declaration of vamp procedures 77a>+≡*

```

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

```

95c *<Interfaces of vamp procedures 94b>+≡*

```

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.

95d *<Implementation of vamp procedures 77c>+≡*

```

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 98b>
do j = 1, ndim
  if (j == d) then
    <call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 97c>
  else
    <call copy_division (gs%div(j), g%div(j)) 98a>
  end if
end do
if (d == 0) then
  <Handle g%calls_per_cell for d == 0 96a>
end if
<Copy the rest of g to the gs 96b>
end subroutine vamp_fork_grid_single

Divide the sampling points among identical grids
96a <Handle g%calls_per_cell for d == 0 96a>≡
  if (any (stratified_division (g%div))) then
    call raise_exception (exc, EXC_FATAL, FN, &
      "d == 0 incompatiple 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

96b <Copy the rest of g to the gs 96b>≡
  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
96c <Copy the rest of g to the gs 96b>+≡
  gs%mu(1) = 0.0
  gs%mu(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

```

97a *<Copy the rest of g to the gs 96b>+≡*

```

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

```

97b *<Copy the rest of g to the gs 96b>+≡*

```

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.

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

```

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 97d>

```

97d *<Bail out if exception exc raised 97d>≡*

```

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.

```

98a  <call copy_division (gs%div(j), g%div(j)) 98a>≡
      do i = 1, num_grids
        call copy_division (gs(i)%div(j), g%div(j))
      end do

98b  <Allocate or resize the divisions 98b>≡
      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

98c  <Implementation of vamp procedures 77c>+≡
      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)) 98d>
          else
            <call sum_division (g%div(j), gs%div(j)) 99a>
          end if
        end do
        <Combine the rest of gs onto g 99b>
      end subroutine vamp_join_grid_single

98d  <call join_division (g%div(j), gs%div(j)) 98d>≡
      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 97d>
99a <call sum_division (g%div(j), gs%div(j)) 99a>≡
    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)
99b <Combine the rest of gs onto g 99b>≡
    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_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.

```

99c <Idioms 99c>≡
    type(vamp_grid), dimension(:), allocatable :: gx
    integer, dimension(:,:), allocatable :: dim
    ...
    allocate (gx(vamp_fork_grid_joints (dim)))
    call vamp_fork_grid (g, gs, gx, dim, exc)

```

---

<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.

```

...
call vamp_join_grid (g, gs, gx, dim, exc)
100a ⟨Implementation of vamp procedures 77c⟩+≡
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
100b ⟨Declaration of vamp procedures 77a⟩+≡
public :: vamp_fork_grid_joints

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

100c ⟨Implementation of vamp procedures 77c⟩+≡
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

```

101a *⟨Implementation of vamp procedures 77c⟩*+≡

```

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

```

#### 5.2.4 Parallel Execution

101b *⟨Declaration of vamp procedures 77a⟩*+≡

```

public :: vamp_sample_grid_parallel
public :: vamp_distribute_work

```

HPF [9, 10, 14]:

101c *<Implementation of vamp procedures 77c>+≡*

```

subroutine vamp_sample_grid_parallel &
  (rng, g, func, prc_index, 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
  integer, intent(in) :: prc_index
  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, prc_index, &
           channel, weights, grids, exc)
      end do
    end if
  end do

```

```

    <Gather exceptions in vamp_sample_grid_parallel 103a>
    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, prc_index, channel, weights, grids, exc)
end if
<Bail out if exception exc raised 97d>
call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
<Trace results of vamp_sample_grid 104d>
<Exit iterate if accuracy has been reached 95a>
if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
deallocate (d)
<Copy results of vamp_sample_grid to dummy variables 94c>
end subroutine vamp_sample_grid_parallel
103a <Gather exceptions in vamp_sample_grid_parallel 103a>≡
    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.

```

103b <Implementation of vamp procedures 77c>+≡
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 104a⟩
end do try
end subroutine vamp_distribute_work
104a ⟨Accept distribution among n workers 104a⟩≡
    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
104b ⟨Accept distribution among n workers 104a⟩+≡
    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

```

### 5.2.5 Diagnostics

```

104c ⟨Declaration of vamp types 104c⟩≡
    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
104d ⟨Trace results of vamp_sample_grid 104d⟩≡
    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

105a <Declaration of vamp procedures 77a>+≡
    public :: vamp_create_history, vamp_copy_history, vamp_delete_history
    public :: vamp_terminate_history
    public :: vamp_get_history, vamp_get_history_single

105b <Interfaces of vamp procedures 94b>+≡
    interface vamp_get_history
        module procedure vamp_get_history_single
    end interface

105c <Implementation of vamp procedures 77c>+≡
    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

105d <Implementation of vamp procedures 77c>+≡
    elemental subroutine vamp_terminate_history (h)
        type(vamp_history), intent(inout) :: h
        h%calls = 0.0
    end subroutine vamp_terminate_history

105e <Implementation of vamp procedures 77c>+≡

```

```

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 106a
    call copy_history (h%div, summarize_division (g%div))
  end if
end subroutine vamp_get_history_single

106a Adjust h%div iff necessary 106a ≡
  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

106b Declaration of vamp procedures 77a +≡
  public :: vamp_print_history, vamp_write_history
  private :: vamp_print_one_history, vamp_print_histories
  ! private :: vamp_write_one_history, vamp_write_histories

106c Interfaces of vamp procedures 94b +≡
  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

106d Implementation of vamp procedures 77c +≡
  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
    if (h(i)%stratified) then
        s = "*"
    else
        s = ""
    end if
    print "(1X,A8,1X,I2,I9,A1,1X,E11.4,A1,E8.2,A1," &
        // "1X,E13.6,A1,E8.2,A1,F5.1,1X,F5.3)", pfx, &
        i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
        h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &
        h(i)%integral / h(i)%f_max
end do iterations
print "(1X,A78)", repeat("-", 78)
if (all (h%verbose) .and. (imax >= 1)) then
    if (associated (h(1)%div)) then
        allocate (h_tmp(imax))
        dimensions: do j = 1, size (h(1)%div)
            do i = 1, imax
                call copy_history (h_tmp(i), h(i)%div(j))
            end do
            if (present (tag)) then
                write (unit = pfx, fmt = "(A,A1,I2.2)") &
                    trim (tag(1:min(len_trim(tag),8))), "#", j
            else
                write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
            end if
        end do
    end if
end if

```

```

        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

```

108a *<Variables in vamp 78a>+≡*

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

108b *<Implementation of vamp procedures 77c>+≡*

```

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

```



108c *<Implementation of vamp procedures 77c>+≡*

```

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
    end if

```

```

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,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
write (u, "(1X,A78)") repeat ("-", 78)
if (all (h%verbose) .and. (imax >= 1)) then
    if (associated (h(1)%div)) then
        allocate (h_tmp(imax))
        dimensions: do j = 1, size (h(1)%div)
            do i = 1, imax
                call copy_history (h_tmp(i), h(i)%div(j))
            end do
            if (present (tag)) then
                write (unit = pfx, fmt = "(A,A1,I2.2)") &
                    trim (tag(1:min(len_trim(tag),8))), "#", j
            else
                write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
            end if
            call write_history (u, h_tmp, tag = pfx)
        print "(1X,A78)", repeat ("-", 78)
        end do dimensions
    end if
end if

```

```

        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

```

### 5.2.6 Multi Channel

[22]

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

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

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.

111a  $\langle$ Declaration of `vamp` types 104c $\rangle + \equiv$

```
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
```

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

111b  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$

```
public :: vamp_multi_channel, vamp_multi_channel0
```

111c  $\langle$ Implementation of `vamp` procedures 77c $\rangle + \equiv$

```
pure function vamp_multi_channel &
  (func, prc_index, phi, ihp, jacobian, x, weights, channel, grids) result (w_x)
  integer, intent(in) :: prc_index
  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
   $\langle$ Interface declaration for func 22 $\rangle$ 
   $\langle$ Interface declaration for phi 31a $\rangle$ 
   $\langle$ Interface declaration for ihp 31b $\rangle$ 
   $\langle$ Interface declaration for jacobian 31c $\rangle$ 
  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, prc_index, i)
end do
w_x = func (phi_x, prc_index, weights, channel, grids) &
    / dot_product (weights, g_phi_x)
end function vamp_multi_channel

```

112a *<Implementation of vamp procedures 77c>+≡*

```

pure function vamp_multi_channel0 &
    (func, prc_index, phi, jacobian, x, weights, channel) result (w_x)
integer, intent(in) :: prc_index
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, prc_index, i)
end do
w_x = func (x_prime, prc_index) / dot_product (weights, g_phi_x)
end function vamp_multi_channel0

```



WK

112b *<Declaration of vamp procedures 77a>+≡*

```

public :: vamp_jacobian, vamp_check_jacobian

```

112c *<Implementation of vamp procedures 77c>+≡*

```

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
  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

```

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

113 *⟨Implementation of vamp procedures 77c⟩+≡*

```

pure subroutine vamp_check_jacobian &
  (rng, n, func, prc_index, phi, channel, region, delta, x_delta)
type(tao_random_state), intent(inout) :: rng
integer, intent(in) :: n
integer, intent(in) :: prc_index

```

```

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), prc_index, 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.

114a <Declaration of vamp procedures (removed from WHIZARD) 114a>≡  
 private :: numeric\_jacobian

114b <Implementation of vamp procedures (removed from WHIZARD) 114b>≡  
 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

```

115a *<Declaration of vamp procedures 77a>+≡*  
 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 [8]) even if the dummy argument is optional itself.

115b *<Implementation of vamp procedures 77c>+≡*  
 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

```

116a *<Implementation of vamp procedures 77c>+≡*

```

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

```

116b *<Declaration of vamp procedures 77a>+≡*

```

public :: vamp_discard_integrals

```

116c *<Implementation of vamp procedures 77c>+≡*

```

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

```

```

        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
117a <Declaration of vamp procedures 77a>+≡
    public :: vamp_update_weights
We must discard the accumulated integrals, because the weight function  $w = f / \sum_i \alpha_i g_i$  changes:
117b <Implementation of vamp procedures 77c>+≡
    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
117c <Declaration of vamp procedures 77a>+≡
    public :: vamp_reshape_grids
117d <Implementation of vamp procedures 77c>+≡
    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

```

118a *<Declaration of vamp procedures 77a>+≡*  
 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`.

118b *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_sample\_grids &  
   (rng, g, func, prc\_index, 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  
 integer, intent(in) :: prc\_index

```

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) 120a>
        else
            call vamp_nullify_variance (g%grids(ch))
            call vamp_nullify_covariance (g%grids(ch))
        end if
    end do
    if (present(eq)) call vamp_apply_equivalences (g, eq)
    if (iteration < iterations) then
        do ch = 1, size (g%grids)
            active(ch) = (integrals(ch) /= 0)
            if (active(ch)) then

```



```

        call vamp_refine_grid (g%grids(ch))
    end if
end do
end if
if (present (exc) .and. (any (excs%level > 0))) then
    call gather_exceptions (exc, excs)
!    return
end if
call vamp_reduce_channels (g, integrals, std_devs, active)
call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
    <Trace results of vamp_sample_grids 123a>
    <Exit iterate if accuracy has been reached 95a>
end do iterate
    <Copy results of vamp_sample_grid to dummy variables 94c>
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`:

```

120a <Sample the grid g%grids(ch) 120a>≡
    call vamp_sample_grid0 &
        (rng, g%grids(ch), func, prc_index, &
        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

120b <Declaration of vamp procedures 77a>+≡
    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

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

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

121a *Implementation of vamp procedures 77c*)+≡

```
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
```

121b *Declaration of vamp procedures 77a*)+≡

```
public :: vamp_refine_weights
```

122a *⟨Implementation of vamp procedures 77c⟩*+≡

```

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

```

122b *⟨Declaration of vamp procedures 77a⟩*+≡

```

private :: vamp_average_iterations_grids

```

122c *⟨Interfaces of vamp procedures 94b⟩*+≡

```

interface vamp_average_iterations
  module procedure vamp_average_iterations_grids
end interface

```

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

122d *⟨Implementation of vamp procedures 77c⟩*+≡

```

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

```

```

123a  <Trace results of vamp_sample_grids 123a>≡
      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

123b  <Declaration of vamp procedures 77a>+≡
      private :: vamp_get_history_multi

123c  <Interfaces of vamp procedures 94b>+≡
      interface vamp_get_history
        module procedure vamp_get_history_multi
      end interface

123d  <Implementation of vamp procedures 77c>+≡
      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

```



```

123e  <Declaration of vamp procedures 77a>+≡
      public :: vamp_sum_channels

```

124 *Implementation of vamp procedures 77c*+≡

```

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

```

### 5.2.7 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.

```

125a  <Declaration of vamp procedures 77a>+≡
      public :: select_rotation_axis
      public :: select_rotation_subspace

125b  <Set iv to the index of the optimal eigenvector 125b>≡
      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

125c  <Implementation of vamp procedures 77c>+≡
      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

```

126a *<Declaration of vamp procedures 77a>+≡*  
 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>

126b *<Set i(1), i(2) to the axes of the optimal plane 126b>≡*  
 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:

126c *<Set i(1), i(2) to the axes of the optimal plane (broken!) 126c>≡*  
 abs\_evec = abs (evecs(:,iv))  
 i(1) = sum (maxloc (abs\_evec))  
 i(2) = sum (maxloc (abs\_evec, mask = abs\_evec < abs\_evec(i(1))))

126d *<Set i(1), i(2) to the axes of the optimal plane 126b>+≡*  
 print \*, iv, evals(iv), " => ", evecs(:,iv)  
 print \*, i(1), abs\_evec(i(1)), ", ", i(2), abs\_evec(i(2))  
 print \*, i(1), evecs(i(1),iv), ", ", i(2), evecs(i(2),iv)

---

<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.

127a  $\langle$ Get  $\cos \theta$  and  $\sin \theta$  from *evecs* 127a $\rangle \equiv$

```
cos_theta = evecs(i(1),iv)
sin_theta = evecs(i(2),iv)
norm = 1.0 / sqrt (cos_theta**2 + sin_theta**2)
cos_theta = cos_theta * norm
sin_theta = sin_theta * norm
```

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

127b  $\langle$ Construct  $\hat{R}(\theta; i, j)$  127b $\rangle \equiv$

```
call unit (r)
r(i(1),i) = (/ cos_theta, - sin_theta /)
r(i(2),i) = (/ sin_theta, cos_theta /)
```

127c  $\langle$ Implementation of *vamp* procedures 77c $\rangle + \equiv$

```
subroutine select_rotation_axis (cov, r, pancake, cigar)
  real(kind=default), dimension(:, :), intent(in) :: cov
  real(kind=default), dimension(:, :), intent(out) :: r
  integer, intent(in), optional :: pancake, cigar
  integer :: num_pancake, num_cigar
  logical :: like_pancake
  real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evecs
  real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
  integer :: iv
  integer, dimension(2) :: i
  real(kind=default) :: cos_theta, sin_theta, norm
   $\langle$ Handle optional pancake and cigar 127d $\rangle$ 
  call diagonalize_real_symmetric (cov, evals, evecs)
   $\langle$ Set iv to the index of the optimal eigenvector 125b $\rangle$ 
   $\langle$ Set i(1), i(2) to the axes of the optimal plane 126b $\rangle$ 
   $\langle$ Get  $\cos \theta$  and  $\sin \theta$  from evecs 127a $\rangle$ 
   $\langle$ Construct  $\hat{R}(\theta; i, j)$  127b $\rangle$ 
end subroutine select_rotation_axis
```

127d  $\langle$ Handle optional *pancake* and *cigar* 127d $\rangle \equiv$

```
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:

128a *<Implementation of vamp procedures 77c>+≡*

```

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

```

128b *<Implementation of vamp procedures 77c>+≡*

```

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 127d>
    call diagonalize_real_symmetric (cov, evals, evecs)
    <Set iv to the index of the optimal eigenvector 125b>
    <Set subspace to the axes of the optimal plane 128c>
    call select_subspace_explicit (cov, r, subspace)
end subroutine select_subspace_guess

```

128c *<Set subspace to the axes of the optimal plane 128c>≡*

```

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

129a <Interfaces of vamp procedures 94b>+≡
    interface select_rotation_subspace
        module procedure select_subspace_explicit, select_subspace_guess
    end interface

129b <Declaration of vamp procedures 77a>+≡
    private :: select_subspace_explicit
    private :: select_subspace_guess

129c <Declaration of vamp procedures 77a>+≡
    public :: vamp_print_covariance

129d <Implementation of vamp procedures 77c>+≡
    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.


130a  $\langle$ Declaration of `vamp` procedures 77a $\rangle + \equiv$

```

! 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!

130b  $\langle$ Initialize clusters 130b $\rangle \equiv$

```

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.

```

131a  <Join closest clusters 131a>≡
      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)

131b  <Join closest clusters 131a>+≡
      cl_pos(gap+1:cl_num-1) = cl_pos(gap+2:cl_num)
      cl(gap+1:cl_num-1,:) = cl(gap+2:cl_num,:)

131c  <Implementation of vamp procedures 77c>+≡
      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 130b>
        do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
          <Join closest clusters 131a>
          print *, cl_num, ": action = ", condense_action (x, cl)
        end do
        cluster_pos = cl_pos(1:cl_num)
        clusters = cl(1:cl_num,:)
      end subroutine condense

131d  <Declaration of vamp procedures 77a>+≡
      ! private :: condense_action
      public :: condense_action

```

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

132a *<Implementation of vamp procedures 77c>+≡*

```
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
```

132b *<ctest.f90 132b>≡*

```
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

```

### 5.2.8 Event Generation

Automagically adaptive tools are not always appropriate for unweighted event generation, but we can give it a try.

133a *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_next\_event

133b *⟨Interfaces of vamp procedures 94b⟩*+≡  
 interface vamp\_next\_event  
 module procedure vamp\_next\_event\_single, vamp\_next\_event\_multi  
 end interface

133c *⟨Declaration of vamp procedures 77a⟩*+≡  
 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.

133d *⟨Implementation of vamp procedures 77c⟩*+≡  
 pure subroutine vamp\_next\_event\_single &  
 (x, rng, g, func, prc\_index, &  
 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) :: prc\_index  
 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) 134a⟩*  
 if (present (weight)) then

```

        <Unconditionally accept weighted event 134b>
    else
        <Maybe accept unweighted event 134c>
    end if
end do rejection
end subroutine vamp_next_event_single

134a <Choose a x and calculate f(x) 134a>≡
    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 87c>
    ! call record_efficiency (g%div, ia, f/g%f_max)

134b <Unconditionally accept weighted event 134b>≡
    weight = f
    exit rejection

134c <Maybe accept unweighted event 134c>≡
    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  $w(x)$ .

```

134d <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_next_event_multi &
        (x, rng, g, func, prc_index, phi, weight, excess, exc)
        real(kind=default), dimension(:), intent(out) :: x

```

```

type(tao_random_state), intent(inout) :: rng
type(vamp_grids), intent(inout) :: g
integer, intent(in) :: prc_index
real(kind=default), intent(out), optional :: weight
real(kind=default), intent(out), optional :: excess
type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>
<Interface declaration for phi 31a>
character(len=*), parameter :: FN = "vamp_next_event_multi"
real(kind=default), dimension(size(x)) :: xi
real(kind=default) :: r, wgt
real(kind=default), dimension(size(g%weights)) :: weights
integer :: channel
<weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  135>
rejection: do
  <Select channel from weights 136a>
  call vamp_next_event_single &
    (xi, rng, g%grids(channel), func, prc_index, wgt, &
      channel, g%weights, g%grids, exc)
  if (present (weight)) then
    <Unconditionally accept weighted multi channel event 136b>
  else
    <Maybe accept unweighted multi channel event 136c>
  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.

```

135 <weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  135> ≡
  if (any (g%grids%f_max > 0)) then
    weights = g%weights * g%grids%f_max
  else
    weights = g%weights
  end if

```



```

end if
weights = weights / sum (weights)
136a <Select channel from weights 136a>≡
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
136b <Unconditionally accept weighted multi channel event 136b>≡
weight = wgt * g%weights(channel) / weights(channel)
exit rejection
136c <Maybe accept unweighted multi channel event 136c>≡
if (wgt > g%grids(channel)%f_max) then
  if (present(excess)) then
    excess = 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 <= wgt) then
  exit rejection
end if
136d <Maybe accept unweighted multi channel event (old version) 136d>≡
if (wgt > g%grids(channel)%f_max) then
  g%grids(channel)%f_max = wgt
  <weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  135>
  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.

137a *<Declaration of vamp procedures 77a>+≡*  
`public :: vamp_warmup_grid, vamp_warmup_grids`

137b *<Implementation of vamp procedures 77c>+≡*  
`pure subroutine vamp_warmup_grid &`  
`(rng, g, func, prc_index, iterations, exc, history)`  
`type(tao_random_state), intent(inout) :: rng`  
`type(vamp_grid), intent(inout) :: g`  
`integer, intent(in) :: prc_index`  
`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, prc_index, &`  
`iterations - 1, exc = exc, history = history)`  
`call vamp_sample_grid0 (rng, g, func, prc_index, exc = exc)`  
`end subroutine vamp_warmup_grid`



WHERE ... END WHERE alert!

137c *<Implementation of vamp procedures 77c>+≡*  
`pure subroutine vamp_warmup_grids &`  
`(rng, g, func, prc_index, iterations, history, histories, exc)`  
`type(tao_random_state), intent(inout) :: rng`  
`type(vamp_grids), intent(inout) :: g`  
`integer, intent(in) :: prc_index`  
`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, prc_index, 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, prc_index, &
             ch, weights, g%grids, exc = exc)
    end if
end do
end subroutine vamp_warmup_grids

```

### 5.2.9 Convenience Routines

- 138a *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_integrate  
 private :: vamp\_integrate\_grid, vamp\_integrate\_region
- 138b *<Interfaces of vamp procedures 94b>+≡*  
 interface vamp\_integrate  
 module procedure vamp\_integrate\_grid, vamp\_integrate\_region  
 end interface
- 138c *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_integrate\_grid &  
 (rng, g, func, prc\_index, 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  
 integer, intent(in) :: prc\_index  
 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, prc_index, calls(1,step), &
                           exc = exc, history = history(it:))
    <Bail out if exception exc raised 97d>
    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, prc_index, calls(1,last_step), &
                       integral, std_dev, avg_chi2, accuracy, exc = exc, &
                       history = history(it:))
end subroutine vamp_integrate_grid

```

139 *<Implementation of vamp procedures 77c>+≡*

```

pure subroutine vamp_integrate_region &
    (rng, region, func, prc_index, 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
integer, intent(in) :: prc_index
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, prc_index, 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

140a <Declaration of vamp procedures 77a>+≡
    public :: vamp_integratex
    private :: vamp_integratex_region

140b <Interfaces of vamp procedures 94b>+≡
    interface vamp_integratex
        module procedure vamp_integratex_region
    end interface

140c <Implementation of vamp procedures 77c>+≡
    subroutine vamp_integratex_region &
        (rng, region, func, prc_index, 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
    integer, intent(in) :: prc_index
    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, prc_index, calls(:,:), num_div = num_div, &
         exc = exc, history = history(it:))
    <Bail out if exception exc raised 97d>
    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, prc_index, calls(:, :, step), num_div = num_div, &
     exc = exc, history = history(it:))
  <Bail out if exception exc raised 97d>
  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, prc_index, 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

```

### 5.2.10 I/O

- 141a *<Declaration of vamp procedures 77a>+≡*
- ```

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

```
- 141b *<Declaration of vamp procedures 77a>+≡*
- ```

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

```

142a *<Interfaces of vamp procedures 94b>+≡*

```

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

```

142b *<Interfaces of vamp procedures 94b>+≡*

```

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

```

142c *<Implementation of vamp procedures 77c>+≡*

```

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) "sum_integral = ", g%sum_integral
write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
write (unit = unit, fmt = double_fmt) "calls = ", g%calls
write (unit = unit, fmt = double_fmt) "dv2g = ", g%dv2g
write (unit = unit, fmt = double_fmt) "jacobi = ", g%jacobi
write (unit = unit, fmt = double_fmt) "f_min = ", g%f_min
write (unit = unit, fmt = double_fmt) "f_max = ", g%f_max
write (unit = unit, fmt = double_fmt) "mu_gi = ", g%mu_gi
write (unit = unit, fmt = double_fmt) "sum_mu_gi = ", g%sum_mu_gi
write (unit = unit, fmt = descr_fmt) "begin g%num_div"
do i = 1, size (g%div)
    write (unit = unit, fmt = integer_array_fmt) i, g%num_div(i)
end do
write (unit = unit, fmt = descr_fmt) "end g%num_div"
write (unit = unit, fmt = descr_fmt) "begin g%div"
do i = 1, size (g%div)
    call write_division (g%div(i), unit, write_integrals)
end do
write (unit = unit, fmt = descr_fmt) "end g%div"
if (associated (g%map)) then
    write (unit = unit, fmt = descr_fmt) "begin g%map"
    do i = 1, size (g%div)
        do j = 1, size (g%div)
            write (unit = unit, fmt = double_array2_fmt) i, j, g%map(i,j)
        end do
    end do
    write (unit = unit, fmt = descr_fmt) "end g%map"
else
    write (unit = unit, fmt = descr_fmt) "empty g%map"
end if
if (associated (g%mu_x)) then
    write (unit = unit, fmt = descr_fmt) "begin g%mu_x"
    do i = 1, size (g%div)
        write (unit = unit, fmt = double_array_fmt) i, g%mu_x(i)
        write (unit = unit, fmt = double_array_fmt) i, g%sum_mu_x(i)
    do j = 1, size (g%div)
        write (unit = unit, fmt = double_array2_fmt) i, j, g%mu_xx(i,j)

```



```

        write (unit = unit, fmt = double_array2_fmt) i, j, g%sum_mu_xx(i,j)
    end do
end do
write (unit = unit, fmt = descr_fmt) "end g%mu_x"
else
    write (unit = unit, fmt = descr_fmt) "empty g%mu_x"
end if
write (unit = unit, fmt = descr_fmt) "end type(vamp_grid)"
end subroutine write_grid_unit

```

144a *<Variables in vamp 78a>+≡*

```

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,e30.22)", &
    double_array_fmt =   "(1x,i17,1x,e30.22)", &
    double_array2_fmt =  "(2(1x,i8),1x,e30.22)"

```

144b *<Implementation of vamp procedures 77c>+≡*

```

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 146a>
    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%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. 146b>
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. 146c>
        end if
        read (unit = unit, fmt = descr_fmt) chdum
    end subroutine read_grid_unit

146a <Insure that size (g%div) == ndim 146a>≡
    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

146b <Insure that associated (g%map) == .false. 146b>≡
    if (associated (g%map)) then
        deallocate (g%map)
    end if

146c <Insure that associated (g%mu_x) == .false. 146c>≡
    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

146d <Implementation of vamp procedures 77c>+≡
    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

```

147a *<Implementation of vamp procedures 77c>+≡*

```

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

```

147b *<Implementation of vamp procedures 77c>+≡*

```

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

```

148a *⟨Implementation of vamp procedures 77c⟩*+≡

```

subroutine read_grids_unit (g, unit, read_integrals)
  type(vamp_grids), intent(inout) :: g
  integer, intent(in) :: unit
  logical, intent(in), optional :: read_integrals
  character(len=*), parameter :: FN = "vamp_read_grids"
  character(len=80) :: chdum
  integer :: i, nch, idum
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = integer_fmt) chdum, nch
  if (associated (g%grids)) then
    if (size (g%grids) /= nch) then
      call vamp_delete_grid (g%grids)
      deallocate (g%grids, g%weights, g%num_calls)
      allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
      call vamp_create_empty_grid (g%grids)
    end if
  else
    allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
    call vamp_create_empty_grid (g%grids)
  end if
  read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
  read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
  read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
  read (unit = unit, fmt = descr_fmt) chdum
  do i = 1, nch
    read (unit = unit, fmt = double_array_fmt) idum, g%weights(i)
  end do
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = descr_fmt) chdum
  do i = 1, nch
    read (unit = unit, fmt = integer_array_fmt) idum, g%num_calls(i)
  end do
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = descr_fmt) chdum
  do i = 1, nch
    call read_grid_unit (g%grids(i), unit, read_integrals)
  end do
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = descr_fmt) chdum
end subroutine read_grids_unit

```

148b *⟨Implementation of vamp procedures 77c⟩*+≡

```

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

```

149a *⟨Implementation of vamp procedures 77c⟩+≡*

```

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

```

149b *⟨Implementation of vamp procedures 77c⟩+≡*

```

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%sum_integral
write (unit = unit) g%sum_weights
write (unit = unit) g%sum_chi2
write (unit = unit) g%calls
write (unit = unit) g%dv2g
write (unit = unit) g%jacobi
write (unit = unit) g%f_min
write (unit = unit) g%f_max

```

```

write (unit = unit) g%mu_gi
write (unit = unit) g%sum_mu_gi
do i = 1, size (g%div)
  write (unit = unit) g%num_div(i)
end do
do i = 1, size (g%div)
  call write_division_raw (g%div(i), unit, write_integrals)
end do
if (associated (g%map)) then
  write (unit = unit) MAGIC_GRID_MAP
  do i = 1, size (g%div)
    do j = 1, size (g%div)
      write (unit = unit) g%map(i,j)
    end do
  end do
else
  write (unit = unit) MAGIC_GRID_EMPTY
end if
if (associated (g%mu_x)) then
  write (unit = unit) MAGIC_GRID_MU_X
  do i = 1, size (g%div)
    write (unit = unit) g%mu_x(i)
    write (unit = unit) g%sum_mu_x(i)
    do j = 1, size (g%div)
      write (unit = unit) g%mu_xx(i,j)
      write (unit = unit) g%sum_mu_xx(i,j)
    end do
  end do
else
  write (unit = unit) MAGIC_GRID_EMPTY
end if
write (unit = unit) MAGIC_GRID_END
end subroutine write_grid_raw_unit

```

150a *⟨Constants in vamp 150a⟩*≡

```

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

```

150b *⟨Implementation of vamp procedures 77c⟩*+≡

```

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 146a>
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%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

```



```

        end do
    else if (magic == MAGIC_GRID_EMPTY) then
        <Insure that associated (g%map) == .false. 146b>
    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. 146c>
    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

152 <Implementation of vamp procedures 77c>+≡
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

153a  <Implementation of vamp procedures 77c>+≡
    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

153b  <Implementation of vamp procedures 77c>+≡
    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

153c  <Constants in vamp 150a>+≡
    integer, parameter, private :: MAGIC_GRIDS = 33333333
    integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1

```

```

integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2
154  <Implementation of vamp procedures 77c>+≡
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

155a  <Implementation of vamp procedures 77c>+≡
    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

155b  <Implementation of vamp procedures 77c>+≡
    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

```

### 5.2.11 Marshaling

```

155c  <Declaration of vamp procedures 77a>+≡
    public :: vamp_marshall_grid_size, vamp_marshall_grid, vamp_unmarshal_grid

155d  <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_marshall_grid (g, ibuf, dbuf)
        type(vamp_grid), intent(in) :: g
        integer, dimension(:), intent(inout) :: ibuf
        real(kind=default), dimension(:), intent(inout) :: dbuf
        integer :: i, iwords, dwords, iidx, didx, ndim
        ndim = size (g%div)
        ibuf(1) = g%num_calls
        ibuf(2) = g%calls_per_cell
        ibuf(3) = ndim
        if (g%stratified) then

```

```

        ibuf(4) = 1
    else
        ibuf(4) = 0
    end if
    if (g%all_stratified) then
        ibuf(5) = 1
    else
        ibuf(5) = 0
    end if
    if (g%quadrupole) then
        ibuf(6) = 1
    else
        ibuf(6) = 0
    end if
    dbuf(1:2) = g%mu
    dbuf(3) = g%sum_integral
    dbuf(4) = g%sum_weights
    dbuf(5) = g%sum_chi2
    dbuf(6) = g%calls
    dbuf(7) = g%dv2g
    dbuf(8) = g%jacobi
    dbuf(9) = g%f_min
    dbuf(10) = g%f_max
    dbuf(11) = g%mu_gi
    dbuf(12) = g%sum_mu_gi
    ibuf(7:6+ndim) = g%num_div
    iidx = 7 + ndim
    didx = 13
    do i = 1, ndim
        call marshal_division_size (g%div(i), iwords, dwords)
        ibuf(iidx) = iwords
        ibuf(iidx+1) = dwords
        iidx = iidx + 2
        call marshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
                               dbuf(didx:didx-1+dwords))

        iidx = iidx + iwords
        didx = didx + dwords
    end do
    if (associated (g%map)) then
        ibuf(iidx) = 1
        dbuf(didx:didx-1+ndim**2) = reshape (g%map, (/ ndim**2 /))
        didx = didx + ndim**2
    else

```

```

        ibuf(iidx) = 0
    end if
    iidx = iidx + 1
    if (associated (g%mu_x)) then
        ibuf(iidx) = 1
        dbuf(didx:didx-1+ndim) = g%mu_x
        didx = didx + ndim
        dbuf(didx:didx-1+ndim) = g%sum_mu_x
        didx = didx + ndim
        dbuf(didx:didx-1+ndim**2) = reshape (g%mu_xx, (/ ndim**2 /))
        didx = didx + ndim**2
        dbuf(didx:didx-1+ndim**2) = reshape (g%sum_mu_xx, (/ ndim**2 /))
        didx = didx + ndim**2
    else
        ibuf(iidx) = 0
    end if
    iidx = iidx + 1
end subroutine vamp_marshall_grid

```

157a *⟨Implementation of vamp procedures 77c⟩*+≡

```

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

```

157b *⟨Implementation of vamp procedures 77c⟩*+≡

```

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 146a>
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. 146b>
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. 146c>
    end if
    iidx = iidx + 1
end subroutine vamp_unmarshal_grid

159a <Declaration of vamp procedures 77a>+≡
    public :: vamp_marshal_history_size, vamp_marshal_history
    public :: vamp_unmarshal_history

159b <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_marshal_history (h, ibuf, dbuf)
        type(vamp_history), intent(in) :: h
        integer, dimension(:), intent(inout) :: ibuf
        real(kind=default), dimension(:), intent(inout) :: dbuf
        integer :: j, ndim, iidx, didx, iwords, dwords
        if (h%verbose .and. (associated (h%div))) then
            ndim = size (h%div)
        else
            ndim = 0
        end if
        ibuf(1) = ndim
        ibuf(2) = h%calls
        if (h%stratified) then
            ibuf(3) = 1
        else
            ibuf(3) = 0
        end if
        dbuf(1) = h%integral
        dbuf(2) = h%std_dev
        dbuf(3) = h%avg_integral
        dbuf(4) = h%avg_std_dev
        dbuf(5) = h%avg_chi2
        dbuf(6) = h%f_min
        dbuf(7) = h%f_max
        iidx = 4

```



```

didx = 8
do j = 1, ndim
  call marshal_div_history_size (h%div(j), iwords, dwords)
  ibuf(iidx) = iwords
  ibuf(iidx+1) = dwords
  iidx = iidx + 2
  call marshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                           dbuf(didx:didx-1+dwords))

  iidx = iidx + iwords
  didx = didx + dwords
end do
end subroutine vamp_marshal_history

```

160a *⟨Implementation of vamp procedures 77c⟩+≡*

```

pure subroutine vamp_marshal_history_size (h, iwords, dwords)
  type(vamp_history), intent(in) :: h
  integer, intent(out) :: iwords, dwords
  integer :: i, ndim, iw, dw
  if (h%verbose .and. (associated (h%div))) then
    ndim = size (h%div)
  else
    ndim = 0
  end if
  iwords = 3
  dwords = 7
  do i = 1, ndim
    call marshal_div_history_size (h%div(i), iw, dw)
    iwords = iwords + 2 + iw
    dwords = dwords + dw
  end do
end subroutine vamp_marshal_history_size

```

160b *⟨Implementation of vamp procedures 77c⟩+≡*

```

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

```

### 5.2.12 Boring Copying and Deleting of Objects

161 *Implementation of vamp procedures 77c* +≡

```

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%sum_integral = rhs%sum_integral
  lhs%sum_weights = rhs%sum_weights
  lhs%sum_chi2 = rhs%sum_chi2
  lhs%calls = rhs%calls
  lhs%num_calls = rhs%num_calls
  call copy_array_pointer (lhs%num_div, rhs%num_div)
  lhs%dv2g = rhs%dv2g
  lhs%jacobi = rhs%jacobi

```

```

lhs%f_min = rhs%f_min
lhs%f_max = rhs%f_max
lhs%mu_gi = rhs%mu_gi
lhs%sum_mu_gi = rhs%sum_mu_gi
lhs%calls_per_cell = rhs%calls_per_cell
lhs%stratified = rhs%stratified
lhs%all_stratified = rhs%all_stratified
lhs%quadrupole = rhs%quadrupole
if (associated (lhs%div)) then
    if (size (lhs%div) /= ndim) then
        call delete_division (lhs%div)
        deallocate (lhs%div)
        allocate (lhs%div(ndim))
    end if
else
    allocate (lhs%div(ndim))
end if
call copy_division (lhs%div, rhs%div)
if (associated (rhs%map)) then
    call copy_array_pointer (lhs%map, rhs%map)
else if (associated (lhs%map)) then
    deallocate (lhs%map)
end if
if (associated (rhs%mu_x)) then
    call copy_array_pointer (lhs%mu_x, rhs%mu_x)
    call copy_array_pointer (lhs%mu_xx, rhs%mu_xx)
    call copy_array_pointer (lhs%sum_mu_x, rhs%sum_mu_x)
    call copy_array_pointer (lhs%sum_mu_xx, rhs%sum_mu_xx)
else if (associated (lhs%mu_x)) then
    deallocate (lhs%mu_x, lhs%mu_xx, lhs%sum_mu_x, lhs%sum_mu_xx)
end if
end subroutine vamp_copy_grid

```

162 *⟨Implementation of vamp procedures 77c⟩+≡*  
 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

163a <Implementation of vamp procedures 77c>+≡
    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

163b <Implementation of vamp procedures 77c>+≡
    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

163c <Implementation of vamp procedures 77c>+≡
    elemental subroutine vamp_copy_history (lhs, rhs)
        type(vamp_history), intent(inout) :: lhs
        type(vamp_history), intent(in) :: rhs
        lhs%calls = rhs%calls
        lhs%stratified = rhs%stratified
        lhs%verbose = rhs%verbose
        lhs%integral = rhs%integral

```

```

lhs%std_dev = rhs%std_dev
lhs%avg_integral = rhs%avg_integral
lhs%avg_std_dev = rhs%avg_std_dev
lhs%avg_chi2 = rhs%avg_chi2
lhs%f_min = rhs%f_min
lhs%f_max = rhs%f_max
if (rhs%verbose) then
  if (associated (lhs%div)) then
    if (size (lhs%div) /= size (rhs%div)) then
      deallocate (lhs%div)
      allocate (lhs%div(size(rhs%div)))
    end if
  else
    allocate (lhs%div(size(rhs%div)))
  end if
  call copy_history (lhs%div, rhs%div)
end if
end subroutine vamp_copy_history

```

164a *⟨Implementation of vamp procedures 77c⟩*+≡

```

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:

164b *⟨vampi.f90 164b⟩*≡

```

! vampi.f90 --

```

*⟨Coryleft notice 1⟩*

```
module vamp_serial_mpi
  use vamp, &
    <vamp0_* => vamp_* 166b>
    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.

```
165a <vampi.f90 164b>+≡
  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 166a>
    <Interfaces of vampi procedures 170c>
    <Parameters in vampi 166d>
    <Declaration of vampi types 170f>
    character(len=*), public, parameter :: VAMPI_RCS_ID = &
      "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    <Implementation of vampi procedures 166c>
  end module vamp_parallel_mpi
```

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

```
165b <vampi.f90 164b>+≡
  module vampi
    use vamp_serial_mpi !NODEP!
    use vamp_parallel_mpi !NODEP!
    public
  end module vampi
```

### 5.3.1 Parallel Execution

### Single Channel

- 166a**  $\langle$ Declaration of `vampi` procedures **166a** $\rangle \equiv$
- ```
public :: vamp_create_grid
public :: vamp_discard_integral
public :: vamp_reshape_grid
public :: vamp_sample_grid
public :: vamp_delete_grid
```
- 166b**  $\langle$ `vamp0_* => vamp_*` **166b** $\rangle \equiv$
- ```
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, &
```
- 166c**  $\langle$ Implementation of `vampi` procedures **166c** $\rangle \equiv$
- ```
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
```
- 166d**  $\langle$ Parameters in `vampi` **166d** $\rangle \equiv$
- ```
integer, public, parameter :: VAMP_ROOT = 0
```
- 166e**  $\langle$ Implementation of `vampi` procedures **166c** $\rangle + \equiv$
- ```
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

```

167a *<Implementation of vampi procedures 166c>+≡*

```

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.

167b *<Implementation of vampi procedures 166c>+≡*

```

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
  end if
end do

```

```

end do
call vamp_join_grid (g, gs, gx, d, exc)
call vamp0_delete_grid (gs)
deallocate (gs, gx)
call vamp_refine_grid (g)
call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
if (present (history)) then
    if (iteration <= size (history)) then
        call vamp_get_history &
            (history(iteration), g, &
                local_integral, local_std_dev, local_avg_chi2)
    else
        call raise_exception (exc, EXC_WARN, FN, "history too short")
    end if
    call vamp_terminate_history (history(iteration+1:))
end if
if (present (accuracy)) then
    if (local_std_dev <= accuracy * local_integral) then
        call raise_exception (exc, EXC_INFO, FN, &
            "requested accuracy reached")
        exit iterate
    end if
end if
else if (proc_id < num_workers) then
    call vamp_send_grid (g, VAMP_ROOT, 0)
end if
end do iterate
if (proc_id == VAMP_ROOT) then
    deallocate (d)
    if (present (integral)) then
        integral = local_integral
    end if
    if (present (std_dev)) then
        std_dev = local_std_dev
    end if
    if (present (avg_chi2)) then
        avg_chi2 = local_avg_chi2
    end if
end if
end subroutine vamp_sample_grid

```

169 *⟨Implementation of vampi procedures 166c⟩+≡*  
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

170a <Declaration of vampi procedures 166a>+≡
    public :: vamp_print_history
    private :: vamp_print_one_history, vamp_print_histories

170b <vamp0_* => vamp_* 166b>+≡
    vamp0_print_history => vamp_print_history, &

170c <Interfaces of vampi procedures 170c>≡
    interface vamp_print_history
        module procedure vamp_print_one_history, vamp_print_histories
    end interface

170d <Implementation of vampi procedures 166c>+≡
    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

170e <Implementation of vampi procedures 166c>+≡
    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*

```

170f <Declaration of vampi types 170f>≡
    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

```

171a  $\langle \text{vamp0\_} * \Rightarrow \text{vamp\_} * \text{ 166b} \rangle + \equiv$   
 $\text{vamp0\_grids} \Rightarrow \text{vamp\_grids}, \&$

Partially duplicate the API of vamp:

171b  $\langle \text{Declaration of vampi procedures 166a} \rangle + \equiv$   

```

public :: vamp_create_grids
public :: vamp_discard_integrals
public :: vamp_update_weights
public :: vamp_refine_weights
public :: vamp_delete_grids
public :: vamp_sample_grids

```

171c  $\langle \text{vamp0\_} * \Rightarrow \text{vamp\_} * \text{ 166b} \rangle + \equiv$   

```

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

171d  $\langle \text{Implementation of vampi procedures 166c} \rangle + \equiv$   

```

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

172a <Implementation of vampi procedures 166c>+≡
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

172b <Implementation of vampi procedures 166c>+≡
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

172c <Implementation of vampi procedures 166c>+≡
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

```

173a *<Implementation of vampi procedures 166c>+≡*

```

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.

173b *<Implementation of vampi procedures 166c>+≡*

```

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
    end if
end subroutine vamp_sample_grids

```

```

        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 174b>
        else
            <Distribute each grid among processes 178b>
        end if
        <Exit iterate if accuracy has been reached (MPI) 177c>
    end do iterate
    <Copy results of vamp_sample_grids to dummy variables 177b>
end subroutine vamp_sample_grids

```

Setting VAMP\_MAX\_WASTE to 1 disables the splitting of grids, which doesn't work yet.

174a *<Parameters in vampi 166d>+≡*  
 real(kind=default), private, parameter :: VAMP\_MAX\_WASTE = 1.0  
 ! real(kind=default), private, parameter :: VAMP\_MAX\_WASTE = 0.3

174b *<Distribute complete grids among processes 174b>≡*  
 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) 175a>*  
 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:

174c *<Distribute complete grids among processes 174b>+≡*  
 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 176b⟩
        end if
    end if
end do

```

therefore we use vamp\_sample\_grid0 instead of vamp0\_sample\_grid:

```

175a ⟨Sample g%g0%grids(ch) 175a⟩≡
    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

175b ⟨Distribute complete grids among processes 174b⟩+≡
    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 176c⟩
            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

```



```

        end if
    end if

```

This would be cheaper than `vamp_broadcast_grid`, but we need the latter to support the adaptive multi channel sampling:

- 176a** *⟨Ship g%g0%grids from the root to the assigned processor 176a⟩*≡
- ```

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

```
- 176b** *⟨Ship the result for channel #ch back to the root 176b⟩*≡
- ```

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

```
- 176c** *⟨Receive the result for channel #ch at the root 176c⟩*≡
- ```

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

```
- 176d** *⟨Declaration of vampi procedures 166a⟩*+≡
- ```

private :: object

```
- 176e** *⟨Implementation of vampi procedures 166c⟩*+≡
- ```

pure function object (ch, obj) result (tag)
    integer, intent(in) :: ch, obj
    integer :: tag
    tag = 100 * ch + obj
end function object

```

```

177a  <Parameters in vampi 166d>+≡
      integer, public, parameter :: &
          TAG_INTEGRAL = 1, &
          TAG_STD_DEV = 2, &
          TAG_GRID = 3, &
          TAG_HISTORY = 6, &
          TAG_NEXT_FREE = 9

177b  <Copy results of vamp_sample_grids to dummy variables 177b>≡
      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

177c  <Exit iterate if accuracy has been reached (MPI) 177c>≡
      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.

```

177d  <Declaration of vampi procedures 166a>+≡
      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.

```

177e  <Implementation of vampi procedures 166c>+≡
      pure subroutine schedule (jobs, num_procs, assign, waste)

```

```

real(kind=default), dimension(:), intent(in) :: jobs
integer, intent(in) :: num_procs
integer, dimension(:), intent(out) :: assign
real(kind=default), intent(out), optional :: waste
integer, dimension(size(jobs)) :: idx
real(kind=default), dimension(size(jobs)) :: sjobs
real(kind=default), dimension(num_procs) :: fill
integer :: job, proc
sjobs = jobs / sum (jobs) * num_procs
idx = (/ (job, job = 1, size(jobs)) /)
call sort (sjobs, idx, reverse = .true.)
fill = 0.0
fill(VAMP_ROOT+1) = 0.1
do job = 1, size (sjobs)
    proc = sum (minloc (fill))
    fill(proc) = fill(proc) + sjobs(job)
    assign(idx(job)) = proc - 1
end do
<Estimate waste of processor time 178a>
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:

**178a** *<Estimate waste of processor time 178a>*≡

```

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!

**178b** *<Distribute each grid among processes 178b>*≡

```

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
end if

```

### 5.3.2 Event Generation

This is currently only a syntactical translation ...

- 179a *<Declaration of vampi procedures 166a>+≡*  
 public :: vamp\_warmup\_grid  
 public :: vamp\_warmup\_grids  
 public :: vamp\_next\_event  
 private :: vamp\_next\_event\_single, vamp\_next\_event\_multi
- 179b *<vamp0\_\* => vamp\_\* 166b>+≡*  
 vamp0\_warmup\_grid => vamp\_warmup\_grid, &  
 vamp0\_warmup\_grids => vamp\_warmup\_grids, &  
 vamp0\_next\_event => vamp\_next\_event, &
- 179c *<Interfaces of vampi procedures 170c>+≡*  
 interface vamp\_next\_event

```

        module procedure vamp_next_event_single, vamp_next_event_multi
    end interface

180a  <Implementation of vampi procedures 166c>+≡
    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

180b  <Implementation of vampi procedures 166c>+≡
    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

180c  <Implementation of vampi procedures 166c>+≡
    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

```

181a <Implementation of vampi procedures 166c>+≡

```

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

181b <Declaration of vampi procedures 166a>+≡

```

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

```

181c <vamp0\_\* => vamp\_\* 166b>+≡

```

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

```

181d <Interfaces of vampi procedures 170c>+≡

```

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

```

```

182a  <Implementation of vampi procedures 166c>+≡
      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

182b  <Implementation of vampi procedures 166c>+≡
      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

182c  <Implementation of vampi procedures 166c>+≡
      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

182d  <Implementation of vampi procedures 166c>+≡
      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

182e  <Declaration of vampi procedures 166a>+≡
      public :: vamp_write_grids, vamp_read_grids

```

```

private :: write_grids_unit, write_grids_name
private :: read_grids_unit, read_grids_name

183a <vamp0_* => vamp_* 166b>+≡
    vamp0_write_grids => vamp_write_grids, &
    vamp0_read_grids => vamp_read_grids, &

183b <Interfaces of vampi procedures 170c>+≡
    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

183c <Implementation of vampi procedures 166c>+≡
    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

183d <Implementation of vampi procedures 166c>+≡
    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

183e <Implementation of vampi procedures 166c>+≡
    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

```

184a *⟨Implementation of vampi procedures 166c⟩*+≡

```

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

184b *⟨Declaration of vampi procedures 166a⟩*+≡

```

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`:

184c *⟨Implementation of vampi procedures 166c⟩*+≡

```

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

```

185a *⟨Implementation of vampi procedures 166c⟩*+≡

```

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`:

185b *⟨Implementation of vampi procedures (doesn't work with MPICH yet) 185b⟩*≡

```

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 ...

186a *⟨Implementation of vampi procedures (doesn't work with MPICH yet) 185b⟩+≡*

```
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.

186b *⟨Interfaces of vampi procedures 170c⟩+≡*

```
interface vamp_broadcast_grid
  module procedure &
    vamp_broadcast_one_grid, vamp_broadcast_many_grids
end interface
```

186c *⟨Implementation of vampi procedures 166c⟩+≡*

```
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

```

187a *⟨Implementation of vampi procedures 166c⟩*+≡

```

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

```

187b *⟨Implementation of vampi procedures 166c⟩*+≡

```

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

```

188a *<Declaration of vampi procedures 166a>+≡*

```

public :: vamp_send_history
public :: vamp_receive_history

```

188b *<Implementation of vampi procedures 166c>+≡*

```

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

```

188c *<Implementation of vampi procedures 166c>+≡*

```

subroutine vamp_receive_history (g, source, tag, domain, status, error)
    type(vamp_history), intent(inout) :: g
    integer, intent(in) :: source, tag
    integer, intent(in), optional :: domain

```

```

type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
integer, dimension(2) :: words
integer, dimension(:), allocatable :: ibuf
real(kind=default), dimension(:), allocatable :: dbuf
call mpi90_receive (words, source, tag, domain, status, error)
allocate (ibuf(words(1)), dbuf(words(2)))
call mpi90_receive (ibuf, source, tag+1, domain, status, error)
call mpi90_receive (dbuf, source, tag+2, domain, status, error)
call vamp_unmarshal_history (g, ibuf, dbuf)
deallocate (ibuf, dbuf)
end subroutine vamp_receive_history

```

# —6—

## SELF TEST

### 6.1 No Mapping Mode

In this chapter we perform a test of the major features of Vamp. A function with many peaks is integrated with the traditional Vegas algorithm, using a multi-channel approach and in parallel. The function is constructed to have a known analytical integral (which is chosen to be one) in order to be able to gauge the accuracy of the result and error estimate.

#### 6.1.1 Serial Test

```

190a <vamp_test.f90 190a>≡
      ! vamp_test.f90 --
      <Copyleft notice 1>
      <Module vamp_test_functions 190b>
      <Module vamp_tests 194b>

190b <Module vamp_test_functions 190b>≡
      module vamp_test_functions
        use kinds
        use constants, only: PI
        use coordinates
        use vamp, only: vamp_grid, vamp_multi_channel
        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 191a>
      end module vamp_test_functions

```

$$\int_{x_1}^{x_2} dx \frac{1}{(x - x_0)^2 + a^2} = \frac{1}{a} \left( \text{atan} \left( \frac{x_2 - x_0}{a} \right) - \text{atan} \left( \frac{x_1 - x_0}{a} \right) \right) = N(x_0, x_1, x_2, a) \quad (6.1)$$

191a  $\langle$ Implementation of vamp\_test\_functions procedures 191a $\rangle \equiv$

```
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
```

$$\int d^n x f(x) = \int d\Omega_n r^{n-1} dr f(x) = 1 \quad (6.2)$$

191b  $\langle$ Implementation of vamp\_test\_functions procedures 191a $\rangle + \equiv$

```
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
```

191c  $\langle$ Implementation of vamp\_test\_functions procedures 191a $\rangle + \equiv$

```
pure function f (x, prc_index, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: prc_index
  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

```

192 *Implementation of vamp\_test\_functions procedures 191a*  $\vdash \equiv$

```

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:))
  end if
end function phi

```

```

else
  x = 0
end if
end function phi

```

193a  $\langle$ Implementation of vamp\_test\_functions procedures 191a $\rangle + \equiv$

```

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

```

193b  $\langle$ Implementation of vamp\_test\_functions procedures 191a $\rangle + \equiv$

```

pure function j (x, prc_index, channel) result (j_x)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: prc_index
  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)) !  $1/|dr/d\xi_1|$ 
    j_x = j_x / PI !  $1/|d\phi/d\xi_2|$ 
  end if
end function j

```

```

        j_x = j_x * cartesian_to_spherical_cos_j (x(1:channel))
    else
        j_x = 0
    end if
end function j

```

194a *⟨Implementation of vamp\_test\_functions procedures 191a⟩*  $\equiv$

```

pure function w (x, prc_index, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: prc_index
    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, prc_index, phi, ihp, j, x, weights, channel, grids)
end function w

```

194b *⟨Module vamp\_tests 194b⟩*  $\equiv$

```

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 194c⟩
contains
    ⟨Implementation of procedures in vamp_tests 195a⟩
end module vamp_tests

```

### Verification

194c *⟨Declaration of procedures in vamp\_tests 194c⟩*  $\equiv$

```

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

```

194d *⟨Implementation of procedures in vamp\_tests (broken?) 194d⟩*  $\equiv$

```

subroutine check_jacobians (rng, region, weights, samples)
    type( tao_random_state ), intent(inout) :: rng
    real(kind=default), dimension(:, :), intent(in) :: region
    real(kind=default), dimension(:), intent(in) :: weights
    integer, intent(in) :: samples

```

```

real(kind=default), dimension(size(region,dim=2)) :: x
real(kind=default) :: d
integer :: ch
integer, parameter :: prc_index = 1
do ch = 1, size(weights)
    call vamp_check_jacobian (rng, samples, j, prc_index, phi, ch, region, d, x)
    print *, "channel", ch, ": delta(j)/j=", real(d), ", @x=", real (x)
end do
end subroutine check_jacobians

```

195a *⟨Implementation of procedures in vamp\_tests 195a⟩*≡

```

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

```

195b *⟨Implementation of procedures in vamp\_tests 195a⟩*+≡

```

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*

196a *<Declaration of procedures in vamp\_tests 194c>+≡*  
 public :: single\_channel, multi\_channel

196b *<Implementation of procedures in vamp\_tests 195a>+≡*  
 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  
 integer, parameter :: PRC\_INDEX = 1  
 call vamp\_create\_history (history)  
 call vamp\_create\_grid (gr, region, samples(1))  
 call vamp\_sample\_grid (rng, gr, f, PRC\_INDEX, iterations(1), history = history)  
 call vamp\_discard\_integral (gr, samples(2))  
 call vamp\_sample\_grid &  
 (rng, gr, f, PRC\_INDEX, 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

197a  Implementation of procedures in vamp_tests 195a +=
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 197b
end subroutine multi_channel

197b  Body of multi_channel 197b ≡
    type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
        history
    type(vamp_history), dimension(size(history),size(weights)) :: histories
    integer :: it, nit
    integer, parameter :: PRC_INDEX = 1
    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, PRC_INDEX, 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, PRC_INDEX, 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, PRC_INDEX, 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*

198a *<Declaration of procedures in vamp\_tests 194c>+≡*

```
public :: print_results
```

198b *<Implementation of procedures in vamp\_tests 195a>+≡*

```

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*

198c *<vamp\_test.f90 190a>+≡*

```
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
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 system_clock (start_ticks)
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

200a  $\langle$ vampi\_test.f90 200a $\rangle \equiv$   
! vampi\_test.f90 --  
 $\langle$ Copyleft notice 1 $\rangle$   
 $\langle$ Module vamp\_test\_functions 190b $\rangle$

The following is identical to vamp\_tests, except for use vampi:

200b  $\langle$ vampi\_test.f90 200a $\rangle + \equiv$   
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  
   $\langle$ Declaration of procedures in vamp\_tests 194c $\rangle$   
contains  
   $\langle$ Implementation of procedures in vamp\_tests 195a $\rangle$   
end module vampi\_tests

200c  $\langle$ vampi\_test.f90 200a $\rangle + \equiv$   
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
    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

202a `<vamp_test.out 202a>`≡

## 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

202b `<vamp_test0.f90 202b>`≡

```

! vamp_test0.f90 --
<Copyleft notice 1>
<Module vamp_test0_functions 203>

```

### Single Channel

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

```

203 <Module vamp_test0_functions 203>≡
  module vamp_test0_functions
    use kinds
    use vamp, only: vamp_grid, vamp_multi_channel0
    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 204a>
  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.

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

204a  $\langle$ Implementation of vamp\_test0\_functions procedures 204a $\rangle \equiv$

```

pure function f0 (x, x_min, x_max, x0, g) result (f_x)
  real(kind=default), intent(in) :: x, x_min, x_max
  real(kind=default), dimension(:), intent(in) :: x0, g
  real(kind=default) :: f_x
  complex(kind=default) :: amp
  real(kind=default) :: norm
  integer :: i, j
  amp = sum (1.0 / cmplx (x - x0, g, kind=default))
  norm = 0
  do i = 1, size (x0)
    norm = norm + f_norm (x_min, x_max, x0(i), g(i), x0(i), g(i))
    do j = i + 1, size (x0)
      norm = norm + 2 * f_norm (x_min, x_max, x0(i), g(i), x0(j), g(j))
    end do
  end do
  f_x = amp * conjg (amp) / norm
end function f0

```

$$\int_{x_{\min}}^{x_{\max}} dx \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} = \frac{1}{x_{0,p} - x_{0,q} - i\gamma_p - i\gamma_q} \left( \ln \left( \frac{x_{\max} - x_{0,p} + i\gamma_p}{x_{\min} - x_{0,p} + i\gamma_p} \right) - \ln \left( \frac{x_{\max} - x_{0,q} - i\gamma_q}{x_{\min} - x_{0,q} - i\gamma_q} \right) \right) \quad (6.7)$$

Don't even think of merging the logarithms: it will screw up the Riemann sheet.

204b  $\langle$ Implementation of vamp\_test0\_functions procedures 204a $\rangle + \equiv$

```

pure function f_norm (x_min, x_max, x0p, gp, x0q, gq) &
  result (norm)
  real(kind=default), intent(in) :: x_min, x_max, x0p, gp, x0q, gq
  real(kind=default) :: norm
  norm = real (( log ( cmplx (x_max - x0p, gp, kind=default) &
                        / cmplx (x_min - x0p, gp, kind=default)) &
                - log ( cmplx (x_max - x0q, - gq, kind=default) &
                        / cmplx (x_min - x0q, - gq, kind=default))) &
                / cmplx (x0p - x0q, - gp - gq, kind=default), &
                kind=default)
end function f_norm

```

Since we want to be able to do the integral of  $f$  analytically, it is most

convenient to take a weighted sum of products:

$$f(x_1, \dots, x_{n_d} | x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{\sum_{i=1}^{n_c} c_i} \sum_{i=1}^{n_c} c_i \prod_{j=1}^{n_d} f_0(x_j | x_{\min,j}, x_{\max,j}, x_{0,ij}, \gamma_{ij}) \quad (6.8)$$

Each summand is factorized and therefore very easily integrated by Vegas. A non-trivial sum is more realistic in this respect.

- 205a *⟨Implementation of vamp\_test0\_functions procedures 204a⟩+≡*  

```

pure function f (x, prc_index, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: prc_index
  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

```

205b *⟨Implementation of vamp\_test0\_functions procedures 204a⟩+≡*  

```

subroutine delete_sample ()
  deallocate (c, x_min, x_max, x0, gamma)
end subroutine delete_sample

```

205c *⟨Implementation of vamp\_test0\_functions procedures 204a⟩+≡*  

```

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

$$\begin{aligned} \psi(\xi | x_{\min}, x_{\max}, x_0, \gamma) = &x_0 + \\ &\gamma \cdot \tan \left( \frac{\xi - x_{\min}}{x_{\max} - x_{\min}} \cdot \operatorname{atan} \frac{x_{\max} - x_0}{\gamma} - \frac{x_{\max} - \xi}{x_{\max} - x_{\min}} \cdot \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma} \right) \end{aligned} \quad (6.10)$$

206 *<Implementation of vamp\_test0\_functions procedures 204a>+≡*

```

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

$$\frac{d(\psi^{-1}(x|x_{\min}, x_{\max}, x_0, \gamma))}{dx} = \frac{x_{\max} - x_{\min}}{\operatorname{atan} \frac{x_{\max} - x_0}{\gamma} + \operatorname{atan} \frac{x_0 - x_{\min}}{\gamma}} \frac{\gamma}{(x - x_0)^2 + \gamma^2} \quad (6.13)$$

**207a** *⟨Implementation of vamp\_test0\_functions procedures 204a⟩*  $\equiv$

```

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:

**207b** *⟨Decode channel into ch and p(:) 207b⟩*  $\equiv$

```

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:

**207c** *⟨Implementation of vamp\_test0\_functions procedures 204a⟩*  $\equiv$

```

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(:) 207b⟩
    do j = 1, size (xi)
      if (all (gamma(:,ch,j) > 0)) then
        x(j) = psi (xi(j), x_min(j), x_max(j), &
          x0(p(j),ch,j), gamma(p(j),ch,j))
      else
        x = xi

```



```

        end if
    end do
    else if (channel == channels + 1) then
        x = xi
    else
        x = 0
    end if
end function phi

```

similarly for the Jacobians:

208a *⟨Implementation of vamp\_test0\_functions procedures 204a⟩*+≡

```

pure recursive function g (x, prc_index, channel) result (g_x)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: prc_index
    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
        ⟨Decode channel into ch and p(:) 207b⟩
        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

```

208b *⟨Implementation of vamp\_test0\_functions procedures 204a⟩*+≡

```

pure function w (x, prc_index, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: prc_index
    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, prc_index, phi, g, x, weights, channel)
end function w

```

### *Driver Routines*

**209a**  $\langle \text{vamp\_test0.f90 202b} \rangle + \equiv$

```

module vamp_tests0
   $\langle \text{Modules used by vamp\_tests0 209b} \rangle$ 
  use vamp
  implicit none
  private
   $\langle \text{Declaration of procedures in vamp\_tests0 210a} \rangle$ 
contains
   $\langle \text{Implementation of procedures in vamp\_tests0 210b} \rangle$ 
end module vamp_tests0

```

**209b**  $\langle \text{Modules used by vamp\_tests0 209b} \rangle \equiv$

```

  use kinds
  use exceptions
  use histograms
  use tao_random_numbers
  use vamp_test0_functions !NODEP!

```

### *Verification*

**209c**  $\langle \text{Declaration of procedures in vamp\_tests0 (broken?) 209c} \rangle \equiv$

```

  public :: check_jacobians

```

**209d**  $\langle \text{Implementation of procedures in vamp\_tests0 (broken?) 209d} \rangle \equiv$

```

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 do
    end subroutine check_jacobians

```

### *Integration*

210a *<Declaration of procedures in vamp\_tests0 210a>*≡

```

    public :: single_channel, multi_channel

```

210b *<Implementation of procedures in vamp\_tests0 210b>*≡

```

    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
        integer, parameter :: PRC_INDEX = 1
        call vamp_create_history (history)
        call vamp_create_grid (gr, region, samples(1))
        call vamp_sample_grid (rng, gr, f, PRC_INDEX, iterations(1), history = history)
        call vamp_discard_integral (gr, samples(2))
        call vamp_sample_grid &
            (rng, gr, f, PRC_INDEX, 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

```

211a *⟨Implementation of procedures in vamp\_tests0 210b⟩*+≡

```

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 197b⟩
end subroutine multi_channel

```

211b *⟨Body of multi\_channel 197b⟩*+≡

```

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
integer, parameter :: PRC_INDEX = 1
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, PRC_INDEX, iterations(1) - 1, &
    history = history, histories = histories)

do it = 1, 5
    call vamp_sample_grids (rng, grs, w, PRC_INDEX, 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, PRC_INDEX, 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*

212a *<Declaration of procedures in vamp\_tests0 210a>+≡*

```
public :: single_channel_generator, multi_channel_generator
```

212b *<Implementation of procedures in vamp\_tests0 210b>+≡*

```

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
  integer, parameter :: PRC_INDEX = 1
  call vamp_create_grid (gr, region, samples(1))
  call vamp_sample_grid (rng, gr, f, PRC_INDEX, iterations(1), history = history)
  call vamp_discard_integral (gr, samples(2))
  call vamp_warmup_grid &
    (rng, gr, f, PRC_INDEX, 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, PRC_INDEX, exc = exc)
  call handle_exception (exc)
  call fill_histogram (unweighted, x(1))
  call fill_histogram (reweighted, x(1), 1.0_default / f (x, PRC_INDEX))
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, PRC_INDEX, weight, exc = exc)
  call handle_exception (exc)
  call fill_histogram (weighted, x(1), weight / f (x, PRC_INDEX))
  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

```

**213** *<Implementation of procedures in vamp\_tests0 210b>+≡*

```

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
integer, parameter :: PRC_INDEX = 1
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, PRC_INDEX, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
    call vamp_sample_grids (rng, grs, w, PRC_INDEX, 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, PRC_INDEX, 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, PRC_INDEX, phi, exc = exc)
    call handle_exception (exc)

```

```

        call fill_histogram (unweighted, x(1))
        call fill_histogram (reweighted, x(1), 1.0_default / f (x, PRC_INDEX))
    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, PRC_INDEX, phi, weight, exc = exc)
        call handle_exception (exc)
        call fill_histogram (weighted, x(1), weight / f (x, PRC_INDEX))
        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*

```

215  <vamp_test0.f90 202b>+≡
    program vamp_test0
        <Modules used by vamp_test0 217c>
        implicit none
        <Variables in vamp_test0 217a>
        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 system_clock (ticks0)
        call tao_random_seed (rng, ticks0)

```



```

    <Set up integrand and region in vamp_test0 217e>
    <Execute tests in vamp_test0 216a>
    <Cleanup in vamp_test0 217f>
    if (failures == 0) then
        stop 0
    else if (failures == 1) then
        stop 1
    else
        stop 2
    end if
end program vamp_test0

216a <Execute tests in vamp_test0 216a>≡
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"

216b <Execute tests in vamp_test0 216a>+≡
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"

216c <Execute tests in vamp_test0 216a>+≡
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"

216d <Execute tests in vamp_test0 216a>+≡
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"

216e <Execute tests in vamp_test0 216a>+≡
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"

```

217a *<Variables in vamp\_test0 217a>*≡  
       logical :: do\_print

217b *<Execute command 217b>*≡

217c *<Modules used by vamp\_test0 217c>*≡  
       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!

217d *<Variables in vamp\_test0 217a>*+≡  
       integer :: i, j, ticks, ticks\_per\_second, ticks0  
       integer, dimension(2) :: iterations, samples  
       real(kind=default), dimension(:,,:), allocatable :: region  
       type( tao\_random\_state ) :: rng  
       real(kind=default), parameter :: ACCEPTABLE = 4  
       integer :: failures

217e *<Set up integrand and region in vamp\_test0 217e>*≡  
       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

217f *<Cleanup in vamp\_test0 217f>*≡  
       call delete\_sample ()  
       deallocate (region)

## 6.2.2 Parallel Test

```
218a <vampi_test0.f90 218a>≡
! vampi_test0.f90 --
<Copyleft notice 1>
<Module vamp_test0_functions 203>
module vamp_tests0
  <Modules used by vamp_tests0 209b>
  use vampi
  use mpi90
  implicit none
  private
  <Declaration of procedures in vamp_tests0 210a>
contains
  <Implementation of procedures in vamp_tests0 210b>
end module vamp_tests0

218b <vampi_test0.f90 218a>+≡
program vampi_test0
  <Modules used by vamp_test0 217c>
  use mpi90
  use vampi, only: VAMPI_RCS_ID
  implicit none
  <Variables in vamp_test0 217a>
  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 217e>
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 217b>
  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 217f>
call mpi90_finalize ()
if (proc_id == 0) then
  print *, "bye."
end if
end program vampi_test0

```

### 6.2.3 Output

219 <vamp\_test0.out 219>≡

# —7—

## APPLICATION

### 7.1 *Cross section*

```
220a <application.f90 220a>≡
! application.f90 --
<Copyleft notice 1>
module cross_section
  use kinds
  use constants
  use utils
  use kinematics
  use tao_random_numbers
  use products, only: dot
  use helicity
  use vamp, only: vamp_grid, vamp_probability
  implicit none
  private
  <Declaration of cross_section procedures 221d>
  <Types in cross_section 226c>
  <Variables in cross_section 220b>
contains
  <Implementation of cross_section procedures 222a>
end module cross_section

220b <Variables in cross_section 220b>≡
  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

221a  <XXX Variables in cross_section 221a>≡
      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

221b  <XXX Variables in cross_section 221a>+≡
      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

221c  <Variables in cross_section 220b>+≡
      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

221d  <Declaration of cross_section procedures 221d>≡
      private :: cuts

221e  <XXX Implementation of cross_section procedures 221e>≡
      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

221f  <Variables in cross_section 220b>+≡
      real(kind=default), private, parameter :: &

```

```

E_MIN = 1.0, &
COSTH_SEP_MAX = 0.99, &
COSTH_BEAM_MAX = 0.99

```

**222a** *⟨Implementation of cross\_section procedures 222a⟩*≡

```

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

```

**222b** *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

223a  $\langle$ Declaration of cross\_section procedures 221d $\rangle + \equiv$

```

private :: xsect
 $\phi : [0, 1]^{\otimes 5} \rightarrow [(m_2 + m_3)^2, (\sqrt{s} - m_1)^2] \otimes [t_1^{\min}(s_2), t_1^{\max}(s_2)]$ 
 $\otimes [0, 2\pi] \otimes [-1, 1] \otimes [0, 2\pi]$ 
 $(x_1, \dots, x_5) \mapsto (s_2, t_1, \phi, \cos \theta_3, \phi_3)$ 
 $= (s_2(x_1), x_2 t_1^{\max}(s_2) + (1 - x_2) t_1^{\min}(s_2), 2\pi x_3, 2x_4 - 1, 2\pi x_5)$ 
(7.1)

```

where

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

223b  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  223b $\rangle \equiv$

```

! 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)

```

223c  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 223c $\rangle \equiv$

```

! s2_min = S1_MIN_0
s2_min = 0
s2_max = s
s2 = s2_max * x(1) + s2_min * (1 - x(1))
t1_min = - (s - s2)
t1_max = 0
t1 = t1_max * x(2) + t1_min * (1 - x(2))
phi = 2*PI * x(3)
cos_theta3 = 2 * x(4) - 1
phi3 = 2*PI * x(5)

```



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

i.e.

$$J_\phi(x_1, \dots, x_5) = 8\pi^2 \cdot \left| \frac{ds_2}{dx_1} \right| \cdot (t_1^{\max}(s_2) - t_1^{\min}(s_2)) \quad (7.4)$$

```

224a  <Adjust Jacobian 224a>≡
      p%jacobian = p%jacobian &
        * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))

224b  <Implementation of cross_section procedures 222a>+≡
      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 ↔ m_b, m_1 ↔ m_2 for channel #1 224c>
      <Set (s_2, t_1, φ, cos θ_3, φ_3) from (x_1, ..., x_5) 223b>
      p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
      <Adjust Jacobian 224a>
      <p_1 ↔ p_2 for channel #2 225a>
      end function phase_space

224c  <m_a ↔ m_b, m_1 ↔ m_2 for channel #1 224c>≡
      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

```

225a  $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 225a} \rangle \equiv$

```

    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

```

225b  $\langle \text{Declaration of cross\_section procedures 221d} \rangle + \equiv$

```

private :: jacobian

```

225c  $\langle \text{Implementation of cross\_section procedures 222a} \rangle + \equiv$

```

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

```

226a  $\langle$ Declaration of cross\_section procedures 221d $\rangle + \equiv$

```

private :: phase_space, phase_space_massless

```

226b  $\langle$ Implementation of cross\_section procedures 222a $\rangle + \equiv$

```

pure function phase_space_massless (x, channel) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: channel
  type(LIPS3) :: p
  real(kind=default) :: s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s = S_0
   $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 223c $\rangle$ 
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3)
   $\langle$ Adjust Jacobian 224a $\rangle$ 
   $\langle p_1 \leftrightarrow p_2$  for channel #2 225a $\rangle$ 
end function phase_space_massless

```

226c  $\langle$ Types in cross\_section 226c $\rangle \equiv$

```

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

```

226d  $\langle$ Types in cross\_section 226c $\rangle + \equiv$

```

type, public :: x5
! private
  real(kind=default), dimension(5) :: x
  real(kind=default) :: jacobian
end type x5

```

226e  $\langle$ Declaration of cross\_section procedures 221d $\rangle + \equiv$

```

private :: invariants_from_p, invariants_to_p
private :: invariants_from_x, invariants_to_x

```

226f  $\langle$ Implementation of cross\_section procedures 222a $\rangle + \equiv$

```

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

```

227a *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

227b *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

228 *⟨Implementation of cross\_section procedures 222a⟩* +≡

```

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

```

229a *⟨Declaration of cross\_section procedures 221d⟩*+≡

```
public :: sigma, sigma_raw, sigma_massless
```

229b *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

229c *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

230a *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

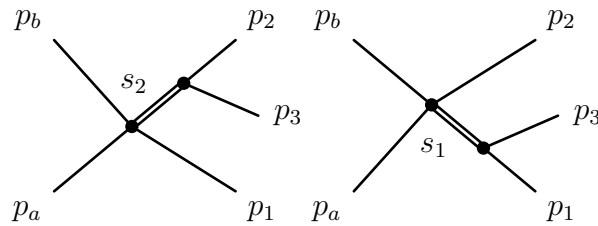
```

230b *⟨Declaration of cross\_section procedures 221d⟩*+≡

```

public :: w

```



230c *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

**231** *⟨Implementation of cross\_section procedures 222a⟩+≡*

```

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

```



```

232a  <Declaration of cross_section procedures 221d>+≡
      public :: sigma_rambo

232b  <Declaration of cross_section procedures 221d>+≡
      public :: check_kinematics
      private :: print_LIPS3_m5i2a3

232c  <Implementation of cross_section procedures 222a>+≡
      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

232d  <Implementation of cross_section procedures 222a>+≡
      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

```

233a *<Declaration of cross\_section procedures 221d>+≡*

```
public :: phi12, phi21, phi1, phi2
public :: g12, g21, g1, g2
```

233b *<Implementation of cross\_section procedures 222a>+≡*

```
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
```

233c *<Implementation of cross\_section procedures 222a>+≡*

```
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

```

234a *⟨Implementation of cross\_section procedures 222a⟩+≡*

```

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

```

234b *⟨Implementation of cross\_section procedures 222a⟩+≡*

```

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

```

234c *⟨Implementation of cross\_section procedures 222a⟩+≡*

```

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

```

235a *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

235b *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

235c *⟨Implementation of cross\_section procedures 222a⟩*+≡

```

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

```

236a *<Declaration of cross\_section procedures 221d>+≡*

```
public :: wx
```

236b *<Implementation of cross\_section procedures 222a>+≡*

```

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

```

237 <application.f90 220a>+≡

```

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 240a
case (CMD_MASSLESS)
  Application in massless single channel mode 240b
case (CMD_MULTI)
  Application in multi channel mode 241
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 242>
case (CMD_COMPARE)
  <Application in single channel mode 240a>
  single_integral = integral
  single_standard_dev = standard_dev
  <Application in Rambo mode 242>
  if (proc_id == 0) then
    rambo_integral = integral
    rambo_standard_dev = standard_dev
    integral = &
      (single_integral / single_standard_dev**2 &
       + rambo_integral / rambo_standard_dev**2) &
      / (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    standard_dev = 1.0_double &
      / sqrt (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    chi_squared = &
      ((single_integral - integral)**2 / single_standard_dev**2) &
      + ((rambo_integral - integral)**2 / rambo_standard_dev**2)
    print *, "S&R:  ", integral, standard_dev, chi_squared
  end if
case default
  if (proc_id == 0) then
    print *, "???: ", command
    !!! TO BE REMOVED !!!
    call check_kinematics (rng)
    allocate (region(2,5))
    region(1,:) = 0
    region(2,:) = 1
    do i = 1, 10
      call tao_random_number (rng, x)
      call vamp_jacobian (phi12, 0, x, region, jac)
      print *, "12:  ", jac, 1 / g12 (x), jac * g12 (x) - 1
      call vamp_jacobian (phi21, 0, x, region, jac)
      print *, "21:  ", jac, 1 / g21 (x), jac * g21 (x) - 1
      print *, "1:   ", real(x)
      print *, "2:   ", real(phi12(phi21(x,0),0))
      print *, "2':  ", real(phi12(phi21(x,-1),-1))
      print *, "3:   ", real(phi21(phi12(x,0),0))
      print *, "3':  ", real(phi21(phi12(x,-1),-1))
      print *, "2-1: ", real(phi12(phi21(x,0),0) - x)
    end do
  end if
end

```



```

        print *, "3-1: ", real(phi21(phi12(x,0),0) - x)
        print *, "a:   ", real(phi12(x,0))
        print *, "a':  ", real(phi12(x,-1))
        print *, "b:   ", real(phi21(x,0))
        print *, "b':  ", real(phi21(x,-1))
    end do
    deallocate (region)
    ! do i = 2, 5
    !     print *, i, phase_space_volume (i, 200.0_double)
    ! end do
end if
end select
if (proc_id == 0) then
    call system_clock (ticks, ticks_per_second)
    print "(1X,A,F8.2,A)", &
        "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
end if
call mpi90_finalize ()
end program application

```

**240a** *⟨Application in single channel mode 240a⟩≡*

```

    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)

```

**240b** *⟨Application in massless single channel mode 240b⟩≡*

```

    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)

```

241 *⟨Application in multi channel mode 241⟩*≡

```

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)

```

242 *Application in Rambo mode 242*≡

```

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.

```
243a <vamp_kinds.f90 243a>≡
      ! 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 :: quadruple = &
          & 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*

```
243b <constants.f90 243b>≡
      ! 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

```
245a <exceptions.f90 245a>≡
      ! exceptions.f90 --
      <Copyleft notice 1>
      module exceptions
        use kinds
        implicit none
        private
        <Declaration of exceptions procedures 246b>
        <Interfaces of exceptions procedures 360d>
        <Variables in exceptions 245c>
        <Declaration of exceptions types 245b>
        character(len=*, public, parameter :: EXCEPTIONS_RCS_ID = &
          "$Id: exceptions.nw 314 2010-04-17 20:32:33Z ohl $"
        contains
          <Implementation of exceptions procedures 246c>
        end module exceptions

245b <Declaration of exceptions types 245b>≡
      type, public :: exception
        integer :: level = EXC_NONE
        character(len=NAME_LENGTH) :: message = ""
        character(len=NAME_LENGTH) :: origin = ""
      end type exception

245c <Variables in exceptions 245c>≡
      integer, public, parameter :: &
        EXC_NONE = 0, &
        EXC_INFO = 1, &
        EXC_WARN = 2, &
```

```

        EXC_ERROR = 3, &
        EXC_FATAL = 4

```

246a *<Variables in exceptions 245c>+≡*

```

    integer, private, parameter :: EXC_DEFAULT = EXC_ERROR
    integer, private, parameter :: NAME_LENGTH = 64

```

246b *<Declaration of exceptions procedures 246b>≡*

```

    public :: handle_exception

```

246c *<Implementation of exceptions procedures 246c>≡*

```

    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

```

246d *<Declaration of exceptions procedures 246b>+≡*

```

    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.

246e *<Implementation of exceptions procedures 246c>+≡*

```

    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

247a ⟨Implementation of exceptions procedures 246c⟩+≡
  elemental subroutine clear_exception (exc)
    type(exception), intent(inout) :: exc
    exc%level = 0
    exc%message = ""
    exc%origin = ""
  end subroutine clear_exception

247b ⟨Implementation of exceptions procedures 246c⟩+≡
  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`

248 *<Idioms 99c>+≡*

```
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* [15] has always been celebrated as the 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 [23] (but see [15] 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

### *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).

249 *<API documentation 249>*≡  
    `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.

250a  $\langle$ API documentation 249 $\rangle + \equiv$   
`type(tao_random_state) :: s`  
`type(tao_random_raw_state) :: rs`

Subroutines filling arrays of reals and integers:

250b  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_number (a, num = n)`  
`call tao_random_number (s, a, num = n)`

Subroutine for changing the seed:

250c  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_seed (seed = seed)`  
`call tao_random_seed (s, seed = seed)`

Subroutine for changing the luxury. Per default, use all random numbers:

250d  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_luxury ()`  
`call tao_random_luxury (s)`

With an integer argument, use the first n of each fill of the buffer:

250e  $\langle$ API documentation 249 $\rangle + \equiv$   
`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:

250f  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_luxury (x)`  
`call tao_random_luxury (s, x)`

Create a `tao_random_state`

250g  $\langle$ API documentation 249 $\rangle + \equiv$   
`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`

250h  $\langle$ API documentation 249 $\rangle + \equiv$   
`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`

250i  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_destroy (s)`

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

251a  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_copy (lhs, rhs)`  
`lhs = rhs`

251b  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_flush (s)`

251c  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_read (s, unit)`  
`call tao_random_write (s, unit)`

251d  $\langle$ API documentation 249 $\rangle + \equiv$   
`call tao_random_test (name = name)`

Here is a sample application of random number states:

251e  $\langle$ API documentation 249 $\rangle + \equiv$   
`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.

251f  $\langle$ API documentation 249 $\rangle + \equiv$   
`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 wil therefore start with the former.

### C.2.1 Generation of 30-bit Random Numbers

The generator is a subtractive lagged Fibonacci

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

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

**252a**  $\langle$ Parameters in tao\_random\_numbers **252a** $\rangle \equiv$   

```
integer, parameter, private :: K = 100, L = 37
```

Other good choices for  $K$  and  $L$  are (cf. [15], table 1 in section 3.2.2, p. 29)

**252b**  $\langle$ Parameters in tao\_random\_numbers (alternatives) **252b** $\rangle \equiv$   

```
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

**252c**  $\langle$ Variables in 30-bit tao\_random\_numbers **252c** $\rangle \equiv$   

```
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:

**252d**  $\langle$ Parameters in tao\_random\_numbers **252a** $\rangle + \equiv$   

```
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 ...

**253a** *⟨Implementation of 30-bit tao\_random\_numbers 253a⟩*≡  

```

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 253c⟩
end subroutine generate

```

**253b** *⟨Declaration of tao\_random\_numbers 253b⟩*≡  

```

private :: generate
state(1:K) is already set up properly:

```

**253c** *⟨Load a and refresh state 253c⟩*≡  

```

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 new `modulo` intrinsic does the right thing, since it guarantees (unlike Fortran77's `mod`) that  $0 \leq \text{modulo}(a, m) < a$  if  $m > 0$ :

**253d** *⟨Load a and refresh state 253c⟩*+≡  

```

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`.

**253e** *⟨Load a and refresh state 253c⟩*+≡  

```

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 [15]).

**253f** *⟨Implementation of tao\_random\_numbers 253f⟩*≡  

```

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:

254a *⟨Variables in 30-bit tao\_random\_numbers 252c⟩*+≡  
integer(kind=tao\_i32), dimension(K), save, private :: s\_state  
logical, save, private :: s\_virginal = .true.

254b *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
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

254c *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
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.

254d *⟨Implementation of 30-bit tao\_random\_numbers 253a⟩*+≡  
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 255a⟩*  
integer :: seed\_value, j, s, t  
integer(kind=tao\_i32), dimension(2\*K-1) :: x  
*⟨Set up seed\_value from seed or DEFAULT\_SEED 255c⟩*  
*⟨Bootstrap the x buffer 255d⟩*  
*⟨Set up s and t 255f⟩*  
do  
*⟨ $p(z) \rightarrow p(z)^2$  (modulo 2 and  $z^K + z^L + 1$ ) 256a⟩*  
*⟨ $p(z) \rightarrow zp(z)$  (modulo 2 and  $z^K + z^L + 1$ ) 257a⟩*  
*⟨Shift s or t and exit if  $t \leq 0$  257b⟩*  
end do  
*⟨Fill state from x 257c⟩*  
end subroutine seed\_stateless

Any default will do

255a  $\langle$ Parameters local to tao\_random\_seed 255a $\rangle \equiv$   
integer, parameter :: DEFAULT\_SEED = 0

These must not be changed:

255b  $\langle$ Parameters local to tao\_random\_seed 255a $\rangle + \equiv$   
integer, parameter :: MAX\_SEED = 2\*\*30 - 3  
integer, parameter :: TT = 70

255c  $\langle$ Set up seed\_value from seed or DEFAULT\_SEED 255c $\rangle \equiv$   
if (present (seed)) then  
seed\_value = seed  
else  
seed\_value = DEFAULT\_SEED  
end if  
if (seed\_value < 0 .or. seed\_value > MAX\_SEED) then  
!!! print \*, "tao\_random\_seed: seed (", seed\_value, &  
!!! " ) not in [ 0,", MAX\_SEED, "]"!  
seed\_value = modulo (abs (seed\_value), MAX\_SEED + 1)  
!!! print \*, "tao\_random\_seed: seed set to ", seed\_value, "!"  
end if

Fill the array  $x_1, \dots, x_K$  with even integers, shifted cyclically by 29 bits.

255d  $\langle$ Bootstrap the x buffer 255d $\rangle \equiv$   
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:

255e  $\langle$ Bootstrap the x buffer 255d $\rangle + \equiv$   
x(2) = x(2) + 1

255f  $\langle$ Set up s and t 255f $\rangle \equiv$   
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  $\pmod{2}$  below.

$$\text{256a } \langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ 256a)} \equiv \\ \mathbf{x(3:2*K-1:2)} = \mathbf{x(2:K)}$$

The coefficients of the odd powers (those with the even indices) have not been changed yet. Set them to a flipped version of the other coefficients with the least significant bit set to 0.

$$\begin{aligned} x_2 &\leftarrow \text{even } x_{2K-1} \\ x_4 &\leftarrow \text{even } x_{2K-3} \\ &\dots \\ x_{K+L-1} &\leftarrow \text{even } x_{K-L+2} \end{aligned} \tag{C.3}$$

Note that the array notation is unambiguous because  $2K - 1$  is odd and source and destination are therefore interleaved:

$$\text{256b } \langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ 256a)} \equiv \\ \mathbf{x(2:K+L-1:2)} = \mathbf{x(2*K-1:K-L+2:-2)} - \text{modulo } (\mathbf{x(2*K-1:K-L+2:-2)}, 2\_tao\_i32)$$

The Fortran program in [15] reads

$$\text{256c } \langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ (DEK, Fortran) 256c)} \equiv \\ \text{do } j = 2*K-1, K-L+1, -2 \\ \quad \mathbf{x(2*K+1-j)} = \mathbf{x(j)} - \text{mod } (\mathbf{x(j)}, 2) \\ \text{end do}$$

i.e.

$$\text{256d } \langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ (alternative) 256d)} \equiv \\ \mathbf{x(2:K+L:2)} = \mathbf{x(2*K-1:K-L+1:-2)} - \text{modulo } (\mathbf{x(2*K-1:K-L+1:-2)}, 2)$$

which is equivalent, as long as  $K + L$  is odd. This is the case most of the time. The version used above is the direct translation of the C version

$$\text{256e } \langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ (DEK, C) 256e)} \equiv \\ \text{for } (j = 2*K-2; j > K-L; j -= 2) \\ \quad \mathbf{x[2*K-1-j]} = \text{evenize } (\mathbf{x[j]});$$



I should decide from theoretical considerations whether the difference matters and if so, which is the correct version. At least I should inform DEK of the inconsistency.

Let's return to the coefficients for  $n > K$  generated by the shifting above. Subtract  $z^n(z^K + z^L + 1) = z^n z^K (1 + z^{-(K-L)} + z^{-K})$  iff the coefficient of  $z^n z^K$  doesn't vanish  $\pmod{2}$  after squaring. The coefficient of  $z^n z^K$  is left alone, because it doesn't belong to  $p(z)$  anyway.

```

256f   $\langle p(z) \rightarrow p(z)^2 \text{ (modulo 2 and } z^K + z^L + 1) \text{ 256a} \rangle + \equiv$ 
      do j= 2*K-1, K+1, -1
        if (modulo (x(j), int(2, tao_i32)) == 1) then
          x(j-(K-L)) = modulo (x(j-(K-L)) - x(j), M)
          x(j-K) = modulo (x(j-K) - x(j), M)
        end if
      end do

257a   $\langle p(z) \rightarrow zp(z) \text{ (modulo 2 and } z^K + z^L + 1) \text{ 257a} \rangle \equiv$ 
      if (modulo (s, 2) == 1) then
        x(2:K+1) = x(1:K)
        x(1) = x(K+1)
        if (modulo (x(K+1), 2_tao_i32) == 1) then
          x(L+1) = modulo (x(L+1) - x(K+1), M)
        end if
      end if

257b   $\langle \text{Shift s or t and exit if } t \leq 0 \text{ 257b} \rangle \equiv$ 
      if (s /= 0) then
        s = s / 2
      else
        t = t - 1
      end if
      if (t <= 0) then
        exit
      end if

257c   $\langle \text{Fill state from x 257c} \rangle \equiv$ 
      state(K-L+1:K) = x(1:L)
      state(1:K-L) = x(L+1:K)

257d   $\langle \text{Interfaces of tao\_random\_numbers 257d} \rangle \equiv$ 
      interface tao_random_seed
        module procedure  $\langle \text{Specific procedures for tao\_random\_seed 257f} \rangle$ 
      end interface

257e   $\langle \text{Declaration of tao\_random\_numbers 253b} \rangle + \equiv$ 
      private ::  $\langle \text{Specific procedures for tao\_random\_seed 257f} \rangle$ 

257f   $\langle \text{Specific procedures for tao\_random\_seed 257f} \rangle \equiv$ 
      seed_static, seed_state, seed_raw_state

```

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

$$X_j = (X_{j-K} + X_{j-L}) \bmod 1 \quad (\text{C.4})$$

```

257g   $\langle \text{Variables in 52-bit tao\_random\_numbers 257g} \rangle \equiv$ 
      real(kind=tao_r64), parameter, private :: M = 1.0_tao_r64

```

The state of the internal routines

```

258a <Variables in 52-bit tao_random_numbers 257g>+≡
      real(kind=tao_r64), dimension(K), save, private :: s_state
      logical, save, private :: s_virginal = .true.

258b <Implementation of 52-bit tao_random_numbers 258b>≡
      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 258c>
      end subroutine generate

```

That's almost identical to the 30-bit version, except that the relative sign is flipped:

```

258c <Load 52-bit a and refresh state 258c>≡
      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.

```

258d <Implementation of 52-bit tao_random_numbers 258b>+≡
      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 255a>
        <Variables local to 52-bit tao_random_seed 259b>
        <Set up seed_value from seed or DEFAULT_SEED 255c>
        <Bootstrap the x and x1 buffers 259d>
        <Set up s and t 255f>
      do
        <52-bit  $p(z) \rightarrow p(z)^2$  (modulo 2 and  $z^K + z^L + 1$ ) 259g>
        <52-bit  $p(z) \rightarrow zp(z)$  (modulo 2 and  $z^K + z^L + 1$ ) 260a>
        <Shift s or t and exit if t ≤ 0 257b>
      end do
      <Fill state from x 257c>

```

```

        end subroutine seed_stateless

259a   $\langle$ Declaration of tao_random_numbers 253b $\rangle + \equiv$ 
        private :: seed_stateless

259b   $\langle$ Variables local to 52-bit tao_random_seed 259b $\rangle \equiv$ 
        real(kind=tao_r64), parameter :: ULP = 2.0_tao_r64**(-52)

259c   $\langle$ Variables local to 52-bit tao_random_seed 259b $\rangle + \equiv$ 
        real(kind=tao_r64), dimension(2*K-1) :: x, x1
        real(kind=tao_r64) :: ss
        integer :: seed_value, t, s, j

259d   $\langle$ Bootstrap the x and x1 buffers 259d $\rangle \equiv$ 
        x1 = 0
        x1(2) = ULP

259e   $\langle$ Bootstrap the x and x1 buffers 259d $\rangle + \equiv$ 
        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

259f   $\langle$ Bootstrap the x and x1 buffers 259d $\rangle + \equiv$ 
        x(2) = x(2) + ULP

259g   $\langle$ 52-bit  $p(z) \rightarrow p(z)^2$  (modulo 2 and  $z^K + z^L + 1$ ) 259g $\rangle \equiv$ 
        x1(3:2*K-1:2) = x1(2:K)
        x(3:2*K-1:2) = x(2:K)

```

This works because  $2*K-1$  is odd (the same problem as on page 256 arises here as well)

```

259h   $\langle$ 52-bit  $p(z) \rightarrow p(z)^2$  (modulo 2 and  $z^K + z^L + 1$ ) 259g $\rangle + \equiv$ 
        x1(2:K+L-1:2) = 0.0
        x(2:K+L-1:2) = x(2*K-1:K-L+2:-2) - x1(2*K-1:K-L+2:-2)
        do j = 2*K-1, K+1, -1
            if (x1(j) /= 0) then
                x1(j-(K-L)) = ULP - x1(j-(K-L))
                x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
                x1(j-K) = ULP - x1(j-K)
                x(j-K) = modulo (x(j-K) + x(j), M)
            end if
        end do

```

260a  $\langle 52\text{-bit } p(z) \rightarrow zp(z) \text{ (modulo 2 and } z^K + z^L + 1) \text{ 260a} \rangle \equiv$

```

    if (modulo (s, 2) == 1) then
        x1(2:K+1) = x1(1:K)
        x1(1) = x1(K+1)
        x(2:K+1) = x(1:K)
        x(1) = x(K+1)
        if (x1(K+1) /= 0) then
            x1(L+1) = ULP - x1(L+1)
            x(L+1) = modulo (x(L+1) + x(K+1), M)
        end if
    end if
end if

```

### C.3 The State

260b  $\langle \text{Declaration of 30-bit tao\_random\_numbers types 260b} \rangle \equiv$

```

type, public :: tao_random_raw_state
private
    integer(kind=tao_i32), dimension(K) :: x
end type tao_random_raw_state

```

260c  $\langle \text{Declaration of 30-bit tao\_random\_numbers types 260b} \rangle + \equiv$

```

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

```

260d  $\langle \text{Declaration of 52-bit tao\_random\_numbers types 260d} \rangle \equiv$

```

type, public :: tao_random_raw_state
private
    real(kind=tao_r64), dimension(K) :: x
end type tao_random_raw_state

```

260e  $\langle \text{Declaration of 52-bit tao\_random\_numbers types 260d} \rangle + \equiv$

```

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

261a *<Interfaces of tao\_random\_numbers 257d>+≡*  
`interface tao_random_create`  
`module procedure <Specific procedures for tao_random_create 261c>`  
`end interface`

261b *<Declaration of tao\_random\_numbers 253b>+≡*  
`private :: <Specific procedures for tao_random_create 261c>`

261c *<Specific procedures for tao\_random\_create 261c>≡*  
`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.

261d *<Implementation of tao\_random\_numbers 253f>+≡*  
`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`

261e *<Implementation of tao\_random\_numbers 253f>+≡*  
`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`

261f *<Implementation of tao\_random\_numbers 253f>+≡*  
`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

```

262a *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 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

262b *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 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

262c *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 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

262d *⟨Interfaces of tao\_random\_numbers 257d⟩*+≡  
 interface tao\_random\_destroy  
   module procedure destroy\_state, destroy\_raw\_state  
end interface

262e *⟨Declaration of tao\_random\_numbers 253b⟩*+≡  
 private :: destroy\_state, destroy\_raw\_state

263a *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 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

263b *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 elemental subroutine destroy\_raw\_state (s)  
   type(tao\_random\_raw\_state), intent(inout) :: s  
 end subroutine destroy\_raw\_state

### C.3.3 Copying

263c *⟨Interfaces of tao\_random\_numbers 257d⟩*+≡  
 interface tao\_random\_copy  
   module procedure *⟨Specific procedures for tao\_random\_copy 263f⟩*  
 end interface

263d *⟨Interfaces of tao\_random\_numbers 257d⟩*+≡  
 interface assignment(=)  
   module procedure *⟨Specific procedures for tao\_random\_copy 263f⟩*  
 end interface

263e *⟨Declaration of tao\_random\_numbers 253b⟩*+≡  
 public :: assignment(=)  
 private :: *⟨Specific procedures for tao\_random\_copy 263f⟩*

263f *⟨Specific procedures for tao\_random\_copy 263f⟩*≡  
 copy\_state, copy\_raw\_state, &  
 copy\_raw\_state\_to\_state, copy\_state\_to\_raw\_state

263g *⟨Implementation of tao\_random\_numbers 253f⟩*+≡  
 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



264a *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

264b *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

264c *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

264d *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

264e *<Interfaces of tao\_random\_numbers 257d>+≡*  
 interface tao\_random\_write  
   module procedure &  
     write\_state\_unit, write\_state\_name, &  
     write\_raw\_state\_unit, write\_raw\_state\_name  
 end interface

264f *<Declaration of tao\_random\_numbers 253b>+≡*  
 private :: write\_state\_unit, write\_state\_name  
 private :: write\_raw\_state\_unit, write\_raw\_state\_name

```

265a  <Interfaces of tao_random_numbers 257d>+≡
      interface tao_random_read
        module procedure &
          read_state_unit, read_state_name, &
          read_raw_state_unit, read_raw_state_name
      end interface

265b  <Declaration of tao_random_numbers 253b>+≡
      private :: read_state_unit, read_state_name
      private :: read_raw_state_unit, read_raw_state_name

265c  <Implementation of tao_random_numbers 253f>+≡
      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

265d  <Implementation of tao_random_numbers 253f>+≡
      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

```

266a *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

266b *<Implementation of tao\_random\_numbers 253f>+≡*  
 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

266c *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*  
 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

266d *<Declaration of 30-bit tao\_random\_numbers 266d>≡*  
 private :: write\_state\_array

266e *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*  
 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

266f *<Declaration of 30-bit tao\_random\_numbers 266d>+≡*  
 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 ...

- 267a *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  

```

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

```
- 267b *<Declaration of 52-bit tao\_random\_numbers 267b>≡*  

```

private :: write_state_array

```
- 267c *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  

```

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

```
- 267d *<Declaration of 52-bit tao\_random\_numbers 267b>+≡*  

```

private :: read_state_array

```
- 267e *<Implementation of tao\_random\_numbers 253f>+≡*  

```

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 = iostat)
    if (status == 0) then
      if (exists .and. .not. is_open) then
        u = i
        if (present (iostat)) then
          iostat = 0
        end if
      end if
    end if
  end do

```

```

        return
    end if
end if
end do
if (present (iostat)) then
    iostat = -1
end if
u = -1
end subroutine find_free_unit

```

268a *<Variables in tao\_random\_numbers 268a>*≡  
integer, parameter, private :: MIN\_UNIT = 11, MAX\_UNIT = 99

268b *<Declaration of tao\_random\_numbers 253b>*+≡  
private :: find\_free\_unit

268c *<Implementation of tao\_random\_numbers 253f>*+≡  
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

268d *<Implementation of tao\_random\_numbers 253f>*+≡  
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

268e *<Implementation of tao\_random\_numbers 253f>*+≡  
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

```

269a *<Implementation of tao\_random\_numbers 253f>+≡*

```

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!

269b *<Interfaces of tao\_random\_numbers 257d>+≡*

```

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

```

269c *<Declaration of tao\_random\_numbers 253b>+≡*

```

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

```

269d *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*

```

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

270a <Implementation of 30-bit tao_random_numbers 253a>+≡
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

270b <Implementation of 30-bit tao_random_numbers 253a>+≡
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

270c <Implementation of 30-bit tao_random_numbers 253a>+≡
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

270d <Implementation of 30-bit tao_random_numbers 253a>+≡
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

```

271a *⟨Implementation of 30-bit tao\_random\_numbers 253a⟩*+≡

```

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

```

271b *⟨Implementation of 52-bit tao\_random\_numbers 258b⟩*+≡

```

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

```

271c *⟨Implementation of 52-bit tao\_random\_numbers 258b⟩*+≡

```

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

```

271d *⟨Implementation of 52-bit tao\_random\_numbers 258b⟩*+≡

```

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

```



272a *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  

```

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

```

272b *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  

```

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

```

272c *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  

```

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

272d *<tao\_random\_numbers.f90 272d>≡*  

```

! 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 253b>
  <Declaration of 30-bit tao_random_numbers 266d>
  <Interfaces of tao_random_numbers 257d>
  <Interfaces of 30-bit tao_random_numbers 279f>
  <Parameters in tao_random_numbers 252a>
  <Variables in tao_random_numbers 268a>

```

```

    <Variables in 30-bit tao_random_numbers 252c>
    <Declaration of 30-bit tao_random_numbers types 260b>
    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 253f>
    <Implementation of 30-bit tao_random_numbers 253a>
end module tao_random_numbers

273a <tao52_random_numbers.f90 273a>≡
    ! 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 253b>
    <Declaration of 52-bit tao_random_numbers 267b>
    <Interfaces of tao_random_numbers 257d>
    <Interfaces of 52-bit tao_random_numbers 280d>
    <Parameters in tao_random_numbers 252a>
    <Variables in tao_random_numbers 268a>
    <Variables in 52-bit tao_random_numbers 257g>
    <Declaration of 52-bit tao_random_numbers types 260d>
    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 253f>
    <Implementation of 52-bit tao_random_numbers 258b>
end module tao52_random_numbers

Ten functions are exported

273b <Declaration of tao_random_numbers 253b>+≡
    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  $0 \leq r < 2^{30} = 1073741824$ :

```

274a <Implementation of 30-bit tao_random_numbers 253a>+≡
      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_* 274b>
      end subroutine integer_stateless

274b <Body of tao_random_* 274b>≡
      <Step last and reload buffer iff necessary 274d>
      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`.

```

274c <Variables in 30-bit tao_random_numbers 252c>+≡
      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.

```

274d <Step last and reload buffer iff necessary 274d>≡
      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.

```

274e <Implementation of 30-bit tao_random_numbers 253a>+≡
      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_* 274b>
end subroutine real_stateless

```

A random real  $r \in [0, 1)$ .

275a <Implementation of 52-bit tao\_random\_numbers 258b>+≡

```

    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_* 274b>
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.

275b <Variables in 52-bit tao\_random\_numbers 257g>+≡

```

    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  $j_1, \dots, j_\nu$  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`  $\nu$  times.

275c <Implementation of 30-bit tao\_random\_numbers 253a>+≡

```

    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 275d>
end subroutine integer_array_stateless

```

275d <Body of tao\_random\*\_array 275d>≡

```

    integer :: nu, done, todo, chunk
    <Set nu to num or size(v) 276a>
    <Prepare array buffer and done, todo, chunk 276b>

```

```

v(1:chunk) = NORM * buffer(last+1:last+chunk)
do
  <Update last, done and todo and set new chunk 276c>
  <Reload buffer or exit 276d>
  v(done+1:done+chunk) = NORM * buffer(1:chunk)
end do

```

```

276a <Set nu to num or size(v) 276a>≡
  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.

```

276b <Prepare array buffer and done, todo, chunk 276b>≡
  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.

```

276c <Update last, done and todo and set new chunk 276c>≡
  last = last + chunk
  done = done + chunk
  todo = todo - chunk
  chunk = min (todo, buffer_end)

```

```

276d <Reload buffer or exit 276d>≡
  if (chunk <= 0) then
    exit
  end if
  call generate (buffer, state)
  last = 0

```

```

276e <Implementation of 30-bit tao_random_numbers 253a>+≡
  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 275d>
end subroutine real_array_stateless

```

Fill the array  $v_1, \dots, v_\nu$  with uniform deviates  $v_i \in [0, 1)$ .

277a <Implementation of 52-bit tao\_random\_numbers 258b>+≡

```

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 275d>
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:

277b <Implementation of 30-bit tao\_random\_numbers 253a>+≡

```

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

```

277c <Implementation of 30-bit tao\_random\_numbers 253a>+≡

```

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

```

277d <Implementation of 52-bit tao\_random\_numbers 258b>+≡

```

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

278a  ⟨Implementation of 30-bit tao_random_numbers 253a⟩+≡
    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

278b  ⟨Implementation of 30-bit tao_random_numbers 253a⟩+≡
    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

278c  ⟨Implementation of 52-bit tao_random_numbers 258b⟩+≡
    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:

```

278d  ⟨Initialize a virginal random number generator 278d⟩≡
    if (s_virginal) then
        call tao_random_seed ()
    end if

278e  ⟨Implementation of 30-bit tao_random_numbers 253a⟩+≡
    subroutine integer_static (r)
        integer, intent(out) :: r
        ⟨Initialize a virginal random number generator 278d⟩
        call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
    end subroutine integer_static

```

279a *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*  
 subroutine real\_static (r)  
   real(kind=default), intent(out) :: r  
   *<Initialize a virginal random number generator 278d>*  
   call real\_stateless (s\_state, s\_buffer, s\_buffer\_end, s\_last, r)  
 end subroutine real\_static

279b *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  
 subroutine real\_static (r)  
   real(kind=default), intent(out) :: r  
   *<Initialize a virginal random number generator 278d>*  
   call real\_stateless (s\_state, s\_buffer, s\_buffer\_end, s\_last, r)  
 end subroutine real\_static

279c *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*  
 subroutine integer\_array\_static (v, num)  
   integer, dimension(:), intent(out) :: v  
   integer, optional, intent(in) :: num  
   *<Initialize a virginal random number generator 278d>*  
   call integer\_array\_stateless &  
     (s\_state, s\_buffer, s\_buffer\_end, s\_last, v, num)  
 end subroutine integer\_array\_static

279d *<Implementation of 30-bit tao\_random\_numbers 253a>+≡*  
 subroutine real\_array\_static (v, num)  
   real(kind=default), dimension(:), intent(out) :: v  
   integer, optional, intent(in) :: num  
   *<Initialize a virginal random number generator 278d>*  
   call real\_array\_stateless &  
     (s\_state, s\_buffer, s\_buffer\_end, s\_last, v, num)  
 end subroutine real\_array\_static

279e *<Implementation of 52-bit tao\_random\_numbers 258b>+≡*  
 subroutine real\_array\_static (v, num)  
   real(kind=default), dimension(:), intent(out) :: v  
   integer, optional, intent(in) :: num  
   *<Initialize a virginal random number generator 278d>*  
   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

279f *<Interfaces of 30-bit tao\_random\_numbers 279f>≡*  
 interface tao\_random\_number



```

        module procedure <Specific procedures for 30-bit tao_random_number 280a>
    end interface

280a <Specific procedures for 30-bit tao_random_number 280a>≡
    integer_static, integer_state, &
    integer_array_static, integer_array_state, &
    real_static, real_state, real_array_static, real_array_state
    These are not exported

280b <Declaration of 30-bit tao_random_numbers 266d>+≡
    private :: &
        integer_stateless, integer_array_stateless, &
        real_stateless, real_array_stateless

280c <Declaration of 30-bit tao_random_numbers 266d>+≡
    private :: <Specific procedures for 30-bit tao_random_number 280a>

280d <Interfaces of 52-bit tao_random_numbers 280d>≡
    interface tao_random_number
        module procedure <Specific procedures for 52-bit tao_random_number 280e>
    end interface

280e <Specific procedures for 52-bit tao_random_number 280e>≡
    real_static, real_state, real_array_static, real_array_state
    Thes are not exported

280f <Declaration of 52-bit tao_random_numbers 267b>+≡
    private :: real_stateless, real_array_stateless

280g <Declaration of 52-bit tao_random_numbers 267b>+≡
    private :: <Specific procedures for 52-bit tao_random_number 280e>

```

### C.4.6 *Luxury*

```

280h <Implementation of tao_random_numbers 253f>+≡
    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

281a <Implementation of tao_random_numbers 253f>+≡
    elemental subroutine luxury_state (s)
        type(tao_random_state), intent(inout) :: s
        call luxury_state_integer (s, size (s%buffer))
    end subroutine luxury_state

281b <Implementation of tao_random_numbers 253f>+≡
    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

281c <Implementation of tao_random_numbers 253f>+≡
    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

281d <Implementation of tao_random_numbers 253f>+≡
    subroutine luxury_static ()
        <Initialize a virginal random number generator 278d>
        call luxury_static_integer (size (s_buffer))
    end subroutine luxury_static

281e <Implementation of tao_random_numbers 253f>+≡
    subroutine luxury_static_integer (consumption)
        integer, intent(in) :: consumption
        <Initialize a virginal random number generator 278d>
        call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
    end subroutine luxury_static_integer

281f <Implementation of tao_random_numbers 253f>+≡
    subroutine luxury_static_real (consumption)
        real(kind=default), intent(in) :: consumption
        <Initialize a virginal random number generator 278d>
        call luxury_static_integer (int (consumption * size (s_buffer)))
    end subroutine luxury_static_real

281g <Interfaces of tao_random_numbers (unused luxury) 281g>≡
    interface tao_random_luxury
        module procedure <Specific procedures for tao_random_luxury 282c>
    end interface

```

282a *<Declaration of tao\_random\_numbers (unused luxury) 282a>*≡  
private :: luxury\_stateless

282b *<Declaration of tao\_random\_numbers (unused luxury) 282a>*+≡  
private :: *<Specific procedures for tao\_random\_luxury 282c>*

282c *<Specific procedures for tao\_random\_luxury 282c>*≡  
luxury\_static, luxury\_state, &  
luxury\_static\_integer, luxury\_state\_integer, &  
luxury\_static\_real, luxury\_state\_real

## C.5 Testing

### C.5.1 30-bit

282d *<Implementation of 30-bit tao\_random\_numbers 253a>*+≡  
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,')!')"  
*<Parameters in tao\_random\_test 282e>*  
integer, parameter :: &  
A\_2027082 = 461390032  
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 ..."  
*<Perform simple tests of tao\_random\_numbers 283a>*  
*<Perform more tests of tao\_random\_numbers 283d>*  
end subroutine tao\_random\_test

282e *<Parameters in tao\_random\_test 282e>*≡  
integer, parameter :: &  
SEED = 310952, &  
N = 2009, M = 1009, &  
N\_SHORT = 1984

DEK's "official" test expects  $a_{1009 \cdot 2009 + 1} = a_{2027082} = 461390032$ :

```

283a <Perform simple tests of tao_random_numbers 283a>≡
      ! 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 283b>

283b <Test a(1) = A_2027082 283b>≡
      if (a(1) == A_2027082) then
        print OK, a(1)
      else
        print NOT_OK, a(1), A_2027082
      end if

```

Deja vu all over again, but 2027081 is factored the other way around this time

```

283c <Perform simple tests of tao_random_numbers 283a>+≡
      call tao_random_seed (SEED)
      do i = 1, M+1
        call tao_random_number (a)
      end do
      <Test a(1) = A_2027082 283b>

```

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

```

283d <Perform more tests of tao_random_numbers 283d>≡
      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 283b>

```

and restart the saved generator

```

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

```

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

```
284a <Perform more tests of tao_random_numbers 283d>+≡
  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 283b>
    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 283b>
  end if
```

And finally using marshaling/unmarshaling:

```
284b <Perform more tests of tao_random_numbers 283d>+≡
  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 283b>
  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 283b>
```

### C.5.2 52-bit

DEK's "official" test expects  $x_{1009:2009+1} = x_{2027082} = 0.27452626307394156768$ :

```

284c <Implementation of 52-bit tao_random_numbers 258b>+≡
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 282e>
  real(kind=default), parameter :: &
    A_2027082 = 0.27452626307394156768_default
  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 283a>
  <Perform more tests of tao_random_numbers 283d>
end subroutine tao_random_test

```

### C.5.3 Test Program

```

285 <tao_test.f90 285>≡
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")
end program tao_test

```

# —D—

## SPECIAL FUNCTIONS

```

286a  <specfun.f90 286a>≡
      ! specfun.f90 --
      <Copyleft notice 1>
      module specfun
        use kinds
        ! use constants
        implicit none
        private
        <Declaration of specfun procedures 286b>
        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 287c>
      end module specfun

```

The algorithm is stolen from the FORTRAN version in routine C303 of the CERN library [24]. It has an accuracy which is approximately one digit less than machine precision.

```

286b  <Declaration of specfun procedures 286b>≡
      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  $\Gamma$  into [3, 4]:

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

287a  $\langle$  Pull  $u$  into the intervall  $[3, 4]$  287a  $\rangle \equiv$

```

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:

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

287b  $\langle$  Clenshaw's recurrence formula 287b  $\rangle \equiv$

```

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.

287c  $\langle$  Implementation of specfun procedures 287c  $\rangle \equiv$

```

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  $\Gamma(x)$  288a  $\rangle$ 
  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] 287a>
    g = 2*u - 7
    <Clenshaw's recurrence formula 287b>
    if (x < 0) then
        g = PI / (sin (PI * x) * g)
    end if
end function gamma

288a <c0/2, c1, c2, ..., c15 for  $\Gamma(x)$  288a>≡
    (/ 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

```

288b <stest.f90 288b>≡
    ! stest.f90 --
    <Copyleft notice 1>
    module stest_functions
        use kinds
        use constants
        use specfun
    end module

```

```

private
  <Declaration of stest_functions procedures 289a>
contains
  <Implementation of stest_functions procedures 289b>
end module stest_functions

```

289a <Declaration of stest\_functions procedures 289a>≡  
 public :: gauss\_multiplication

Gauss' multiplication fomula can serve as a non-trivial test

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \quad (\text{D.4})$$

289b <Implementation of stest\_functions procedures 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

289c <stest.f90 288b>+≡  
 program stest  
 use kinds  
 use specfun  
 use stest\_functions !NODEP!  
 implicit none  
 integer :: i, steps  
 real(kind=default) :: x, g, xmin, xmax  
 xmin = -4.5  
 xmax = 4.5  
 steps = 100 ! 9  
 do i = 0, steps  
 x = xmin + ((xmax - xmin) / real (steps)) \* i  
 print "(f6.3,4(1x,e9.2))", x, &  
 gauss\_multiplication (x, 2), &  
 gauss\_multiplication (x, 3), &  
 gauss\_multiplication (x, 4), &

```
        gauss_multiplication (x, 5)
    end do
end program stest
```

# —E—

## STATISTICS

**291a**  $\langle \text{vamp\_stat.f90 291a} \rangle \equiv$   
`! vamp_stat.f90 --`  
 $\langle \text{Copyleft notice 1} \rangle$   
`module vamp_stat`  
`use kinds`  
`implicit none`  
`private`  
 $\langle \text{Declaration of vamp\_stat procedures 291b} \rangle$   
`character(len=*), public, parameter :: VAMP_STAT_RCS_ID = &`  
`"$Id: vamp_stat.nw 314 2010-04-17 20:32:33Z ohl $"`  
`contains`  
 $\langle \text{Implementation of vamp\_stat procedures 291c} \rangle$   
`end module vamp_stat`

**291b**  $\langle \text{Declaration of vamp\_stat procedures 291b} \rangle \equiv$   
`public :: average, standard_deviation, value_spread`

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

**291c**  $\langle \text{Implementation of vamp\_stat procedures 291c} \rangle \equiv$   
`pure function average (x) result (a)`  
`real(kind=default), dimension(:), intent(in) :: x`  
`real(kind=default) :: a`  
`integer :: n`  
`n = size (x)`  
`if (n == 0) then`  
`a = 0.0`  
`else`  
`a = sum (x) / n`  
`end if`  
`end function average`

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

292a *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
    s = huge (s)
  else
    s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
                  0.0_default))
  end if
end function standard_deviation

```

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

292b *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread

```

292c *<Declaration of vamp\_stat procedures 291b>+≡*

```

public :: standard_deviation_percent, value_spread_percent

```

292d *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
  else
    s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent

```

292e *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x

```

```

real(kind=default) :: s
real(kind=default) :: abs_avg
abs_avg = abs (average (x))
if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
else
    s = 100.0 * value_spread (x) / abs_avg
end if
end function value_spread_percent

```

# —F—

## HISTOGRAMMING

⚠ Merged WK's improvements for WHIZARD. TODO *after* merging:

1. bins3 is a bad undescriptive name
2. bins3 should be added to histogram2
3. write\_histogram2\_unit for symmetry.

⚠ There's almost no sanity checking. If you call one of these functions on a histogram that has not been initialized, you loose. — *Big time.*

```

294a <histograms.f90 294a>≡
    ! histograms.f90 --
    <Copyleft notice 1>
    module histograms
    use kinds
    use utils, only: find_free_unit
    implicit none
    private
    <Declaration of histograms procedures 295b>
    <Interfaces of histograms procedures 295c>
    <Variables in histograms 295e>
    <Declaration of histograms types 294b>
    character(len=*), public, parameter :: HISTOGRAMS_RCS_ID = &
        "$Id: histograms.nw 314 2010-04-17 20:32:33Z ohl $"
    contains
    <Implementation of histograms procedures 295f>
    end module histograms

294b <Declaration of histograms types 294b>≡
    type, public :: histogram
    private
    integer :: n_bins
    real(kind=default) :: x_min, x_max

```

```

        real(kind=default), dimension(:), pointer :: bins => null ()
        real(kind=default), dimension(:), pointer :: bins2 => null ()
        real(kind=default), dimension(:), pointer :: bins3 => null ()
    end type histogram

```

295a *<Declaration of histograms types 294b>+≡*

```

    type, public :: histogram2
    private
        integer, dimension(2) :: n_bins
        real(kind=default), dimension(2) :: x_min, x_max
        real(kind=default), dimension(:,:), pointer :: bins => null ()
        real(kind=default), dimension(:,:), pointer :: bins2 => null ()
    end type histogram2

```

295b *<Declaration of histograms procedures 295b>≡*

```

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

```

295c *<Interfaces of histograms procedures 295c>≡*

```

    interface create_histogram
        module procedure create_histogram1, create_histogram2
    end interface
    interface fill_histogram
        module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
    end interface
    interface delete_histogram
        module procedure delete_histogram1, delete_histogram2
    end interface
    interface write_histogram
        module procedure write_histogram1, write_histogram2
        module procedure write_histogram1_unit
    end interface

```

295d *<Declaration of histograms procedures 295b>+≡*

```

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

```

295e *<Variables in histograms 295e>≡*

```

    integer, parameter, private :: N_BINS_DEFAULT = 10

```

295f *<Implementation of histograms procedures 295f>≡*

```

    elemental subroutine create_histogram1 (h, x_min, x_max, nb)
        type(histogram), intent(out) :: h
    end subroutine

```



```

real(kind=default), intent(in) :: x_min, x_max
integer, intent(in), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
h%bins = 0
h%bins2 = 0
allocate (h%bins3(0:h%n_bins+1))
h%bins3 = 0
end subroutine create_histogram1

```

296a *⟨Implementation of histograms procedures 295f⟩* +=

```

pure subroutine create_histogram2 (h, x_min, x_max, nb)
type(histogram2), intent(out) :: h
real(kind=default), dimension(:), intent(in) :: x_min, x_max
integer, intent(in), dimension(:), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
          h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
h%bins = 0
h%bins2 = 0
end subroutine create_histogram2

```

296b *⟨Implementation of histograms procedures 295f⟩* +=

```

elemental subroutine fill_histogram1 (h, x, weight, excess)
type(histogram), intent(inout) :: h
real(kind=default), intent(in) :: x
real(kind=default), intent(in), optional :: weight
real(kind=default), intent(in), optional :: excess
integer :: i
if (x < h%x_min) then
    i = 0
else if (x > h%x_max) then
    i = h%n_bins + 1

```

```

else
    i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
!WK! i = min (max (i, 0), h%n_bins + 1)
end if
if (present (weight)) then
    h%bins(i) = h%bins(i) + weight
    h%bins2(i) = h%bins2(i) + weight*weight
else
    h%bins(i) = h%bins(i) + 1
    h%bins2(i) = h%bins2(i) + 1
end if
if (present (excess)) h%bins3(i) = h%bins3(i) + excess
end subroutine fill_histogram1

```

297a *⟨Implementation of histograms procedures 295f⟩*+≡  
 elemental subroutine fill\_histogram2s (h, x1, x2, weight)  
 type(histogram2), intent(inout) :: h  
 real(kind=default), intent(in) :: x1, x2  
 real(kind=default), intent(in), optional :: weight  
 call fill\_histogram2v (h, (/ x1, x2 /), weight)  
 end subroutine fill\_histogram2s

297b *⟨Implementation of histograms procedures 295f⟩*+≡  
 pure subroutine fill\_histogram2v (h, x, weight)  
 type(histogram2), intent(inout) :: h  
 real(kind=default), dimension(:), intent(in) :: x  
 real(kind=default), intent(in), optional :: weight  
 integer, dimension(2) :: i  
 i = 1 + h%n\_bins \* (x - h%x\_min) / (h%x\_max - h%x\_min)  
 i = min (max (i, 0), h%n\_bins + 1)  
 if (present (weight)) then  
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight  
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight\*weight  
 else  
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1  
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1  
 end if  
 end subroutine fill\_histogram2v

297c *⟨Implementation of histograms procedures 295f⟩*+≡  
 elemental subroutine delete\_histogram1 (h)  
 type(histogram), intent(inout) :: h  
 deallocate (h%bins, h%bins2)  
 deallocate (h%bins3)  
 end subroutine delete\_histogram1

```

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

298b  <Implementation of histograms procedures 295f>+≡
      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 if

```

```

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

```

299a *<Declaration of histograms procedures 295b>+≡*  
 !WK! public :: write\_histogram1\_unit



I don't like the `format` statement with the line number. Use a character constant instead (after we have merged with WHIZARD's branch).

299b *<Implementation of histograms procedures 295f>+≡*

```

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 write_histogram1_unit

```

```

        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

```

300a *<Declaration of histograms procedures 295b>+≡*  
 private :: midpoint

300b *<Interfaces of histograms procedures 295c>+≡*  
 interface midpoint  
 module procedure midpoint1, midpoint2  
 end interface

300c *<Declaration of histograms procedures 295b>+≡*  
 private :: midpoint1, midpoint2

300d *<Implementation of histograms procedures 295f>+≡*  
 elemental function midpoint1 (h, bin) result (x)  
 type(histogram), intent(in) :: h  
 integer, intent(in) :: bin  
 real(kind=default) :: x  
 x = h%x\_min + (h%x\_max - h%x\_min) \* (bin - 0.5) / h%n\_bins  
 end function midpoint1

300e *<Implementation of histograms procedures 295f>+≡*  
 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

```

301  <Implementation of histograms procedures 295f>+≡
      subroutine write_histogram2 (h, name, over)
        type(histogram2), intent(in) :: h
        character(len=*), intent(in), optional :: name
        logical, intent(in), optional :: over
        integer :: i1, i2, iounit
        if (present (name)) then
          call find_free_unit (iounit)
          if (iounit > 0) then
            open (unit = iounit, action = "write", status = "replace", &
                  file = name)
            if (present (over)) then
              if (over) then
                write (unit = iounit, fmt = *) &
                  "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
                do i2 = 1, h%n_bins(2)
                  write (unit = iounit, fmt = *) &
                    "x1 underflow", midpoint (h, i2, 2), &
                    h%bins(0,i2), sqrt (h%bins2(0,i2))
                end do
                do i1 = 1, h%n_bins(1)
                  write (unit = iounit, fmt = *) &
                    "x2 underflow", midpoint (h, i1, 1), &
                    h%bins(i1,0), sqrt (h%bins2(i1,0))
                end do
              end if
            end if
            do i1 = 1, h%n_bins(1)
              do i2 = 1, h%n_bins(2)
                write (unit = iounit, fmt = *) &
                  midpoint (h, i1, 1), midpoint (h, i2, 2), &
                  h%bins(i1,i2), sqrt (h%bins2(i1,i2))
              end do
            end do
            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

```

304a  <utils.f90 304a>≡
      ! utils.f90 --
      <Copyleft notice 1>
      module utils
        use kinds
        implicit none
        private
        <Declaration of utils procedures 304b>
        <Parameters in utils 311c>
        <Variables in utils 312b>
        <Interfaces of utils procedures 304c>
        character(len=*), public, parameter :: UTILS_RCS_ID = &
          "$Id: utils.nw 314 2010-04-17 20:32:33Z ohl $"
      contains
        <Implementation of utils procedures 305c>
      end module utils

```

### *G.1 Memory Management*

```

304b  <Declaration of utils procedures 304b>≡
      public :: create_array_pointer
      private :: create_integer_array_pointer
      private :: create_real_array_pointer
      private :: create_integer_array2_pointer
      private :: create_real_array2_pointer

304c  <Interfaces of utils procedures 304c>≡
      interface create_array_pointer
        module procedure &
          create_integer_array_pointer, &

```

```

        create_real_array_pointer, &
        create_integer_array2_pointer, &
        create_real_array2_pointer
    end interface
305a  <Body of create_*_array_pointer 305a>≡
    if (associated (lhs)) then
        if (size (lhs) /= n) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb:n+lb-1))
            else
                allocate (lhs(n))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb:n+lb-1))
        else
            allocate (lhs(n))
        end if
    end if
    lhs = 0
305b  <Body of create_*_array2_pointer 305b>≡
    if (associated (lhs)) then
        if (any (ubound (lhs) /= n)) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
            else
                allocate (lhs(n(1),n(2)))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
        else
            allocate (lhs(n(1),n(2)))
        end if
    end if
    lhs = 0
305c  <Implementation of utils procedures 305c>≡
    pure subroutine create_integer_array_pointer (lhs, n, lb)

```

```

integer, dimension(:), pointer :: lhs
integer, intent(in) :: n
integer, intent(in), optional :: lb
<Body of create_*_array_pointer 305a>
end subroutine create_integer_array_pointer

```

306a <Implementation of utils procedures 305c>+≡

```

pure subroutine create_real_array_pointer (lhs, n, lb)
  real(kind=default), dimension(:), pointer :: lhs
  integer, intent(in) :: n
  integer, intent(in), optional :: lb
  <Body of create_*_array_pointer 305a>
end subroutine create_real_array_pointer

```

306b <Implementation of utils procedures 305c>+≡

```

pure subroutine create_integer_array2_pointer (lhs, n, lb)
  integer, dimension(:,:), pointer :: lhs
  integer, dimension(:), intent(in) :: n
  integer, dimension(:), intent(in), optional :: lb
  <Body of create_*_array2_pointer 305b>
end subroutine create_integer_array2_pointer

```

306c <Implementation of utils procedures 305c>+≡

```

pure subroutine create_real_array2_pointer (lhs, n, lb)
  real(kind=default), dimension(:,:), pointer :: lhs
  integer, dimension(:), intent(in) :: n
  integer, dimension(:), intent(in), optional :: lb
  <Body of create_*_array2_pointer 305b>
end subroutine create_real_array2_pointer

```

Copy an allocatable array component of a derived type, reshaping the target if necessary. The target can be disassociated, but its association *must not* be undefined.

306d <Declaration of utils procedures 304b>+≡

```

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

```

306e <Interfaces of utils procedures 304c>+≡

```

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

```

```

        copy_real_array2_pointer
    end interface

307a  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
        integer, dimension(:), pointer :: lhs
        integer, dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_integer_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
    end subroutine copy_integer_array_pointer

307b  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_real_array_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:), pointer :: lhs
        real(kind=default), dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_real_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
    end subroutine copy_real_array_pointer

307c  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
        integer, dimension(:, :), pointer :: lhs
        integer, dimension(:, :), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_integer_array2_pointer &
            (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
    end subroutine copy_integer_array2_pointer

307d  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:, :), pointer :: lhs
        real(kind=default), dimension(:, :), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_real_array2_pointer &
            (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
    end subroutine copy_real_array2_pointer

```

## G.2 Sorting

```

307e  <Declaration of utils procedures 304b>+≡
    public :: swap

```

```

        private :: swap_integer, swap_real
308a  <Interfaces of utils procedures 304c>+≡
        interface swap
            module procedure swap_integer, swap_real
        end interface
308b  <Implementation of utils procedures 305c>+≡
        elemental subroutine swap_integer (a, b)
            integer, intent(inout) :: a, b
            integer :: tmp
            tmp = a
            a = b
            b = tmp
        end subroutine swap_integer
308c  <Implementation of utils procedures 305c>+≡
        elemental subroutine swap_real (a, b)
            real(kind=default), intent(inout) :: a, b
            real(kind=default) :: tmp
            tmp = a
            a = b
            b = tmp
        end subroutine swap_real
Straight insertion:
308d  <Implementation of utils procedures 305c>+≡
        pure subroutine sort_real (key, reverse)
            real(kind=default), dimension(:), intent(inout) :: key
            logical, intent(in), optional :: reverse
            logical :: rev
            integer :: i, j
            <Set rev to reverse or .false. 308e>
            do i = 1, size (key) - 1
                <Set j to minloc(key) 309a>
                if (j /= i) then
                    call swap (key(i), key(j))
                end if
            end do
        end subroutine sort_real
308e  <Set rev to reverse or .false. 308e>≡
        if (present (reverse)) then
            rev = reverse
        else
            rev = .false.
        end if

```

```

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

309b  <Implementation of utils procedures 305c>+≡
      pure subroutine sort_real_and_real_array (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        real(kind=default), dimension(:, :), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(:, i), table(:, j))
          end if
        end do
      end subroutine sort_real_and_real_array

309c  <Implementation of utils procedures 305c>+≡
      pure subroutine sort_real_and_integer (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        integer, dimension(:), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(i), table(j))
          end if
        end do
      end subroutine sort_real_and_integer

309d  <Declaration of utils procedures 304b>+≡
      public :: sort
      private :: sort_real, sort_real_and_real_array, sort_real_and_integer

```

310a *⟨Interfaces of utils procedures 304c⟩*+≡  

```

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

```

### *G.3 Mathematics*

310b *⟨Declaration of utils procedures 304b⟩*+≡  

```

public :: outer_product

```

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

310c *⟨Implementation of utils procedures 305c⟩*+≡  

```

pure function outer_product (x, y) result (xy)
  real(kind=default), dimension(:), intent(in) :: x, y
  real(kind=default), dimension(size(x),size(y)) :: xy
  xy = spread (x, dim=2, ncopies=size(y)) &
    * spread (y, dim=1, ncopies=size(x))
end function outer_product

```

Greatest common divisor and least common multiple

310d *⟨Declaration of utils procedures 304b⟩*+≡  

```

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

```

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

310e *⟨Implementation of utils procedures 305c⟩*+≡  

```

pure recursive function gcd_internal (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
  if (n <= 0) then
    gcd_m_n = m
  else
    gcd_m_n = gcd_internal (n, modulo (m, n))
  end if
end function gcd_internal

```

Wrap an elemental procedure around the recursive procedure:

310f *⟨Implementation of utils procedures 305c⟩*+≡  

```

elemental function gcd (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n

```

```

gcd_m_n = gcd_internal (m, n)
end function gcd

```

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

311a *<Implementation of utils procedures 305c>+≡*

```

elemental function lcm (m, n) result (lcm_m_n)
  integer, intent(in) :: m, n
  integer :: lcm_m_n
  lcm_m_n = (m * n) / gcd (m, n)
end function lcm

```

A very simple minded factorization procedure, that is not fool proof at all. It maintains  $n == \text{product}(\text{factors}(1:i))$ , however, and will work in all cases of practical relevance.

311b *<Implementation of utils procedures 305c>+≡*

```

pure subroutine factorize (n, factors, i)
  integer, intent(in) :: n
  integer, dimension(:), intent(out) :: factors
  integer, intent(out) :: i
  integer :: nn, p
  nn = n
  i = 0
  do p = 1, size (PRIMES)
    try: do
      if (modulo (nn, PRIMES(p)) == 0) then
        i = i + 1
        factors(i) = PRIMES(p)
        nn = nn / PRIMES(p)
        if (i >= size (factors)) then
          factors(i) = nn
          return
        end if
      else
        exit try
      end if
    end do try
    if (nn == 1) then
      return
    end if
  end do
end subroutine factorize

```

311c *<Parameters in utils 311c>≡*

```

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

```



## G.4 I/O

**312a** *⟨Declaration of utils procedures 304b⟩*+≡  
public :: find\_free\_unit

**312b** *⟨Variables in utils 312b⟩*≡  
integer, parameter, private :: MIN\_UNIT = 11, MAX\_UNIT = 99

**312c** *⟨Implementation of utils procedures 305c⟩*+≡  
subroutine find\_free\_unit (u, iostat)  
integer, intent(out) :: u  
integer, intent(out), optional :: iostat  
logical :: exists, is\_open  
integer :: i, status  
do i = MIN\_UNIT, MAX\_UNIT  
inquire (unit = i, exist = exists, opened = is\_open, &  
iostat = status)  
if (status == 0) then  
if (exists .and. .not. is\_open) then  
u = i  
if (present (iostat)) then  
iostat = 0  
end if  
return  
end if  
end if  
end do  
if (present (iostat)) then  
iostat = -1  
end if  
u = -1  
end subroutine find\_free\_unit

# —H— LINEAR ALGEBRA

```

313a <linalg.f90 313a>≡
! linalg.f90 --
<Coyleft notice 1>
module linalg
  use kinds
  use utils
  implicit none
  private
  <Declaration of linalg procedures 313b>
  character(len=*), public, parameter :: LINALG_RCS_ID = &
    "$Id: linalg.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    <Implementation of linalg procedures 314>
end module linalg

```

## *H.1 LU Decomposition*

```

313b <Declaration of linalg procedures 313b>≡
  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.

314 *Implementation of linalg procedures 314*  $\equiv$

```

pure subroutine lu_decompose (a, pivots, eps, l, u)
  real(kind=default), dimension(:, :), intent(inout) :: a
  integer, dimension(:), intent(out), optional :: pivots
  real(kind=default), intent(out), optional :: eps
  real(kind=default), dimension(:, :), intent(out), optional :: l, u
  real(kind=default), dimension(size(a,dim=1)) :: vv
  integer, dimension(size(a,dim=1)) :: p
  integer :: j, pivot
  <eps = 1 315a>
  vv = maxval (abs (a), dim=2)
  if (any (vv == 0.0)) then
    a = 0.0
    <pivots = 0 and eps = 0 315c>
    return
  end if
  vv = 1.0 / vv
  do j = 1, size (a, dim=1)
    pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
    if (j /= pivot) then
      call swap (a(pivot,:), a(j,:))
      <eps = - eps 315b>
      vv(pivot) = vv(j)
    end if
    p(j) = pivot
    if (a(j,j) == 0.0) then
      a(j,j) = tiny (a(j,j))

```

```

        end if
        a(j+1:,j) = a(j+1:,j) / a(j,j)
        a(j+1:,j+1:) &
            = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
    end do
    <Return optional arguments in lu_decompose 315d>
end subroutine lu_decompose

315a <eps = 1 315a>≡
    if (present (eps)) then
        eps = 1.0
    end if

315b <eps = - eps 315b>≡
    if (present (eps)) then
        eps = - eps
    end if

315c <pivots = 0 and eps = 0 315c>≡
    if (present (pivots)) then
        pivots = 0
    end if
    if (present (eps)) then
        eps = 0
    end if

315d <Return optional arguments in lu_decompose 315d>≡
    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

```

## H.2 Determinant

**316a**  $\langle$ Declaration of `linalg` procedures **313b** $\rangle + \equiv$   
`public :: determinant`

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

**316b**  $\langle$ Implementation of `linalg` procedures **314** $\rangle + \equiv$   
`pure subroutine determinant (a, det)`  
`real(kind=default), dimension(:, :), intent(in) :: a`  
`real(kind=default), intent(out) :: det`  
`real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu`  
`integer :: i`  
`lu = a`  
`call lu_decompose (lu, eps = det)`  
`do i = 1, size (a, dim = 1)`  
`det = det * lu(i,i)`  
`end do`  
`end subroutine determinant`

## H.3 Diagonalization

The code is an implementation of the algorithm presented in [16, 17], but independent from the code presented in [18] to avoid legal problems.

A Jacobi rotation around the angle  $\phi$  in row  $p$  and column  $q$

$$P(\phi; p, q) = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & \cos \phi & \cdots & \sin \phi \\ & & \vdots & 1 & \vdots \\ & & -\sin \phi & \cdots & \cos \phi \\ & & & & \ddots & \\ & & & & & 1 \end{pmatrix} \quad (\text{H.4})$$

results in

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

**317a** *<Declaration of linalg procedures 313b>+≡*

```
public :: diagonalize_real_symmetric
```

**317b** *<Implementation of linalg procedures 314>+≡*

```
pure subroutine diagonalize_real_symmetric (a, eval, evec, num_rot)
  real(kind=default), dimension(:, :), intent(in) :: a
  real(kind=default), dimension(:), intent(out) :: eval
  real(kind=default), dimension(:, :), intent(out) :: evec
  integer, intent(out), optional :: num_rot
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: aa
  real(kind=default) :: off_diagonal_norm, threshold, &
    c, g, h, s, t, tau, cot_2phi
  logical, dimension(size(eval),size(eval)) :: upper_triangle
  integer, dimension(size(eval)) :: one_to_ndim
  integer :: p, q, ndim, j, sweep
  integer, parameter :: MAX_SWEEPS = 50
  ndim = size (eval)
  one_to_ndim = (/ (j, j=1,ndim) /)
  upper_triangle = &
    spread (one_to_ndim, dim=1, ncopies=ndim) &
    > spread (one_to_ndim, dim=2, ncopies=ndim)
  aa = a
  call unit (evec)
<Initialize num_rot 320e>
  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  $A'_{pq} = 0$  318⟩
        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
318 ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  318⟩≡
    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  $A'_{pq} = 0$  319a⟩
        ⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  319c⟩
        ⟨ $V' = V \cdot P(\phi; p, q)$  320d⟩
        ⟨Update num_rot 320f⟩
    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

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

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

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

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

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

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

**319b**  $\langle \text{Determine } \phi \text{ for the Jacobi rotation } P(\phi; p, q) \text{ with } A'_{pq} = 0 \text{ 319a} \rangle + \equiv$   
`c = 1.0 / sqrt (1.0 + t**2)`  
`s = t * c`  
`tau = s / (1.0 + c)`

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

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

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

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

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

**320b**  $\langle$  *Implementation of linalg procedures 314*  $\rangle + \equiv$   
`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`

**320c**  $\langle$  *Declaration of linalg procedures 313b*  $\rangle + \equiv$   
`private :: jacobi_rotation`

**320d**  $\langle V' = V \cdot P(\phi; p, q)$  **320d**  $\rangle \equiv$   
`call jacobi_rotation (s, tau, evec(:,p), evec(:,q))`

**320e**  $\langle$  *Initialize num\_rot 320e*  $\rangle \equiv$   
`if (present (num_rot)) then`  
`num_rot = 0`  
`end if`

**320f**  $\langle$  *Update num\_rot 320f*  $\rangle \equiv$   
`if (present (num_rot)) then`  
`num_rot = num_rot + 1`  
`end if`

321a *<Implementation of linalg procedures 314>+≡*

```
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
```

321b *<Implementation of linalg procedures 314>+≡*

```
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
```

321c *<Declaration of linalg procedures 313b>+≡*

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

## H.4 Test

321d *<la\_sample.f90 321d>≡*

```
! la_sample.f90 --
<Copyleft notice 1>
program la_sample
  use kinds
  use utils
  use tao_random_numbers
  use linalg
  implicit none
  integer, parameter :: N = 200
  real(kind=default), dimension(N,N) :: a, evec, a0, l, u, NAG_bug
  real(kind=default), dimension(N) :: b, eval
  real(kind=default) :: d
  integer :: i
  call system_clock (i)
  call tao_random_seed (i)
  print *, i
  do i = 1, N
```

```

        call tao_random_number (a(:,i))
    end do
    NAG_bug = (a + transpose (a)) / 2
    a = NAG_bug
    a0 = a
    call lu_decompose (a, l=l, u=u)
    a = matmul (l, u)
    print *, maxval (abs(a-a0))
    call determinant (a, d)
    print *, d
    call diagonalize_real_symmetric (a, eval, evec)
    print *, product (eval)
    stop
    call sort (eval, evec)
    do i = 1, N
        b = matmul (a, evec(:,i)) - eval(i) * evec(:,i)
        write (unit = *, fmt = "(A,I3, 2(A,E11.4))") &
            "eval #", i, " = ", eval(i), ", |(A-lambda)V|_infty = ", &
            maxval (abs(b)) / maxval (abs(evec(:,i)))
    end do
end program la_sample

```

# —I—

## PRODUCTS

```
323 <products.f90 323>≡
! products.f90 --
<Copyleft notice 1>
module products
  use kinds
  implicit none
  private
  public :: dot, sp, spc
  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)) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
      - cmplx (q(2), q(3)) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
  end function sp
  pure function spc (p, q) result (spcpq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: spcpq
    spcpq = conjg (sp (p, q))
  end function spc
end module products
```

# —J—

## KINEMATICS

```

324a <kinematics.f90 324a>≡
    ! kinematics.f90 --
    <Copyleft notice 1>
    module kinematics
        use kinds
        use constants
        use products, only: dot
        use specfun, only: gamma
        implicit none
        private
        <Declaration of kinematics procedures 324b>
        <Interfaces of kinematics procedures 324c>
        <Declaration of kinematics types 326g>
        character(len=*), public, parameter :: KINEMATICS_RCS_ID = &
            "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
    contains
        <Implementation of kinematics procedures 325a>
    end module kinematics

```

### *J.1 Lorentz Transformations*

```

324b <Declaration of kinematics procedures 324b>≡
    public :: boost_velocity
    private :: boost_one_velocity, boost_many_velocity
    public :: boost_momentum
    private :: boost_one_momentum, boost_many_momentum

324c <Interfaces of kinematics procedures 324c>≡
    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  $\beta$ :

$$p'_0 = \gamma (p_0 - \vec{\beta} \vec{p}) \quad (\text{J.1a})$$

$$\vec{p}' = \gamma (\vec{p}_{\parallel} - \vec{\beta} p_0) + \vec{p}_{\perp} \quad (\text{J.1b})$$

with  $\gamma = 1/\sqrt{1 - \vec{\beta}^2}$ ,  $\vec{p}_{\parallel} = \vec{\beta}(\vec{\beta} \vec{p})/\vec{\beta}^2$  and  $\vec{p}_{\perp} = \vec{p} - \vec{p}_{\parallel}$ . Using  $1/\vec{\beta}^2 = \gamma^2/(\gamma + 1) \cdot 1/(\gamma - 1)$  and  $\vec{b} = \gamma \vec{\beta}$  this can be rewritten as

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

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

**325a**  $\langle \text{Implementation of kinematics procedures } \text{325a} \rangle \equiv$

```

pure function boost_one_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(0:3) :: p_prime
  real(kind=default), dimension(1:3) :: b
  real(kind=default) :: gamma, b_dot_p
  gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
  b = gamma * beta
  b_dot_p = dot_product (b, p(1:3))
  p_prime(0) = gamma * p(0) - b_dot_p
  p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
end function boost_one_velocity

```

**325b**  $\langle \text{Implementation of kinematics procedures } \text{325a} \rangle + \equiv$

```

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  $\vec{\beta} = \vec{q}/|q_0|$ :

```

326a <Implementation of kinematics procedures 325a>+≡
    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

326b <Implementation of kinematics procedures 325a>+≡
    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

```

326c <Implementation of kinematics procedures 325a>+≡
    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

326d <Declaration of kinematics procedures 324b>+≡
    public :: lambda

326e <Declaration of kinematics procedures 324b>+≡
    public :: two_to_three
    private :: two_to_three_massive, two_to_three_massless

326f <Interfaces of kinematics procedures 324c>+≡
    interface two_to_three
        module procedure two_to_three_massive, two_to_three_massless
    end interface

326g <Declaration of kinematics types 326g>≡
    type, public :: LIPS3
        real(kind=default), dimension(3,0:3) :: p
        real(kind=default) :: jacobian
    end type LIPS3

```

$$dLIPS_3 = \int \frac{d^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{d^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{d^3\vec{p}_3}{(2\pi)^3 2E_3} (2\pi)^4 \delta^4(p_1 + p_2 + p_3 - p_a - p_b) \quad (J.4)$$

The jacobian is given by

$$dLIPS_3 = \frac{1}{(2\pi)^5} \int d\phi dt_1 ds_2 d\Omega_3^{[23]} \frac{1}{32\sqrt{ss_2}} \frac{|p_3^{[23]}|}{|p_a^{[ab]}|} \quad (J.5)$$

where  $\vec{p}_i^{[jk]}$  denotes the momentum of particle  $i$  in the center of mass system of particles  $j$  and  $k$ .

**327a** *⟨Implementation of kinematics procedures 325a⟩* +≡  

```

pure function two_to_three_massive &
  (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
    s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
    1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3,2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive

```

A specialized version for massless particles can be faster, because the kinematics is simpler:

**327b** *⟨Implementation of kinematics procedures 325a⟩* +≡  

```

pure function two_to_three_massless (s, t1, s2, phi, cos_theta3, phi3) &
  result (p)
  real(kind=default), intent(in) :: s, t1, s2, phi, cos_theta3, phi3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: pa_abs, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (s) / 2
  p1_abs = (s - s2) / (2 * sqrt (s))

```



```

    p3_abs = sqrt (s2) / 2
    p%jacobian = 1.0 / ((2*PI)**5 * 32 * s)
    cos_theta = 1 + t1 / (2*pa_abs*p1_abs)
    p%p(1,0) = p1_abs
    p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p23(1:3) = - p%p(1,1:3)
    p23(0) = on_shell (p23, sqrt (s2))
    p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3)
end function two_to_three_massless

328a  <Declaration of kinematics procedures 324b>+≡
      public :: one_to_two
      private :: one_to_two_massive, one_to_two_massless

328b  <Interfaces of kinematics procedures 324c>+≡
      interface one_to_two
        module procedure one_to_two_massive, one_to_two_massless
      end interface

328c  <Implementation of kinematics procedures 325a>+≡
      pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi, m1, m2
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: s, p1_abs
        s = dot (p12, p12)
        p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,1:3) = - p(1,1:3)
        p(1,0) = on_shell (p(1,:), m1)
        p(2,0) = on_shell (p(2,:), m2)
        p = boost_momentum (p, - p12)
      end function one_to_two_massive

328d  <Implementation of kinematics procedures 325a>+≡
      pure function one_to_two_massless (p12, cos_theta, phi) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: p1_abs
        p1_abs = sqrt (dot (p12, p12)) / 2
        p(1,0) = p1_abs
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,0) = p1_abs
        p(2,1:3) = - p(1,1:3)
        p = boost_momentum (p, - p12)

```

```

end function one_to_two_massless

329a <Declaration of kinematics procedures 324b>+≡
public :: polar_to_cartesian, on_shell

329b <Implementation of kinematics procedures 325a>+≡
pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
  real(kind=default), intent(in) :: v_abs, cos_theta, phi
  real(kind=default), dimension(3) :: v
  real(kind=default) :: sin_phi, cos_phi, sin_theta
  sin_theta = sqrt (1.0 - cos_theta**2)
  cos_phi = cos (phi)
  sin_phi = sin (phi)
  v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
end function polar_to_cartesian

329c <Implementation of kinematics procedures 325a>+≡
pure function on_shell (p, m) result (E)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), intent(in) :: m
  real(kind=default) :: E
  E = sqrt (m**2 + dot_product (p(1:3), p(1:3)))
end function on_shell

```

### *J.3 Massive 3-Particle Phase Space Revisited*

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

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

```

329d <kinematics.f90 324a>+≡
module phase_space
  use kinds
  use constants
  use kinematics !NODEP!
  use tao_random_numbers
  implicit none
  private

```

```

    <Declaration of phase_space procedures 331b>
    <Interfaces of phase_space procedures 331c>
    <Declaration of phase_space types 330a>
    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 331d>
end module phase_space

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

```

330a <Declaration of phase\_space types 330a>≡

```

type, public :: LIPS3_unit
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_unit

```

330b <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_unit_massless
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_unit_massless

LIPS3_s2_t1_angles : (s2, t1, ϕ, cos θ3, ϕ3) (J.9)

```

330c <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_s2_t1_angles
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles

```

330d <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_s2_t1_angles_massless
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles_massless

LIPS3_momenta : (p1, p2, p3) (J.10)

```

330e <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_momenta
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default), dimension(2) :: mass_in
  real(kind=default), dimension(3) :: mass_out
  real(kind=default) :: jacobian
end type LIPS3_momenta

331a <Declaration of phase_space types 330a>+≡
type, public :: LIPS3_momenta_massless
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default) :: jacobian
end type LIPS3_momenta_massless

331b <Declaration of phase_space procedures 331b>≡
public :: random_LIPS3
private :: random_LIPS3_unit, random_LIPS3_unit_massless

331c <Interfaces of phase_space procedures 331c>≡
interface random_LIPS3
  module procedure random_LIPS3_unit, random_LIPS3_unit_massless
end interface

331d <Implementation of phase_space procedures 331d>≡
pure subroutine random_LIPS3_unit (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit

331e <Implementation of phase_space procedures 331d>+≡
pure subroutine random_LIPS3_unit_massless (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit_massless), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit_massless

331f <Declaration of phase_space procedures 331b>+≡
private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0

331g <(Unused) Interfaces of phase_space procedures 331g>≡
interface assignment(=)
  module procedure &
    LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
end interface

```

```

332a  <Implementation of phase_space procedures 331d>+≡
      pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
        type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
        type(LIPS3_unit), intent(in) :: unit
      end subroutine LIPS3_unit_to_s2_t1_angles

332b  <Implementation of phase_space procedures 331d>+≡
      pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
        type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
        type(LIPS3_unit_massless), intent(in) :: unit
      end subroutine LIPS3_unit_to_s2_t1_angles_m0

```

## J.4 Massless $n$ -Particle Phase Space: *RAMBO*

```

332c  <Declaration of kinematics procedures 324b>+≡
      public :: massless_isotropic_decay

```

The massless *RAMBO* algorithm [25]:

```

332d  <Implementation of kinematics procedures 325a>+≡
      pure function massless_isotropic_decay (roots, ran) result (p)
        real (kind=default), intent(in) :: roots
        real (kind=default), dimension(:,,:), intent(in) :: ran
        real (kind=default), dimension(size(ran,dim=1),0:3) :: p
        real (kind=default), dimension(size(ran,dim=1),0:3) :: q
        real (kind=default), dimension(0:3) :: qsum
        real (kind=default) :: cos_theta, sin_theta, phi, qabs, x, r, z
        integer :: k
        <Generate isotropic null vectors 332e>
        <Boost and rescale the vectors 333a>
      end function massless_isotropic_decay

```

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

```

332e  <Generate isotropic null vectors 332e>≡
      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 [25]. The transformation is really a Lorentz boost (as can be seen easily).

333a  $\langle$ Boost and rescale the vectors 333a $\rangle \equiv$

```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
  r = dot (q(k,:), qsum) / qabs
  z = (q(k,0) + r) / (qsum(0) + qabs)
  p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
  p(k,0) = x * r
enddo
```

333b  $\langle$ Declaration of kinematics procedures 324b $\rangle + \equiv$

```
public :: phase_space_volume
```

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

333c  $\langle$ Implementation of kinematics procedures 325a $\rangle + \equiv$

```
pure function phase_space_volume (n, roots) result (volume)
  integer, intent(in) :: n
  real (kind=default), intent(in) :: roots
  real (kind=default) :: volume
  real (kind=default) :: nd
  nd = n
  volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

## J.5 Tests

333d  $\langle$ ktest.f90 333d $\rangle \equiv$

```
program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default) :: &
    ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: t1_min, t1_max
  real(kind=default), dimension(5) :: r
  type(LIPS3) :: p
```

```

integer :: i
character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
ma = 1.0
mb = 1.0
m1 = 10.0
m2 = 20.0
m3 = 30.0
s = 100.0 ** 2
do i = 1, 10
  call tao_random_number (r)
  s2 = (r(1) * (sqrt (s) - m1) + (1 - r(1)) * (m2 + m3)) ** 2
  t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1 = r(2) * t1_max + (1 - r(2)) * t1_min
  phi = 2*PI * r(3)
  cos_theta3 = 2 * r(4) - 1
  phi3 = 2*PI * r(5)
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
  print fmt, "p1      = ", p%p(1,:)
  print fmt, "p2      = ", p%p(2,:)
  print fmt, "p3      = ", p%p(3,:)
  print fmt, "p1,2,3^2 = ", dot (p%p(1,:), p%p(1,)), &
    dot (p%p(2,:), p%p(2,)), dot (p%p(3,:), p%p(3,))
  print fmt, "sum(p)   = ", p%p(1,:) + p%p(2,:) + p%p(3,:)
  print fmt, "|J|     = ", p%jacobian
end do
end program ktest

```



Trivial check for typos, should be removed from the finalized program!

334  $\langle$  Trivial ktest.f90 334  $\rangle \equiv$

```

program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default), dimension(0:3) :: p, q, p_prime, p0
  real(kind=default) :: m
  character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
  integer :: i

```

```

do i = 1, 5
  if (i == 1) then
    p = (/ 1.0_double, 0.0_double, 0.0_double, 0.0_double /)
    m = 1.0
  else
    call tao_random_number (p)
    m = sqrt (PI)
  end if
  call tao_random_number (q(1:3))
  q(0) = sqrt (m**2 + dot_product (q(1:3), q(1:3)))
  p_prime = boost_momentum (p, q)
  print fmt, "p    = ", p
  print fmt, "q    = ", q
  print fmt, "p'   = ", p_prime
  print fmt, "p^2  = ", dot (p, p)
  print fmt, "p'^2 = ", dot (p_prime, p_prime)
  if (dot (p, p) > 0.0) then
    p0 = boost_momentum (p, p)
    print fmt, "p0   = ", p0
    print fmt, "p0^2 = ", dot (p0, p0)
  end if
end do
end program ktest

```



# —K—

## COORDINATES

```

336  <coordinates.f90 336>≡
      ! coordinates.f90 --
      <Copyleft notice 1>
      module coordinates
        use kinds
        use constants, only: PI
        use specfun, only: gamma
        implicit none
        private
        <Declaration of coordinates procedures 337a>
      contains
        <Implementation of coordinates procedures 337b>
      end module coordinates

```

### *K.1 Angular Spherical Coordinates*

$$\begin{aligned}
 x_n &= r \cos \theta_{n-2} \\
 x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
 &\dots \\
 x_3 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \cos \theta_1 \\
 x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \cos \phi \\
 x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \sin \phi
 \end{aligned} \tag{K.1}$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} (\sin \theta_i)^i \tag{K.2}$$

We can minimize the number of multiplications by computing the products

$$P_j = \prod_{i=j}^{n-2} \sin \theta_i \quad (\text{K.3})$$

Then

$$\begin{aligned} x_n &= r \cos \theta_{n-2} \\ x_{n-1} &= r P_{n-2} \cos \theta_{n-3} \\ &\dots \\ x_3 &= r P_2 \cos \theta_1 \\ x_2 &= r P_1 \cos \phi \\ x_1 &= r P_1 \sin \phi \end{aligned} \quad (\text{K.4})$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} P_i \quad (\text{K.5})$$

Note that  $\theta_i \in [0, \pi]$  and  $\phi \in [0, 2\pi]$  or  $\phi \in [-\pi, \pi]$ . Therefore  $\sin \theta_i \geq 0$  and

$$\sin \theta_i = \sqrt{1 - \cos^2 \theta_i} \quad (\text{K.6})$$

which is not true for  $\phi$ . Since `sqrt` is typically much faster than `sin` and `cos`, we use (K.6) where ever possible.

```

337a <Declaration of coordinates procedures 337a>≡
      public :: spherical_to_cartesian_2, &
              spherical_to_cartesian, spherical_to_cartesian_j

337b <Implementation of coordinates procedures 337b>≡
      pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(theta)) :: cos_theta
        real(kind=default), dimension(size(theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (theta) + 2
        cos_theta = cos (theta)
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
          product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do

```

```

if (present (x)) then
  x(1) = r * product_sin_theta(1) * sin (phi)
  x(2) = r * product_sin_theta(1) * cos (phi)
  x(3:) = r * product_sin_theta(2:n-1) * cos_theta
end if
if (present (jacobian)) then
  jacobian = r**(n-1) * product (product_sin_theta)
end if
end subroutine spherical_to_cartesian_2

```



Note that `call` inside of a function breaks F-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where `theta` could not be assumed shape ...

**338a** *⟨Implementation of coordinates procedures 337b⟩+≡*

```

pure function spherical_to_cartesian (r, phi, theta) result (x)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: theta
  real(kind=default), dimension(size(theta)+2) :: x
  call spherical_to_cartesian_2 (r, phi, theta, x = x)
end function spherical_to_cartesian

```

**338b** *⟨Implementation of coordinates procedures 337b⟩+≡*

```

pure function spherical_to_cartesian_j (r, phi, theta) &
  result (jacobian)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: theta
  real(kind=default) :: jacobian
  call spherical_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
end function spherical_to_cartesian_j

```

**338c** *⟨Declaration of coordinates procedures 337a⟩+≡*

```

public :: cartesian_to_spherical_2, &
  cartesian_to_spherical, cartesian_to_spherical_j

```

**338d** *⟨Implementation of coordinates procedures 337b⟩+≡*

```

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))
product_sin_theta(n-1) = 1
do i = n, 3, -1
    cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    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
    phi = atan2 (x(1), x(2))
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 subroutine cartesian_to_spherical_2

```

339a *⟨Implementation of coordinates procedures 337b⟩+≡*

```

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

```

339b *⟨Implementation of coordinates procedures 337b⟩+≡*

```

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

339c *⟨Declaration of coordinates procedures 337a⟩+≡*

```

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

340a *⟨Implementation of coordinates procedures 337b⟩+≡*

```
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
  if (present (jacobian)) then
    jacobian = r**(n-1) * product (product_sin_theta(2:))
  end if
end subroutine spherical_cos_to_cartesian_2
```

340b *⟨Implementation of coordinates procedures 337b⟩+≡*

```
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
```

340c *⟨Implementation of coordinates procedures 337b⟩+≡*

```
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
```

340d *⟨Declaration of coordinates procedures 337a⟩+≡*

```
public :: cartesian_to_spherical_cos_2, &
  cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
```

341a *<Implementation of coordinates procedures 337b>+≡*

```

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))
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
    local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    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
    phi = atan2 (x(1), x(2))
  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 subroutine cartesian_to_spherical_cos_2

```

341b *<Implementation of coordinates procedures 337b>+≡*

```

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

```

341c *<Implementation of coordinates procedures 337b>+≡*

```

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*

**342a** *⟨Declaration of coordinates procedures 337a⟩+≡*  

```
public :: surface
```

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

**342b** *⟨Implementation of coordinates procedures 337b⟩+≡*  

```
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

```
343a  <mpi90.f90 343a>≡
      ! mpi90.f90 --
      <Copyleft notice 1>
      module mpi90
        use kinds
        use mpi
        implicit none
        private
        <Declaration of mpi90 procedures 343b>
        <Interfaces of mpi90 procedures 346c>
        <Parameters in mpi90 (never defined)>
        <Variables in mpi90 (never defined)>
        <Declaration of mpi90 types 348b>
        character(len=*), public, parameter :: MPI90_RCS_ID = &
          "$Id: mpi90.nw 314 2010-04-17 20:32:33Z ohl $"
      contains
        <Implementation of mpi90 procedures 344a>
      end module mpi90
```

### *L.1 Basics*

```
343b  <Declaration of mpi90 procedures 343b>≡
      public :: mpi90_init
      public :: mpi90_finalize
      public :: mpi90_abort
      public :: mpi90_print_error
      public :: mpi90_size
      public :: mpi90_rank
```



```

344a  <Implementation of mpi90 procedures 344a>≡
      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) 344b>
      end subroutine mpi90_init

344b  <Handle local_error (no mpi90_abort) 344b>≡
      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

344c  <Handle local_error 344c>≡
      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

344d  <Implementation of mpi90 procedures 344a>+≡
      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 344c>
      end subroutine mpi90_finalize

344e  <Implementation of mpi90 procedures 344a>+≡
      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 345b>
call mpi_abort (local_domain, local_code, local_error)
<Handle local_error (no mpi90_abort) 344b>
end subroutine mpi90_abort

```

345a <Implementation of mpi90 procedures 344a>+≡

```

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

```

345b <Set default for domain 345b>≡

```

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

```

345c <Implementation of mpi90 procedures 344a>+≡

```

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 345b>
    call mpi_comm_size (local_domain, sz, local_error)
    <Handle local_error 344c>
end subroutine mpi90_size

346a <Implementation of mpi90 procedures 344a>+≡
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 345b>
  call mpi_comm_rank (local_domain, rank, local_error)
  <Handle local_error 344c>
end subroutine mpi90_rank

```

## *L.2 Point to Point*

```

346b <Declaration of mpi90 procedures 343b>+≡
  public :: mpi90_send
  public :: mpi90_receive
  public :: mpi90_receive_pointer

346c <Interfaces of mpi90 procedures 346c>≡
  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

346d <Implementation of mpi90 procedures 344a>+≡
  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

346e <Implementation of mpi90 procedures 344a>+≡
  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

347a ⟨Implementation of mpi90 procedures 344a⟩+≡
    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 347b⟩
    end subroutine mpi90_send_integer_array

347b ⟨Body of mpi90_send_*_array 347b⟩≡
    integer :: local_domain, local_error
    external mpi_send
    ⟨Set default for domain 345b⟩
    call mpi_send (buffer, size (buffer), datatype, target, tag, &
        local_domain, local_error)
    ⟨Handle local_error 344c⟩

347c ⟨Implementation of mpi90 procedures 344a⟩+≡
    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 347b⟩
    end subroutine mpi90_send_double_array

347d ⟨Implementation of mpi90 procedures 344a⟩+≡
    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

348a  <Implementation of mpi90 procedures 344a>+≡
        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

348b  <Declaration of mpi90 types 348b>≡
        type, public :: mpi90_status
            integer :: count, source, tag, error
        end type mpi90_status

348c  <Implementation of mpi90 procedures 344a>+≡
        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

348d  <Interfaces of mpi90 procedures 346c>+≡
        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

348e  <Set defaults for source, tag and domain 348e>≡
        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 345b>
349a <Implementation of mpi90 procedures 344a>+≡
    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
349b <Implementation of mpi90 procedures 344a>+≡
    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 349c>
    end subroutine mpi90_receive_integer_array
349c <Body of mpi90_receive_*_array 349c>≡
    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 348e>
    call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
        local_domain, local_status, local_error)
    <Handle local_error 344c>
    if (present (status)) then
        call decode_status (status, local_status, datatype)
    end if
349d <Declaration of mpi90 procedures 343b>+≡
    private :: decode_status

```

 Can we ignore ierror???

```

349e <Implementation of mpi90 procedures 344a>+≡
    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

```

350a *<Implementation of mpi90 procedures 344a>+≡*

```

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 349c>
end subroutine mpi90_receive_double_array

```

350b *<Implementation of mpi90 procedures 344a>+≡*

```

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

```

350c *<Implementation of mpi90 procedures 344a>+≡*

```

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

```

351a *<Interfaces of mpi90 procedures 346c>+≡*

```

interface mpi90_receive_pointer
    module procedure &
        mpi90_receive_integer_pointer, mpi90_receive_double_pointer
end interface

```

351b *<Implementation of mpi90 procedures 344a>+≡*

```

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 351c>
end subroutine mpi90_receive_integer_pointer

```

351c *<Body of mpi90\_receive\_\*\_pointer 351c>≡*

```

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 348e>

```

351d *<Body of mpi90\_receive\_\*\_pointer 351c>+≡*

```

call mpi_probe (local_source, local_tag, local_domain, &
    local_status, local_error)
<Handle local_error 344c>

```

 Can we ignore ierror???

351e *<Body of mpi90\_receive\_\*\_pointer 351c>+≡*

```

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

352a  <Body of mpi90_receive_*_pointer 351c>+≡
      call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
                    local_domain, local_status, local_error)

352b  <Body of mpi90_receive_*_pointer 351c>+≡
      <Handle local_error 344c>
      if (present (status)) then
        call decode_status (status, local_status, datatype)
      end if

352c  <Implementation of mpi90 procedures 344a>+≡
      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 351c>
      end subroutine mpi90_receive_double_pointer

```

### *L.3 Collective Communication*

```

352d  <Declaration of mpi90 procedures 343b>+≡
      public :: mpi90_broadcast

352e  <Interfaces of mpi90 procedures 346c>+≡
      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

352f  <Set default for domain 345b>+≡
      if (present (domain)) then
        local_domain = domain
      end if

```

```

else
    local_domain = MPI_COMM_WORLD
end if

353a  ⟨Implementation of mpi90 procedures 344a⟩+≡
    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

353b  ⟨Implementation of mpi90 procedures 344a⟩+≡
    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

353c  ⟨Implementation of mpi90 procedures 344a⟩+≡
    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

353d  ⟨Implementation of mpi90 procedures 344a⟩+≡
    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 354a>
    end subroutine mpi90_broadcast_integer_array

354a <Body of mpi90_broadcast_*_array 354a>≡
    integer :: local_domain, local_error
    external mpi_bcast
    <Set default for domain 345b>
    call mpi_bcast (buffer, size (buffer), datatype, root, &
                    local_domain, local_error)
    <Handle local_error 344c>

354b <Implementation of mpi90 procedures 344a>+≡
    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 354a>
    end subroutine mpi90_broadcast_double_array

354c <Implementation of mpi90 procedures 344a>+≡
    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 354a>
    end subroutine mpi90_broadcast_logical_array

354d <Implementation of mpi90 procedures 344a>+≡
    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

```

355a *<Implementation of mpi90 procedures 344a>+≡*

```

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

```

355b *<Implementation of mpi90 procedures 344a>+≡*

```

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

```

355c *<Implementation of mpi90 procedures 344a>+≡*

```

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

```

355d *<Implementation of mpi90 procedures 344a>+≡*

```

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
356  ⟨Implementation of mpi90 procedures 344a⟩+≡
    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—

## POOR MAN’S ELEMENTAL PROCEDURES

On one hand, I want to take advantage of Fortran95’s improvements, but on the other hand, I want to continue to use F as a style guide and also allow people with Fortran90 compilers to use the library.

### *M.1 m4 Macros*

```
357a <f95.m4 357a>≡
    dnl f95.m4 --
    divert(-1)dnl
    <Kill m4(1) builtins 357b>
    define('_specific_sv','dnl')
    define('_interface_sv','dnl')
    define('_specific_sva','dnl')
    define('_interface_sva','dnl')
    define('_begin_f90','divert(-1)dnl')
    define('_end_f90','divert''dnl')
    divert''dnl

357b <Kill m4(1) builtins 357b>≡
    undefine('eval')

357c <f90.m4 357c>≡
    dnl f90.m4 --
    divert(-1)dnl
    <Kill m4(1) builtins 357b>
    define('pure','')
    define('elemental','')
    define('_specific_sv','private :: $1_s, $1_v')
    define('_interface_sv','interface $1
        module procedure $1_s, $1_v
        end interface''define($1,$1_s)')
    define('_specific_sva','private :: $1_s, $1_v, $1_a')
```

```

define('_interface_sva','interface $1
    module procedure $1_s, $1_v, $1_a
    end interface''define($1,$1_s)')
define('_begin_f90','dnl')
define('_end_f90','dnl')
divert''dnl

```

## M.2 Miscellaneous Utilities

358a *<Implementation of utils procedures 305c>+≡*  
       \_begin\_f90

358b *<Declaration of utils procedures 304b>+≡*  
       \_begin\_f90  
       private :: swap\_integer\_array, swap\_real\_array  
       \_end\_f90

358c *<Interfaces of utils procedures 304c>+≡*  
       \_begin\_f90  
       interface swap  
           module procedure swap\_integer\_array, swap\_real\_array  
       end interface  
       \_end\_f90

358d *<Implementation of utils procedures 305c>+≡*  
       pure subroutine swap\_integer\_array (a, b)  
           integer, dimension(:), intent(inout) :: a, b  
           integer, dimension(max(size(a),size(b))) :: tmp  
           tmp = a  
           a = b  
           b = tmp  
       end subroutine swap\_integer\_array

358e *<Implementation of utils procedures 305c>+≡*  
       pure subroutine swap\_real\_array (a, b)  
           real(kind=default), dimension(:), intent(inout) :: a, b  
           real(kind=default), dimension(max(size(a),size(b))) :: tmp  
           tmp = a  
           a = b  
           b = tmp  
       end subroutine swap\_real\_array

358f *<Declaration of utils procedures 304b>+≡*  
       \_specific\_sva(gcd)  
       \_specific\_sva(lcm)

```

359a  <Interfaces of utils procedures 304c>+≡
      _interface_sva(gcd)
      _interface_sva(lcm)

359b  <Implementation of utils procedures 305c>+≡
      pure function gcd_v (m, n) result (gcd_m_n)
        integer, dimension(:), intent(in) :: m, n
        integer, dimension(size(m)) :: gcd_m_n
        integer :: i
        do i = 1, size (m)
          gcd_m_n(i) = gcd (m(i), n(i))
        end do
      end function gcd_v

359c  <Implementation of utils procedures 305c>+≡
      pure function lcm_v (m, n) result (lcm_m_n)
        integer, dimension(:), intent(in) :: m, n
        integer, dimension(size(m)) :: lcm_m_n
        integer :: i
        do i = 1, size (m)
          lcm_m_n(i) = lcm (m(i), n(i))
        end do
      end function lcm_v

```

This abuses the `_a` suffix, which is used elsewhere for two-dimensional arrays:

```

359d  <Implementation of utils procedures 305c>+≡
      pure function gcd_a (m, n) result (gcd_m_n)
        integer, dimension(:), intent(in) :: m
        integer, intent(in) :: n
        integer, dimension(size(m)) :: gcd_m_n
        integer :: i
        do i = 1, size (m)
          gcd_m_n(i) = gcd (m(i), n)
        end do
      end function gcd_a

359e  <Implementation of utils procedures 305c>+≡
      pure function lcm_a (m, n) result (lcm_m_n)
        integer, dimension(:), intent(in) :: m
        integer, intent(in) :: n
        integer, dimension(size(m)) :: lcm_m_n
        integer :: i
        do i = 1, size (m)
          lcm_m_n(i) = lcm (m(i), n)
        end do
      end function lcm_a

```



360a *<Implementation of utils procedures 305c>+≡*  
       \_end\_f90

### *M.3 Errors and Exceptions*

360b *<Implementation of exceptions procedures 246c>+≡*  
       \_begin\_f90

360c *<Declaration of exceptions procedures 246b>+≡*  
       \_specific\_sv(raise\_exception)  
       \_specific\_sv(clear\_exception)

360d *<Interfaces of exceptions procedures 360d>≡*  
       \_interface\_sv(raise\_exception)  
       \_interface\_sv(clear\_exception)

360e *<Implementation of exceptions procedures 246c>+≡*  
       pure subroutine raise\_exception\_v (exc, level, message, origin)  
           type(exception), dimension(:), intent(inout) :: exc  
           integer, dimension(:), intent(in) :: level  
           character(len=\*), dimension(:), intent(in), optional :: message, origin  
           integer :: i  
           do i = 1, size (exc)  
               call raise\_exception (exc(i), level(i), message(i), origin(i))  
           end do  
       end subroutine raise\_exception\_v

360f *<Implementation of exceptions procedures 246c>+≡*  
       pure subroutine clear\_exception\_v (exc)  
           type(exception), dimension(:), intent(inout) :: exc  
           integer :: i  
           do i = 1, size (exc)  
               call clear\_exception (exc(i))  
           end do  
       end subroutine clear\_exception\_v

360g *<Implementation of exceptions procedures 246c>+≡*  
       \_end\_f90

### *M.4 The Abstract Datatype division*

360h *<Implementation of divisions procedures 38b>+≡*  
       \_begin\_f90

```

361a  <Declaration of divisions procedures 38a>+≡
      _specific_sv(create_division)
      _specific_sv(create_empty_division)
      _specific_sva(copy_division)
      _specific_sv(set_rigid_division)
      _specific_sv(reshape_division)
      _specific_sv(delete_division)

361b  <Interfaces of divisions procedures 61b>+≡
      _interface_sv(create_division)
      _interface_sv(create_empty_division)
      _interface_sva(copy_division)
      _interface_sv(set_rigid_division)
      _interface_sv(reshape_division)
      _interface_sv(delete_division)

361c  <Implementation of divisions procedures 38b>+≡
      pure subroutine create_division_v (d, x_min, x_max, x_min_true, x_max_true)
        type(division_t), dimension(:), intent(out) :: d
        real(kind=default), dimension(:), intent(in) :: x_min, x_max
        real(kind=default), dimension(:), intent(in), optional :: &
          x_min_true, x_max_true
        integer :: j
        do j = 1, size (d)
          if (present (x_min_true) .and. present (x_max_true)) then
            call create_division &
              (d(j), x_min(j), x_max(j), x_min_true(j), x_max_true(j))
          else
            call create_division (d(j), x_min(j), x_max(j))
          end if
        end do
      end subroutine create_division_v

361d  <Implementation of divisions procedures 38b>+≡
      pure subroutine create_empty_division_v (d)
        type(division_t), dimension(:), intent(out) :: d
        integer :: j
        do j = 1, size (d)
          call create_empty_division (d(j))
        end do
      end subroutine create_empty_division_v

361e  <Implementation of divisions procedures 38b>+≡
      pure subroutine copy_division_v (lhs, rhs)
        type(division_t), dimension(:), intent(inout) :: lhs
        type(division_t), dimension(:), intent(in) :: rhs

```

```

integer :: j
do j = 1, size(lhs)
    call copy_division (lhs(j), rhs(j))
end do
end subroutine copy_division_v

```

This abuses the `_a` suffix, which is used elsewhere for two-dimensional arrays:

**362a** *⟨Implementation of divisions procedures 38b⟩+≡*

```

pure subroutine copy_division_a (lhs, rhs)
    type(division_t), dimension(:), intent(inout) :: lhs
    type(division_t), intent(in) :: rhs
    integer :: j
    do j = 1, size(lhs)
        call copy_division (lhs(j), rhs)
    end do
end subroutine copy_division_a

```

**362b** *⟨Implementation of divisions procedures 38b⟩+≡*

```

pure subroutine set_rigid_division_v (d, ng)
    type(division_t), dimension(:), intent(inout) :: d
    integer, dimension(:), intent(in) :: ng
    integer :: j
    do j = 1, size(d)
        call set_rigid_division (d(j), ng(j))
    end do
end subroutine set_rigid_division_v

```

**362c** *⟨Implementation of divisions procedures 38b⟩+≡*

```

pure subroutine reshape_division_v (d, max_num_div, ng, use_variance)
    type(division_t), dimension(:), intent(inout) :: d
    integer, dimension(:), intent(in) :: max_num_div
    integer, dimension(:), intent(in), optional :: ng
    logical, intent(in), optional :: use_variance
    integer :: j
    do j = 1, size(d)
        call reshape_division (d(j), max_num_div(j), ng(j), use_variance)
    end do
end subroutine reshape_division_v

```

**362d** *⟨Implementation of divisions procedures 38b⟩+≡*

```

pure subroutine delete_division_v (d)
    type(division_t), dimension(:), intent(inout) :: d
    integer :: j
    do j = 1, size(d)
        call delete_division (d(j))
    end do

```

```

        end subroutine delete_division_v

363a  <Declaration of divisions procedures 38a>+≡
        _specific_sv(inject_division)
        _specific_sv(inject_division_short)

363b  <Interfaces of divisions procedures 61b>+≡
        _interface_sv(inject_division)
        _interface_sv(inject_division_short)

363c  <Implementation of divisions procedures 38b>+≡
        pure subroutine inject_division_v (d, r, cell, x, x_mid, idx, wgt)
            type(division_t), dimension(:), intent(in) :: d
            real(kind=default), dimension(:), intent(in) :: r
            integer, dimension(:), intent(in) :: cell
            real(kind=default), dimension(:), intent(out) :: x, x_mid
            integer, dimension(:), intent(out) :: idx
            real(kind=default), dimension(:), intent(out) :: wgt
            integer :: j
            do j = 1, size (d)
                call inject_division (d(j), r(j), cell(j), x(j), &
                                     x_mid(j), idx(j), wgt(j))
            end do
        end subroutine inject_division_v

363d  <Implementation of divisions procedures 38b>+≡
        pure subroutine inject_division_short_v (d, r, x, idx, wgt)
            type(division_t), dimension(:), intent(in) :: d
            real(kind=default), dimension(:), intent(in) :: r
            real(kind=default), dimension(:), intent(out) :: x
            integer, dimension(:), intent(out) :: idx
            real(kind=default), dimension(:), intent(out) :: wgt
            integer :: j
            do j = 1, size (d)
                call inject_division_short (d(j), r(j), x(j), idx(j), wgt(j))
            end do
        end subroutine inject_division_short_v

363e  <Declaration of divisions procedures 38a>+≡
        _specific_sv(record_integral)
        _specific_sv(record_variance)
        _specific_sv(clear_integral_and_variance)

363f  <Declaration of divisions procedures (removed from WHIZARD) 60c>+≡
        _specific_sv(record_efficiency)

```

364a  $\langle$ Interfaces of divisions procedures 61b $\rangle + \equiv$   
`_interface_sv(record_integral)`  
`_interface_sv(record_variance)`  
`_interface_sv(clear_integral_and_variance)`

364b  $\langle$ Interfaces of divisions procedures (removed from WHIZARD) 364b $\rangle \equiv$   
`_interface_sv(record_efficiency)`

364c  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$   

```

pure subroutine record_integral_v (d, i, f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: f
  integer :: j
  do j = 1, size (d)
    call record_integral (d(j), i(j), f)
  end do
end subroutine record_integral_v

```

364d  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$   

```

pure subroutine record_variance_v (d, i, var_f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: var_f
  integer :: j
  do j = 1, size (d)
    call record_variance (d(j), i(j), var_f)
  end do
end subroutine record_variance_v

```

364e  $\langle$ Implementation of divisions procedures (removed from WHIZARD) 45b $\rangle + \equiv$   

```

pure subroutine record_efficiency_v (d, i, eff_f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: eff_f
  integer :: j
  do j = 1, size (d)
    call record_efficiency (d(j), i(j), eff_f)
  end do
end subroutine record_efficiency_v

```

364f  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$   

```

pure subroutine clear_integral_and_variance_v (d)
  type(division_t), dimension(:), intent(inout) :: d
  integer :: j
  do j = 1, size (d)

```

```

        call clear_integral_and_variance (d(j))
    end do
end subroutine clear_integral_and_variance_v

365a  <Declaration of divisions procedures 38a>+≡
      _specific_sv(refine_division)

365b  <Interfaces of divisions procedures 61b>+≡
      _interface_sv(refine_division)

365c  <Implementation of divisions procedures 38b>+≡
      pure subroutine refine_division_v (d)
        type(division_t), dimension(:), intent(inout) :: d
        integer :: j
        do j = 1, size (d)
            call refine_division (d(j))
        end do
      end subroutine refine_division_v

365d  <Declaration of divisions procedures 38a>+≡
      _specific_sv(probability)
      _specific_sv(inside_division)
      _specific_sv(stratified_division)
      _specific_sv(volume_division)
      _specific_sv(rigid_division)
      _specific_sv(adaptive_division)
      _specific_sv(quadrapole_division)

365e  <Interfaces of divisions procedures 61b>+≡
      _interface_sv(probability)
      _interface_sv(inside_division)
      _interface_sv(stratified_division)
      _interface_sv(volume_division)
      _interface_sv(rigid_division)
      _interface_sv(adaptive_division)
      _interface_sv(quadrapole_division)

365f  <Implementation of divisions procedures 38b>+≡
      pure function probability_v (d, xi) result (p)
        type(division_t), dimension(:), intent(in) :: d
        real(kind=default), dimension(:), intent(in) :: xi
        real(kind=default), dimension(size(d)) :: p
        integer :: j
        do j = 1, size (d)
            p(j) = probability (d(j), xi(j))
        end do
      end function probability_v

```

```

366a  <Implementation of divisions procedures 38b>+≡
      pure function inside_division_v (d, x) result (theta)
        type(division_t), dimension(:), intent(in) :: d
        real(kind=default), dimension(:), intent(in) :: x
        logical, dimension(size(d)) :: theta
        integer :: j
        do j = 1, size (d)
          theta(j) = inside_division (d(j), x(j))
        end do
      end function inside_division_v

366b  <Implementation of divisions procedures 38b>+≡
      pure function stratified_division_v (d) result (yorn)
        type(division_t), dimension(:), intent(in) :: d
        logical, dimension(size(d)) :: yorn
        integer :: j
        do j = 1, size (d)
          yorn(j) = stratified_division (d(j))
        end do
      end function stratified_division_v

366c  <Implementation of divisions procedures 38b>+≡
      pure function volume_division_v (d) result (vol)
        type(division_t), dimension(:), intent(in) :: d
        real(kind=default), dimension(size(d)) :: vol
        integer :: j
        do j = 1, size(d)
          vol(j) = volume_division (d(j))
        end do
      end function volume_division_v

366d  <Implementation of divisions procedures 38b>+≡
      pure function rigid_division_v (d) result (n)
        type(division_t), dimension(:), intent(in) :: d
        integer, dimension(size(d)) :: n
        integer :: j
        do j = 1, size(d)
          n(j) = rigid_division (d(j))
        end do
      end function rigid_division_v

366e  <Implementation of divisions procedures 38b>+≡
      pure function adaptive_division_v (d) result (n)
        type(division_t), dimension(:), intent(in) :: d
        integer, dimension(size(d)) :: n
        integer :: j

```

```

        do j = 1, size(d)
            n(j) = adaptive_division (d(j))
        end do
    end function adaptive_division_v

367a  <Implementation of divisions procedures 38b>+≡
    pure function quadrupole_division_v (d) result (q)
        type(division_t), dimension(:), intent(in) :: d
        real(kind=default), dimension(size(d)) :: q
        integer :: j
        do j = 1, size (d)
            q(j) = quadrupole_division (d(j))
        end do
    end function quadrupole_division_v

367b  <Declaration of divisions procedures 38a>+≡
    _specific_sv(copy_history)
    _specific_sv(summarize_division)

367c  <Interfaces of divisions procedures 61b>+≡
    _interface_sv(copy_history)
    _interface_sv(summarize_division)

367d  <Implementation of divisions procedures 38b>+≡
    pure subroutine copy_history_v (lhs, rhs)
        type(div_history), dimension(:), intent(inout) :: lhs
        type(div_history), dimension(:), intent(in) :: rhs
        integer :: j
        do j = 1, size (rhs)
            call copy_history (lhs(j), rhs(j))
        end do
    end subroutine copy_history_v

367e  <Implementation of divisions procedures 38b>+≡
    pure function summarize_division_v (d) result (s)
        type(division_t), dimension(:), intent(in) :: d
        type(div_history), dimension(size(d)) :: s
        integer :: j
        do j = 1, size (d)
            s(j) = summarize_division (d(j))
        end do
    end function summarize_division_v

367f  <Implementation of divisions procedures 38b>+≡
    _end_f90

```



## M.5 The Abstract Datatype *vamp\_grid*

- 368a *⟨Implementation of vamp procedures 77c⟩*+≡  
    \_begin\_f90
- 368b *⟨Declaration of vamp procedures 77a⟩*+≡  
    \_specific\_sv(vamp\_create\_empty\_grid)  
    \_specific\_sv(vamp\_nullify\_covariance)  
    \_specific\_sv(vamp\_get\_variance)  
    \_specific\_sv(vamp\_nullify\_variance)
- 368c *⟨Interfaces of vamp procedures 94b⟩*+≡  
    \_interface\_sv(vamp\_create\_empty\_grid)  
    \_interface\_sv(vamp\_nullify\_covariance)  
    \_interface\_sv(vamp\_get\_variance)  
    \_interface\_sv(vamp\_nullify\_variance)
- 368d *⟨Implementation of vamp procedures 77c⟩*+≡  
    pure subroutine vamp\_create\_empty\_grid\_v (g)  
        type(vamp\_grid), dimension(:), intent(inout) :: g  
        integer :: i  
        do i = 1, size (g)  
            call vamp\_create\_empty\_grid (g(i))  
        end do  
    end subroutine vamp\_create\_empty\_grid\_v
- 368e *⟨Implementation of vamp procedures 77c⟩*+≡  
    pure subroutine vamp\_nullify\_covariance\_v (g)  
        type(vamp\_grid), dimension(:), intent(inout) :: g  
        integer :: i  
        do i = 1, size (g)  
            call vamp\_nullify\_covariance (g(i))  
        end do  
    end subroutine vamp\_nullify\_covariance\_v
- 368f *⟨Implementation of vamp procedures 77c⟩*+≡  
    pure function vamp\_get\_variance\_v (g) result (v)  
        type(vamp\_grid), dimension(:), intent(in) :: g  
        real(kind=default), dimension(size(g)) :: v  
        integer :: i  
        do i = 1, size (g)  
            v(i) = vamp\_get\_variance (g(i))  
        end do  
    end function vamp\_get\_variance\_v

369a *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_nullify\_variance\_v (g)  
   type(vamp\_grid), dimension(:), intent(inout) :: g  
   integer :: i  
   do i = 1, size (g)  
     call vamp\_nullify\_variance (g(i))  
 end do  
end subroutine vamp\_nullify\_variance\_v

369b *<Declaration of vamp procedures 77a>+≡*  
 \_specific\_sv(vamp\_copy\_grid)  
 \_specific\_sv(vamp\_delete\_grid)

369c *<Interfaces of vamp procedures 94b>+≡*  
 \_interface\_sv(vamp\_copy\_grid)  
 \_interface\_sv(vamp\_delete\_grid)

369d *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_copy\_grid\_v (lhs, rhs)  
   type(vamp\_grid), dimension(:), intent(inout) :: lhs  
   type(vamp\_grid), dimension(:), intent(in) :: rhs  
   integer :: i  
   do i = 1, size (lhs)  
     call vamp\_copy\_grid (lhs(i), rhs(i))  
 end do  
end subroutine vamp\_copy\_grid\_v

369e *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_delete\_grid\_v (g)  
   type(vamp\_grid), dimension(:), intent(inout) :: g  
   integer :: i  
   do i = 1, size (g)  
     call vamp\_delete\_grid (g(i))  
 end do  
end subroutine vamp\_delete\_grid\_v

369f *<Declaration of vamp procedures 77a>+≡*  
 \_specific\_sv(vamp\_copy\_grids)  
 \_specific\_sv(vamp\_delete\_grids)

369g *<Interfaces of vamp procedures 94b>+≡*  
 \_interface\_sv(vamp\_copy\_grids)  
 \_interface\_sv(vamp\_delete\_grids)

369h *<Implementation of vamp procedures 77c>+≡*  
 pure subroutine vamp\_copy\_grids\_v (lhs, rhs)  
   type(vamp\_grids), dimension(:), intent(inout) :: lhs

```

        type(vamp_grids), dimension(:), intent(in) :: rhs
        integer :: i
        do i = 1, size (lhs)
            call vamp_copy_grids (lhs(i), rhs(i))
        end do
    end subroutine vamp_copy_grids_v
370a  <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_delete_grids_v (g)
        type(vamp_grids), dimension(:), intent(inout) :: g
        integer :: i
        do i = 1, size (g)
            call vamp_delete_grids (g(i))
        end do
    end subroutine vamp_delete_grids_v
370b  <Declaration of vamp procedures 77a>+≡
    _specific_sva(vamp_create_history)
    _specific_sv(vamp_terminate_history)
    _specific_sva(vamp_copy_history)
    _specific_sva(vamp_delete_history)
370c  <Interfaces of vamp procedures 94b>+≡
    _interface_sva(vamp_create_history)
    _interface_sv(vamp_terminate_history)
    _interface_sva(vamp_copy_history)
    _interface_sva(vamp_delete_history)
370d  <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_create_history_v (h, ndim, verbose)
        type(vamp_history), dimension(:), intent(inout) :: h
        integer, intent(in), optional :: ndim
        logical, intent(in), optional :: verbose
        integer :: i
        do i = 1, size (h)
            call vamp_create_history (h(i), ndim, verbose)
        end do
    end subroutine vamp_create_history_v
370e  <Implementation of vamp procedures 77c>+≡
    pure subroutine vamp_create_history_a (h, ndim, verbose)
        type(vamp_history), dimension(:, :), intent(inout) :: h
        integer, intent(in), optional :: ndim
        logical, intent(in), optional :: verbose
        integer :: i
        do i = 1, size (h, dim=2)

```

```

        call vamp_create_history_v (h(:,i), ndim, verbose)
    end do
end subroutine vamp_create_history_a

371a <Implementation of vamp procedures 77c>+≡
pure subroutine vamp_terminate_history_v (h)
    type(vamp_history), dimension(:), intent(inout) :: h
    integer :: i
    do i = 1, size (h)
        call vamp_terminate_history (h(i))
    end do
end subroutine vamp_terminate_history_v

371b <Implementation of vamp procedures 77c>+≡
pure subroutine vamp_copy_history_v (lhs, rhs)
    type(vamp_history), dimension(:), intent(out) :: lhs
    type(vamp_history), dimension(:), intent(in) :: rhs
    integer :: i
    do i = 1, size (rhs)
        call vamp_copy_history (lhs(i), rhs(i))
    end do
end subroutine vamp_copy_history_v

371c <Implementation of vamp procedures 77c>+≡
pure subroutine vamp_copy_history_a (lhs, rhs)
    type(vamp_history), dimension(:, :), intent(out) :: lhs
    type(vamp_history), dimension(:, :), intent(in) :: rhs
    integer :: i
    do i = 1, size (rhs, dim=2)
        call vamp_copy_history_v (lhs(:,i), rhs(:,i))
    end do
end subroutine vamp_copy_history_a

371d <Implementation of vamp procedures 77c>+≡
pure subroutine vamp_delete_history_v (h)
    type(vamp_history), dimension(:), intent(inout) :: h
    integer :: i
    do i = 1, size (h)
        call vamp_delete_history (h(i))
    end do
end subroutine vamp_delete_history_v

371e <Implementation of vamp procedures 77c>+≡
pure subroutine vamp_delete_history_a (h)
    type(vamp_history), dimension(:, :), intent(inout) :: h
    integer :: i

```

```

do i = 1, size (h, dim=2)
  call vamp_delete_history_v (h(:,i))
end do
end subroutine vamp_delete_history_a
372  ⟨Implementation of vamp procedures 77c⟩+≡
      _end_f90

```

# —N— IDEAS

## *N.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.

## *N.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.

## *N.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 ...

## *N.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.

## *N.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).

# —O—

## CROSS REFERENCES

### *O.1 Identifiers*

BUFFER\_SIZE: [59b](#), [60a](#), [106d](#), [108a](#), [108b](#), [108c](#), [265c](#)  
DEFAULT\_BUFFER\_SIZE: [252d](#), [261d](#), [261f](#), [274c](#), [275b](#)  
DEFAULT\_SEED: [255a](#), [255c](#)  
EXC\_DEFAULT: [246a](#), [246e](#)  
EXC\_ERROR: [89b](#), [245c](#), [246a](#), [246c](#)  
EXC\_FATAL: [50a](#), [50b](#), [51a](#), [90a](#), [96a](#), [245c](#), [246c](#)  
EXC\_INFO: [95a](#), [167b](#), [177c](#), [245c](#), [246c](#)  
EXC\_NONE: [245b](#), [245c](#), [246c](#)  
EXC\_WARN: [89b](#), [97d](#), [104d](#), [120a](#), [123a](#), [134c](#), [136c](#), [136d](#), [167b](#), [175a](#), [175b](#),  
[178b](#), [245c](#), [246c](#)  
K: [252a](#), [252b](#), [252a](#), [253c](#), [253d](#), [252a](#), [253e](#), [254a](#), [254d](#), [255d](#), [256a](#), [256b](#),  
[256c](#), [256d](#), [256e](#), [256f](#), [257a](#), [257c](#), [258a](#), [258c](#), [259c](#), [259e](#), [259g](#), [252a](#),  
[259h](#), [260a](#), [260b](#), [260d](#), [261d](#), [261f](#)  
L: [252a](#), [252b](#), [253d](#), [253e](#), [256b](#), [256c](#), [256d](#), [256e](#), [256f](#), [257a](#), [257c](#), [258c](#),  
[259h](#), [260a](#)  
LIPS3: [224b](#), [226b](#), [226f](#), [227a](#), [229b](#), [230a](#), [230c](#), [232c](#), [233b](#), [233c](#), [234a](#),  
[234b](#), [234c](#), [235a](#), [235b](#), [235c](#), [236b](#), [326g](#), [327a](#), [327b](#), [333d](#)  
LIPS3\_m5i2a3: [226c](#), [226f](#), [227a](#), [227b](#), [228](#), [232c](#), [232d](#), [233b](#), [233c](#), [234a](#),  
[234b](#), [234c](#), [235a](#), [235b](#), [235c](#)  
LIPS3\_momenta: [330e](#)  
LIPS3\_momenta\_massless: [331a](#)  
LIPS3\_s2\_t1\_angles: [330c](#), [332a](#)  
LIPS3\_s2\_t1\_angles\_massless: [330d](#), [332b](#)  
LIPS3\_unit: [330a](#), [331d](#), [332a](#)  
LIPS3\_unit\_massless: [330b](#), [331e](#), [332b](#)  
LIPS3\_unit\_to\_s2\_t1\_angles: [331f](#), [331g](#), [332a](#)  
LIPS3\_unit\_to\_s2\_t1\_angles\_m0: [331f](#), [331g](#), [332b](#)



M: [240b](#), [252c](#), [253d](#), [253e](#), [255d](#), [256f](#), [257a](#), [257g](#), [258c](#), [259h](#), [260a](#), [274e](#),  
[276e](#), [282e](#), [283a](#), [283c](#), [283d](#), [283e](#), [284a](#), [284b](#)  
MAX\_SEED: [255b](#), [255c](#)  
MAX\_UNIT: [267e](#), [268a](#), [312b](#), [312c](#)  
MIN\_NUM\_DIV: [46a](#)  
MIN\_UNIT: [267e](#), [268a](#), [312b](#), [312c](#)  
NAME\_LENGTH: [245b](#), [246a](#)  
NUM\_DIV\_DEFAULT: [77c](#), [78a](#), [78a](#)  
PI: [190b](#), [192](#), [193a](#), [193b](#), [223b](#), [223c](#), [224a](#), [225c](#), [226f](#), [227b](#), [228](#), [243b](#),  
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## *Acknowledgements*

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