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

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Abstract

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

Revision Control

```
prelude.nw 314 2010-04-17 20:32:33Z ohl
divisions.nw 314 2010-04-17 20:32:33Z ohl
vamp.nw 317 2010-04-18 00:31:03Z ohl
vampi.nw 314 2010-04-17 20:32:33Z ohl
vamp_test.nw 314 2010-04-17 20:32:33Z ohl
vamp_test0.nw 314 2010-04-17 20:32:33Z ohl
application.nw 314 2010-04-17 20:32:33Z ohl
kinds.nw 314 2010-04-17 20:32:33Z ohl
constants.nw 314 2010-04-17 20:32:33Z ohl
exceptions.nw 314 2010-04-17 20:32:33Z ohl
specfun.nw 314 2010-04-17 20:32:33Z ohl
vamp_stat.nw 314 2010-04-17 20:32:33Z ohl
histograms.nw 314 2010-04-17 20:32:33Z ohl
utils.nw 314 2010-04-17 20:32:33Z ohl
linalg.nw 314 2010-04-17 20:32:33Z ohl
products.nw 314 2010-04-17 20:32:33Z ohl
kinematics.nw 314 2010-04-17 20:32:33Z ohl
coordinates.nw 314 2010-04-17 20:32:33Z ohl
mpi90.nw 314 2010-04-17 20:32:33Z ohl
postlude.nw 314 2010-04-17 20:32:33Z ohl
```

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Program Summary:

- **Title of program:** VAMP, Version 1.0 (October 1999)

- **Program obtainable** by anonymous `ftp` from the host `crunch.ikp.physik.th-darmstadt.de` in the directory `pub/ohl/vamp`.

- **Licensing provisions:** Free software under the GNU General Public License.

- **Programming language used:** From version 2.2.0 of the program: Fortran2003 [8] Until version 2.1.x of the program: Fortran95 [9] (Fortran90 [7] and F [14] versions available as well)

- **Number of program lines in distributed program, including test data, etc.:** ≈ 4300 (excluding comments)

- **Computer/Operating System:** Any with a Fortran95 (or Fortran90 or F) programming environment.

- **Memory required to execute with typical data:** Negligible on the scale of typical applications calling the library.

- **Typical running time:** A small fraction (typically a few percent) of the running time of applications calling the library.

- **Purpose of program:**

- **Nature of physical problem:**

- **Method of solution:**

- **Keywords:** adaptive integration, event generation, parallel processing

INTRODUCTION

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

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

Copyleft

Mention the GNU General Public License (maybe we can switch to the GNU Library General Public License)

1   ⟨*Copyleft notice* 1⟩≡   (37a 70c 167b 192a 202a 204b 220b 222a 245 247a 273d 274a 287a 289b 292a 295a 305a 3

```
! Copyright (C) 1998 by Thorsten Ohl <ohl@hep.tu-darmstadt.de>
!
! VAMP is free software; you can redistribute it and/or modify it
! under the terms of the GNU General Public License as published by
! the Free Software Foundation; either version 2, or (at your option)
! any later version.
!
```

---

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

```
! VAMP is distributed in the hope that it will be useful, but
! WITHOUT ANY WARRANTY; without even the implied warranty of
! MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
! GNU General Public License for more details.
!
! You should have received a copy of the GNU General Public License
! along with this program; if not, write to the Free Software
! Foundation, Inc., 675 Mass Ave, Cambridge, MA 02139, USA.
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Mention that the tangled sources are not the preferred form of distribution:

2 ⟨*Copyleft notice* 1⟩+≡   (37a 70c 167b 192a 202a 204b 220b 222a 245 247a 273d 274a 287a 289b 292a 295a 305a

```
! This version of the source code of vamp has no comments and
! can be hard to understand, modify, and improve.  You should have
! received a copy of the literate 'noweb' sources of vamp that
! contain the documentation in full detail.
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

—2—
Algorithms

The notation has to be synchronized with [3]!

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

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

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

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

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

Where $|X|$ is the size of the point set and $|\mathcal{D}| = \int_{\mathcal{D}} \mathrm{d}x$ 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

$$\mathcal{E}(\langle f\rangle) = E(f) \tag{2.2a}$$
$$\mathcal{E}(\sigma^2(f)) = V(f) \tag{2.2b}$$

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

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

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

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

while the variance transformes non-trivially

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

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

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

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

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

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

A familiar example is given by the map

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

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

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

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

2.2   Stratified Sampling

The technique of importance sampling concentrates the sampling points in the region where the contribution to the integrand is largest. Alternatively we can also concentrates 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 $\mathcal{D}^i$

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

a new estimator is

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

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

where

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

and

$$\sum_{i=1}^{n} N_i = N \tag{2.12}$$

since the expectation is linear

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

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

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

This is minimized for

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

as a simple variation of $\mathcal{V}(\overline{\langle f \rangle})$ shows.
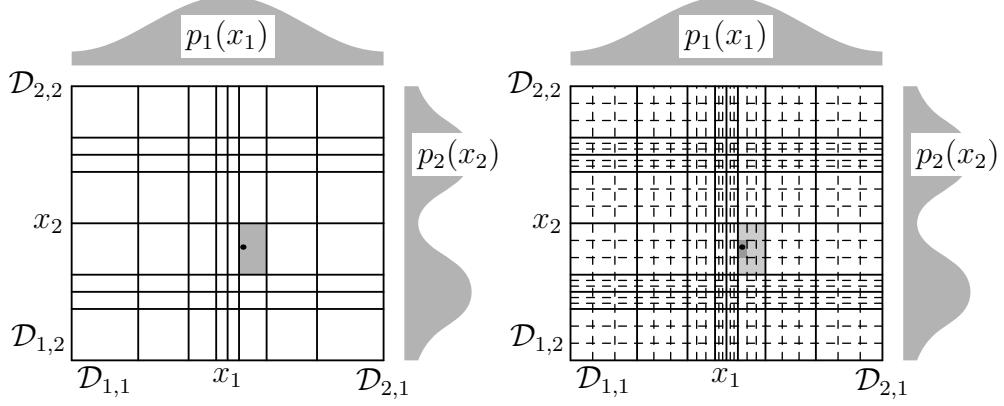
Figure 2.1: `vegas` grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.
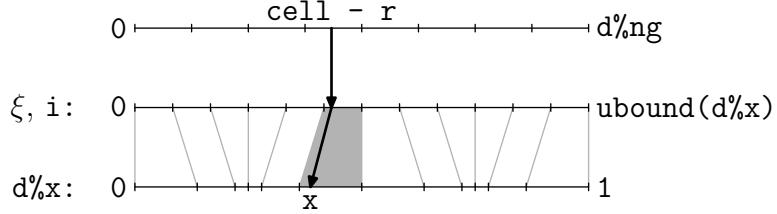
Figure 2.2: One-dimensional illustration of the `vegas` grid structure for pseudo stratified sampling, which is used in high dimensions.

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.

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

The present reimplementation 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

$$n_{\mathrm{div},j} \to \frac{Q_j n_{\mathrm{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\mathrm{dim}}}} \tag{2.16}$$

where we have used the damped standard deviation

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

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 integranted efficiently by Vegas can be enlarged substantially by using multi channel methods. The new class will include almost all integrals appearing in high energy physics simulations.

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

2.5   Revolving

⚠ Under construction!

2.6   Parallelization

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

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

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

2.6.1   Multilinear Structure of the Sampling Algorithm

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

$$S : \pi \times F \to \mathbf{R}$$
$$(p, f) \mapsto I = S(p, f)$$

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

$$S_0 : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} \to R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R}$$
$$(\rho, G, a, f, \mu_1, \mu_2) \mapsto (\rho', G, a', f, \mu_1', \mu_2') = S_0(\rho, G, a, f, \mu_1, \mu_2) \tag{2.18}$$

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

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

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

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

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

$$r : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} \to R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R}$$
$$(\rho, G, a, f, \mu_1, \mu_2) \mapsto (\rho, G', a, f, \mu_1, \mu_2) = r(\rho, G, a, f, \mu_1, \mu_2) \tag{2.20}$$

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

$$S_n = S_0(rS_0)^n \tag{2.21}$$

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:

$$P : R \times \Gamma \times A \times F \times \mathbf{R} \times \mathbf{R} \to \mathbf{R} \times \mathbf{R}$$
$$(\rho, G, a, f, \mu_1, \mu_2) \mapsto (I, \sigma) \tag{2.22}$$

Then

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

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

For parallelization, it is crucial to find a division of S_n or any part of it into *independent* pieces that can be evaluated in parallel. In order to be effective, r has to be applied to *all* of a and therefore a sychronization of G before and after r is appropriately. Forthermore, 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 he 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 proof that it does not change the results, i.e.

$$S_0 = \iota S_0 \phi \tag{2.24}$$

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

However, a reordering of the random number sequence will only change the result by the statistical error, as long as the scale of the allowed reorderings is *bounded* and much smaller than the period of the random number generator [1] Below, we will therefore use the notation $x \approx y$ for "equal for an appropriate finite reordering of the ρ used in calculating x and y". For our porposes, 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

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

where

$$\rho = \bigoplus_i \rho_i \tag{2.25b}$$

$$G = \bigoplus_i G_i \tag{2.25c}$$

$$a = \bigoplus_i a_i \tag{2.25d}$$

$$\mu_n = \bigoplus_i \mu_{n,i} \tag{2.25e}$$

for appropriate definitions of "$\oplus$". For the moments, we have standard addition

$$\mu_{n,1} \oplus \mu_{n,2} = \mu_{n,1} + \mu_{n,2} \tag{2.26}$$

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

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[1] Arbirtrary 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

$$a_1 \oplus a_2 = a_1 + a_2 \tag{2.27}$$

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 corrspond to a sampling of the variance per cell and no longer of function values themselves.

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

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

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

$$G = \bigotimes_{j=1}^{n_{\mathrm{dim}}} D^j \tag{2.28}$$

and decompositions of the D^j induce decompositions of G

$$G_1 \oplus G_2 = \left(\bigotimes_{j=1}^{i-1} D^j \otimes D_1^i \otimes \bigotimes_{i=j+1}^{n_{\dim}} D^j \right) \oplus \left(\bigotimes_{j=1}^{i-1} D^j \otimes D_2^i \otimes \bigotimes_{i=j+1}^{n_{\dim}} D^j \right)$$

$$= \bigotimes_{j=1}^{i-1} D^j \otimes \left(D_1^i \oplus D_2^i \right) \otimes \bigotimes_{j=i+1}^{n_{\dim}} D^j \quad (2.29)$$

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)

$$a = (d^1, \ldots, d^{n_{\dim}}) \tag{2.30}$$

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

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

with "+" denoting the standard addition of the bin contents and "⊕" 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

$$D^i = D_1^i \oplus D_2^i \tag{2.32}$$

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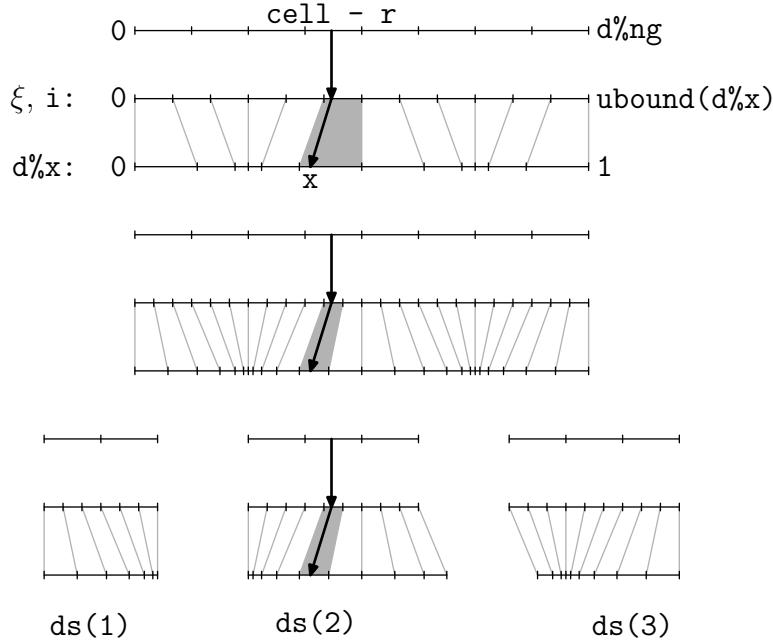
Figure 2.3: Forking one dimension `d` of a grid into three parts `ds(1)`, `ds(2)`, and `ds(3)`. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 2.2).

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

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

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

2.6.2 State and Message Passing

2.6.3 Random Numbers

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

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[2]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 [10, 11, 15] and MPI [12], respectively. From these examples, it should be obvious how to adapt VAMP to other parallel computing paradigms.

Serial

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

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

HPF

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

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

Instead of one random number generator state rng, it takes an array consisting of one state per processor. These rng(:) are assumed to be initialized, such that the resulting sequences are statistically independent. For this purpose, Knuth's random number generator [16] is most convenient and is included with VAMP (see the example on page 16). Before each S_0, the procedure vamp_distribute_work determines a good decomposition of the grid d into size(rng) pieces. This decomposition is encoded in the array d where d(1,:) holds the dimensions along which to split the grid and d(2,:) holds the corrsponding 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)
```

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

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

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

MPI

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

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

17 ⟨*Parallel implementation of* $S_n = S_0(rS_0)^n$ *(MPI)* 17⟩≡

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

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

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

—3—
DESIGN TRADE OFFS

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

- *Ease-Of-Use:* few procedures, few arguments.

- *Parallelizability:* statelessness

- *Performance and Flexibility:* rich interface, functionality.

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

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

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

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

3.1 Programming Language

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

Let us consider the alternatives

- FORTRAN77 is still the dominant language in high energy physics and all running experiment's software environments are based on it. However, the standard [6] is obsolete now and the successors [7, 9] have added many desirable features, while retaining almost all of FORTRAN77 a 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

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

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

`subroutine vamp_delete_grid (g [, exc])`

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

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

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

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

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

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

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

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

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

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

22 ⟨*Interface declaration for* `func` 22⟩≡   (14 15 17 86c 94d 104 113–15 120b 135d 137 139–42 170 176 182 183)

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

4.1.1 Basic Example

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

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

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23a ⟨basic.f90 23a⟩≡   23b ▷

```
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 themselve, but must pass them along). The module tao_random_numbers hosts the random number generator used and vamp is the adaptive interation module proper. Finally, the application module basic_fct has to be imported as well.

23b ⟨basic.f90 23a⟩+≡   ◁ 23a 23c ▷

```
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⟩+≡   ◁ 23b 24a ▷

```
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⟩+≡   ◁23c 24b▷
```
    call tao_random_create (rng, seed=0)
    call clear_exception (exc)
    call vamp_create_grid (grid, domain, num_calls=10000, exc=exc)
    call handle_exception (exc)
```

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

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

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

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

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

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

4.2   Advanced Usage

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

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

4.2.1   Types

`type(vamp_grid)`

`type(vamp_grids)`

`type(vamp_history)`

`type(exception)`

   (from module `exceptions`)

4.2.2   Shared Arguments

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

`real, intent(in) :: accuracy`

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

$$\frac{\texttt{std\_dev}}{\texttt{integral}} < \texttt{accuracy} \tag{4.3}$$

`real, intent(out) :: avg_chi2`

   The average χ^2 of the iterations.

`integer, intent(in) :: channel`

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

`logical, intent(in) :: covariance`

   Collect covariance data.

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

   Exceptional conditions are reported in `exc`.

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

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

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

Diagnostic information for multi channel sampling.

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

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

`real, intent(out) :: integral`

The current best estimate of the integral.

`integer, intent(in) :: iterations`

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

`integer, intent(in) :: num_calls`

The number of sampling points.

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

Number of divisions of the adaptive grid in each dimension.

`logical, intent(in) :: quadrupole`

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

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

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

`real, intent(out) :: std_dev`

The current best estimate of the error on the integral.

`logical, intent(in) :: stratified`

Try to use stratified sampling.

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

...

4.2.3 Single Channel Procedures

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

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

subroutine vamp_create_empty_grid (g)

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

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

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

    func

  S_n with $n =$ iterations

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

    func

  S_0

subroutine vamp_refine_grid (g, [, exc])

  r

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

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

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

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

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

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

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

subroutine vamp_copy_grid (lhs, rhs)

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

subroutine vamp_delete_grid (g)

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

4.2.4   Inout/Output and Marshling

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

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

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

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

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

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

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

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

pure subroutine vamp_marshal_grid (g, integer_buffer,
  double_buffer)
```

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```fortran
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_marshal_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!

```fortran
pure subroutine vamp_marshal_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.

```fortran
pure subroutine vamp_unmarshal_grid (g, integer_buffer,
  double_buffer)

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

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

29 ⟨*MPI communication example* 29⟩≡
```fortran
  call vamp_marshal_grid_size (g, isize, dsize)
```

29

```
allocate (ibuf(isize), dbuf(dsize))
call mpi_comm_rank (MPI_COMM_WORLD, proc_id, errno)
select case (proc_id)
   case (0)
      call vamp_marshal_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_marshal_history_size (g, [, . . .])

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

subroutine vamp_marshal_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

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

31a   ⟨*Interface declaration for* `phi` 31a⟩≡   (113–16 137 183a)
```
interface
   pure function phi (xi, channel) result (x)
     use kinds
     real(kind=default), dimension(:), intent(in) :: xi
     integer, intent(in) :: channel
     real(kind=default), dimension(size(xi)) :: x
   end function phi
end interface
```

31b   ⟨*Interface declaration for* `ihp` 31b⟩≡   (113c)
```
interface
   pure function ihp (x, channel) result (xi)
     use kinds
     real(kind=default), dimension(:), intent(in) :: x
     integer, intent(in) :: channel
     real(kind=default), dimension(size(x)) :: xi
   end function ihp
end interface
```

31c   ⟨*Interface declaration for* `jacobian` 31c⟩≡   (113c 114a)
```
interface
   pure function jacobian (x, data, channel) result (j)
     use kinds
     use vamp_grid_type !NODEP!
     import vamp_data_t
     real(kind=default), dimension(:), intent(in) :: x
     class(vamp_data_t), intent(in) :: data
     integer, intent(in) :: channel
     real(kind=default) :: j
   end function jacobian
end interface

function vamp_multi_channel (func, phi, ihp, jacobian, x,
  weightsl, grids)

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

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```
    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,
  weightsl)

    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

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

```
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
```

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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⟩≡   (37a) 58a ▷

```
type, public :: division_t
!   private
!!! Avoiding a g95 bug
```

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

5.1.1   Creation, Manipulation & Injection

38a   ⟨*Declaration of* divisions *procedures* 38a⟩≡   (37a) 43a▷
```
   public :: create_division, create_empty_division
   public :: copy_division, delete_division
   public :: set_rigid_division, reshape_division
```

38b   ⟨*Implementation of* divisions *procedures* 38b⟩≡   (37a) 39a▷
```
   elemental subroutine create_division &
        (d, x_min, x_max, x_min_true, x_max_true)
     type(division_t), intent(out) :: d
     real(kind=default), intent(in) :: x_min, x_max
     real(kind=default), intent(in), optional :: x_min_true, x_max_true
     allocate (d%x(0:1), d%integral(1), d%variance(1))
   ! allocate (d%efficiency(1))
     d%x(0) = 0.0
     d%x(1) = 1.0
     d%x_min = x_min
     d%x_max = x_max
     d%dx = d%x_max - d%x_min
     d%stratified = .false.
     d%ng = 1
     d%dxg = 1.0 / d%ng
     if (present (x_min_true)) then
        d%x_min_true = x_min_true
     else
        d%x_min_true = x_min
     end if
     if (present (x_max_true)) then
        d%x_max_true = x_max_true
```

```
          else
              d%x_max_true = x_max
          end if
      end subroutine create_division
```

39a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁38b 39b▷
```
      elemental subroutine create_empty_division (d)
        type(division_t), intent(out) :: d
        nullify (d%x, d%integral, d%variance)
      ! nullify (d%efficiency)
      end subroutine create_empty_division
```

39b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁39a 39c▷
```
      elemental subroutine set_rigid_division (d, ng)
        type(division_t), intent(inout) :: d
        integer, intent(in) :: ng
        d%stratified = ng > 1
        d%ng = ng
        d%dxg = real (ubound (d%x, dim=1), kind=default) / d%ng
      end subroutine set_rigid_division
```

$$\mathrm{dxg} = \frac{n_{\mathrm{div}}}{n_g} \tag{5.1}$$

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

39c ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁39b 43b▷
```
      elemental subroutine reshape_division (d, max_num_div, ng, use_variance)
        type(division_t), intent(inout) :: d
        integer, intent(in) :: max_num_div
        integer, intent(in), optional :: ng
        logical, intent(in), optional :: use_variance
        real(kind=default), dimension(:), allocatable :: old_x, m
        integer :: num_div, equ_per_adap
        if (present (ng)) then
           if (max_num_div > 1) then
              d%stratified = ng > 1
           else
              d%stratified = .false.
           end if
        else
           d%stratified = .false.
        end if
        if (d%stratified) then
```

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```
      d%ng = ng
      ⟨Initialize stratified sampling 42⟩
   else
      num_div = max_num_div
      d%ng = 1
   end if
   d%dxg = real (num_div, kind=default) / d%ng
   allocate (old_x(0:ubound(d%x,dim=1)), m(ubound(d%x,dim=1)))
   old_x = d%x
   ⟨Set m to (1, 1, ...) or to rebinning weights from d%variance 40a⟩
   ⟨Resize arrays, iff necessary 40b⟩
   d%x = rebin (m, old_x, num_div)
   deallocate (old_x, m)
end subroutine reshape_division
```

40a ⟨Set m to (1, 1, ...) or to rebinning weights from d%variance 40a⟩≡   (39c)
```
   if (present (use_variance)) then
      if (use_variance) then
         m = rebinning_weights (d%variance)
      else
         m = 1.0
      end if
   else
      m = 1.0
   end if
```

40b ⟨Resize arrays, iff necessary 40b⟩≡   (39c)
```
   if (ubound (d%x, dim=1) /= num_div) then
      deallocate (d%x, d%integral, d%variance)
   !  deallocate (d%efficiency)
      allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
   !  allocate (d%efficiency(num_div))
   end if
```

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

For a low number of sampling points and high dimensions, genuinely stratified sampling is impossible, because we would have to reduce the number n_{div} of adaptive divisions too far. Instead, we keep stratified false which will tell the integration routine not to concentrate the grid in the regions where
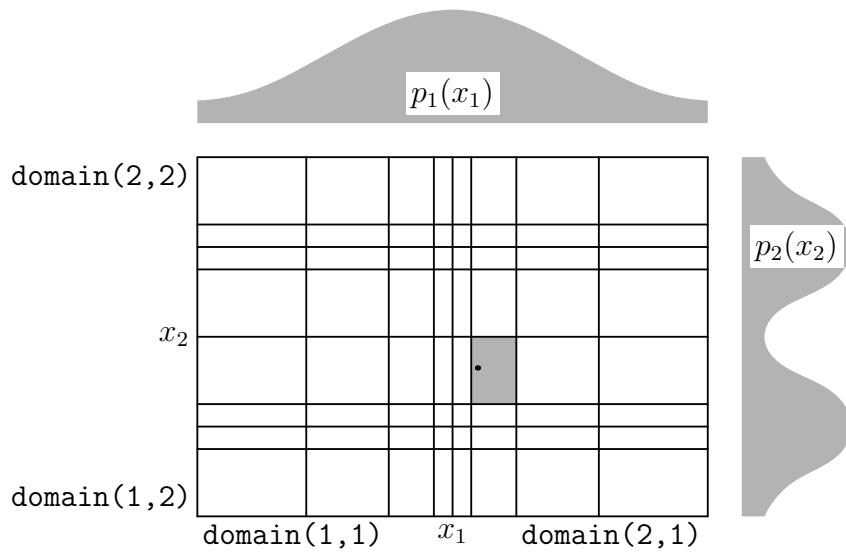
Figure 5.1: `vegas` grid structure for non-stratified sampling. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.
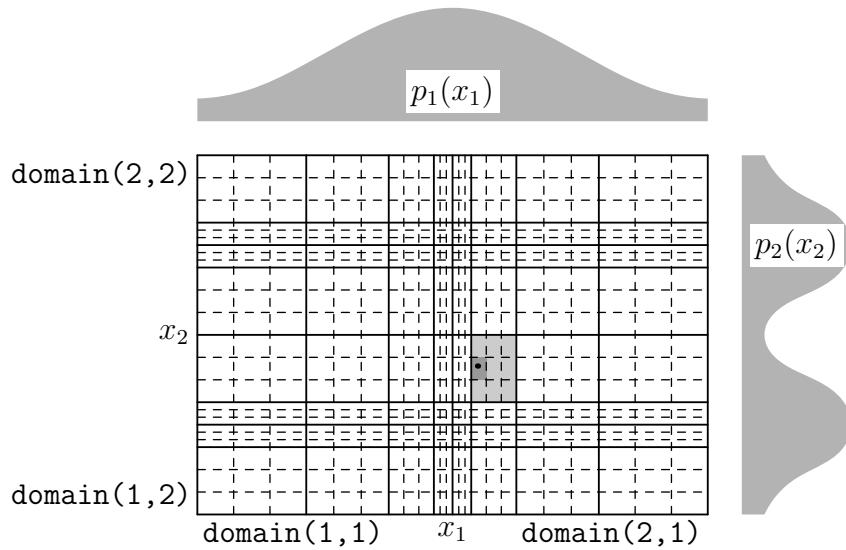
Figure 5.2: `vegas` grid structure for genuinely stratified sampling, which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.

n_{dim}	$N_{\text{calls}}^{\max}(n_g = 25)$
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 $n_{\text{div}}^{\max}$ divisions of the adaptive grid

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

and the corresponding number n_{div} of adaptive divisions

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

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

$$n_g = k \cdot n_{\text{div}} \tag{5.2c}$$

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

```
if (d%ng >= max_num_div / 2) then
   d%stratified = .true.
   equ_per_adap = d%ng / max_num_div + 1
   num_div = d%ng / equ_per_adap
   if (num_div < 2) then
      d%stratified = .false.
      num_div = 2
      d%ng = 1
   else if (mod (num_div,2) == 1) then
      num_div = num_div - 1
      d%ng = equ_per_adap * num_div
   else
```
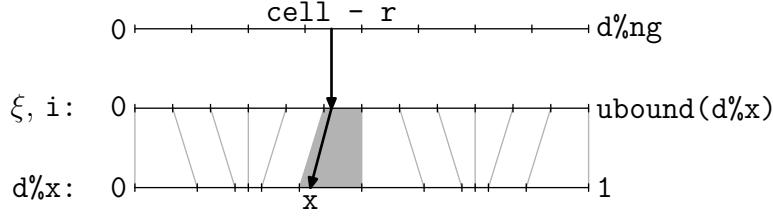
Figure 5.3: One-dimensional illustration of the `vegas` grid structure for pseudo stratified sampling, which is used in high dimensions.

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

Figure 5.3 on page 43 is a one-dimensional illustration of the sampling algorithm. In each cell of the rigid equidistant grid, two random points are selected (or N_{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.

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

43a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁38a 44c▷
    `public :: inject_division, inject_division_short`

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

```
     ⟨Set i, delta_x, x, and wgt from xi 44a⟩
       idx = i
       x_mid = d%x_min + 0.5 * (d%x(i-1) + d%x(i)) * d%dx
     end subroutine inject_division
```

44a   ⟨Set i, delta_x, x, and wgt from xi 44a⟩≡   (43b 44b)
```
       i = max (min (int (xi), ubound (d%x, dim=1)), 1)
       delta_x = d%x(i) - d%x(i-1)
       x = d%x_min + (d%x(i-1) + (xi - i) * delta_x) * d%dx
       wgt = delta_x * ubound (d%x, dim=1)
```

44b   ⟨Implementation of divisions procedures 38b⟩+≡   (37a) ◁43b 44d▷
```
     elemental subroutine inject_division_short (d, r, x, idx, wgt)
       type(division_t), intent(in) :: d
       real(kind=default), intent(in) :: r
       integer, intent(out) :: idx
       real(kind=default), intent(out) :: x, wgt
       real(kind=default) :: delta_x, xi
       integer :: i
       xi = r * ubound (d%x, dim=1) + 1.0
       ⟨Set i, delta_x, x, and wgt from xi 44a⟩
       idx = i
     end subroutine inject_division_short
```

5.1.2   Grid Refinement

44c   ⟨Declaration of divisions procedures 38a⟩+≡   (37a) ◁43a 45d▷
```
     public :: record_integral, record_variance, clear_integral_and_variance
     ! public :: record_efficiency
```

44d   ⟨Implementation of divisions procedures 38b⟩+≡   (37a) ◁44b 45a▷
```
     elemental subroutine record_integral (d, i, f)
       type(division_t), intent(inout) :: d
       integer, intent(in) :: i
       real(kind=default), intent(in) :: f
       d%integral(i) = d%integral(i) + f
       if (.not. d%stratified) then
          d%variance(i) = d%variance(i) + f*f
       end if
     end subroutine record_integral
```

45a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁44d 45c▷
```
  elemental subroutine record_variance (d, i, var_f)
    type(division_t), intent(inout) :: d
    integer, intent(in) :: i
    real(kind=default), intent(in) :: var_f
    if (d%stratified) then
       d%variance(i) = d%variance(i) + var_f
    end if
  end subroutine record_variance
```

45b ⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩≡   60d▷
```
  elemental subroutine record_efficiency (d, i, eff)
    type(division_t), intent(inout) :: d
    integer, intent(in) :: i
    real(kind=default), intent(in) :: eff
  ! d%efficiency(i) = d%efficiency(i) + eff
  end subroutine record_efficiency
```

45c ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁45a 45e▷
```
  elemental subroutine clear_integral_and_variance (d)
    type(division_t), intent(inout) :: d
    d%integral = 0.0
    d%variance = 0.0
  ! d%efficiency = 0.0
  end subroutine clear_integral_and_variance
```

45d ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁44c 47a▷
```
  public :: refine_division
```

45e ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁45c 46b▷
```
  elemental subroutine refine_division (d)
    type(division_t), intent(inout) :: d
    character(len=*), parameter :: FN = "refine_division"
    d%x = rebin (rebinning_weights (d%variance), d%x, size (d%variance))
  end subroutine refine_division
```

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

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

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

46a ⟨*Variables in* `divisions` 46a⟩≡   (37a) 60a ▷
```
integer, private, parameter :: MIN_NUM_DIV = 3
```

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

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

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

---

[1]Some old timers call this a feature, however.

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```
          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⟩+≡   (37a) ◁45d 48a▷
```
  private :: rebinning_weights
```

The NaN test is probably not portable:

47b ⟨*Bail out if* any (d == NaN) 47b⟩≡   (46b)
```
  if (any (d /= d)) then
     m = 1.0
     return
  end if
```

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

47c ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁46b 48e▷
```
  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 ∑ m_k ≥ Δ and keep the surplus in δ 48b⟩
        ⟨Interpolate the new x_i from x_k and δ 48c⟩
    end do
    x_new(num_div) = 1.0
  end function rebin
```

$$\bar{f}_i \approx \frac{m_i}{\Delta x_i}$$

$x_0 \; x_1 \; x_2 \qquad\qquad\qquad x_{n-1} x_n$
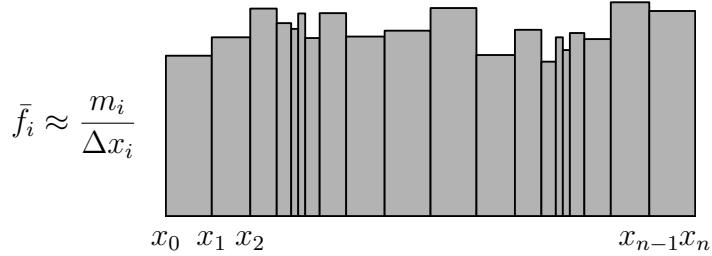
Figure 5.4: Typical weights used in the rebinning algorithm.

48a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁47a 48d▷
```
private :: rebin
```

We increment k until another Δ (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* δ 48b⟩≡   (47c)
```
do
   if (step <= delta) then
      exit
   end if
   k = k + 1
   delta = delta + m(k)
end do
delta = delta - step
```

48c ⟨*Interpolate the new* x_i *from* x_k *and* δ 48c⟩≡   (47c)
```
x_new(i) = x(k) - (x(k) - x(k-1)) * delta / m(k)
```

5.1.3 Probability Density

48d ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁48a 49a▷
```
public :: probability
```

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

and

$$\int_{x_{\min}}^{x_{\max}} \mathrm{d}x \; p(x) = 1 \tag{5.7}$$

48e ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁47c 49b▷
```
elemental function probability (d, x) result (p)
   type(division_t), intent(in) :: d
   real(kind=default), intent(in) :: x
```

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

5.1.4   Quadrupole

49a   ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁48d 49c▷
```fortran
  public :: quadrupole_division
```

49b   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁48e 50a▷
```fortran
  elemental function quadrupole_division (d) result (q)
    type(division_t), intent(in) :: d
    real(kind=default) :: q
    !!!  q = value_spread_percent (rebinning_weights (d%variance))
    q = standard_deviation_percent (rebinning_weights (d%variance))
  end function quadrupole_division
```

5.1.5   Forking and Joining

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

49c   ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁49a 54c▷
```fortran
  public :: fork_division, join_division, sum_division
```

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

50a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡　　　　　(37a) ◁49b 50b▷

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

50b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡　　　　　(37a) ◁50a 55a▷

```
pure subroutine join_division (d, ds, exc)
  type(division_t), intent(inout) :: d
  type(division_t), dimension(:), intent(in) :: ds
  type(exception), intent(inout), optional :: exc
  character(len=*), parameter :: FN = "join_division"
  integer, dimension(size(ds)) :: n0, n1
  integer, dimension(0:size(ds)) :: n, ds_ng
  integer :: i, j, num_div, num_forks, nx
  real(kind=default), dimension(:), allocatable :: d_x, d_integral, d_variance
```

```
  ! real(kind=default), dimension(:), allocatable :: d_efficiency
    num_div = ubound (d%x, dim=1)
    num_forks = size (ds)
    if (d%ng == 1) then
        ⟨Join importance sampling divisions 51b⟩
    else if (num_div >= num_forks) then
        if (modulo (d%ng, num_div) == 0) then
            ⟨Join pure stratified sampling divisions 52c⟩
        else
            ⟨Join pseudo stratified sampling divisions 54b⟩
        end if
    else
        if (present (exc)) then
            call raise_exception (exc, EXC_FATAL, FN, "internal error")
        end if
    end if
  end subroutine join_division
```

Importance Sampling

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

51a   ⟨Fork an importance sampling division 51a⟩≡   (50a)
```
  if (d%stratified) then
      call raise_exception (exc, EXC_FATAL, FN, &
                            "ng == 1 incompatiple 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⟩≡   (50b)
```
  call sum_division (d, ds)
```

Note, however, that this is only legitimate as long as $d\%ng$ == 1 implies $d\%stratified$ == .false., because otherwise the sampling code would be incorrect (cf. var_f on page 90).

Stratified Sampling

For stratified sampling, we have to work a little harder, because there are just two points per cell and we have to slice along the lines of the stratification

grid. Actually, we are slicing along the adaptive grid, since it has a reasonable size. Slicing along the stratification grid could be done using the method below. However, in this case *very* large adaptive grids would be shipped from one process to the other and the comunication costs will outweigh the gains fom paralell processing.

52a ⟨*Setup to fork a pure stratified sampling division* 52a⟩≡ (52)
```
n = (num_div * (/ (j, j=0,num_forks) /)) / num_forks
n0(1:num_forks) = n(0:num_forks-1)
n1(1:num_forks) = n(1:num_forks)
```

52b ⟨*Fork a pure stratified sampling division* 52b⟩≡ (50a)
```
⟨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⟩≡ (50b)
```
⟨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
```
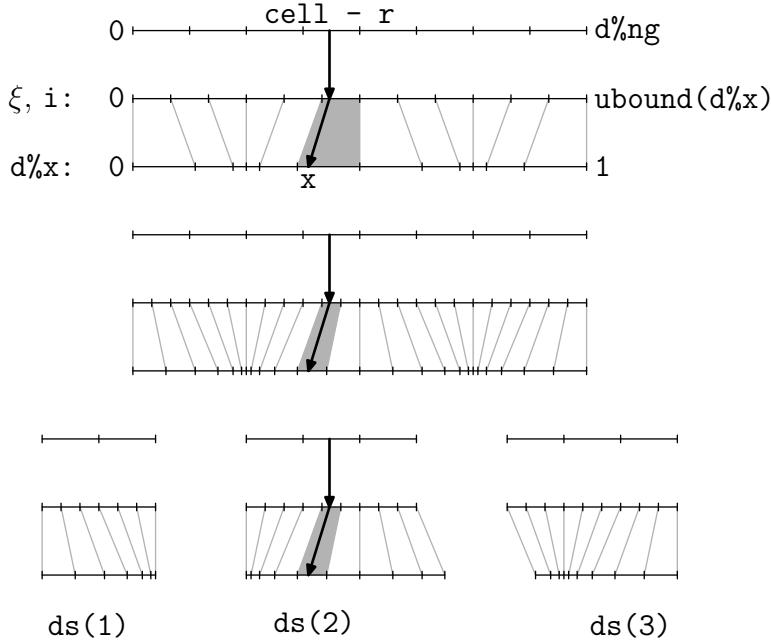
Figure 5.5: Forking one dimension `d` of a grid into three parts `ds(1)`, `ds(2)`, and `ds(3)`. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 5.3).

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

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

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⟩≡ (54)

```
nx = lcm (d%ng / gcd (num_forks, d%ng), num_div)
ds_ng = (d%ng * (/ (j, j=0,num_forks) /)) / num_forks
n = (nx * ds_ng) / d%ng
n0(1:num_forks) = n(0:num_forks-1)
n1(1:num_forks) = n(1:num_forks)
```

54a 〈*Fork a pseudo stratified sampling division* 54a〉≡   (50a)
```
     〈Setup to fork a pseudo stratified sampling division 53〉
     allocate (d_x(0:nx), d_integral(nx), d_variance(nx))
     ! allocate (d_efficiency(nx))
     call subdivide (d_x, d%x)
     call distribute (d_integral, d%integral)
     call distribute (d_variance, d%variance)
     ! call distribute (d_efficiency, d%efficiency)
     do i = 1, num_forks
        call copy_array_pointer (ds(i)%x, d_x(n0(i):n1(i)), lb = 0)
        call copy_array_pointer (ds(i)%integral, d_integral(n0(i)+1:n1(i)))
        call copy_array_pointer (ds(i)%variance, d_variance(n0(i)+1:n1(i)))
     !  call copy_array_pointer (ds(i)%efficiency, d_efficiency(n0(i)+1:n1(i)))
        ds(i)%x = (ds(i)%x - ds(i)%x(0)) / (d_x(n1(i)) - d_x(n0(i)))
     end do
     ds%x_min = d%x_min + d%dx * d_x(n0)
     ds%x_max = d%x_min + d%dx * d_x(n1)
     ds%dx = ds%x_max - ds%x_min
     ds%x_min_true = d%x_min_true
     ds%x_max_true = d%x_max_true
     ds%stratified = d%stratified
     ds%ng = ds_ng(1:num_forks) - ds_ng(0:num_forks-1)
     num_calls = sum_calls ! this is a misnomer, it remains "calls per cell" here
     ds%dxg = real (n1 - n0, kind=default) / ds%ng
     deallocate (d_x, d_integral, d_variance)
     ! deallocate (d_efficiency)
```

54b 〈*Join pseudo stratified sampling divisions* 54b〉≡   (50b)
```
     〈Setup to fork a pseudo stratified sampling division 53〉
     allocate (d_x(0:nx), d_integral(nx), d_variance(nx))
     ! allocate (d_efficiency(nx))
     do i = 1, num_forks
        d_integral(n0(i)+1:n1(i)) = ds(i)%integral
        d_variance(n0(i)+1:n1(i)) = ds(i)%variance
     !  d_efficiency(n0(i)+1:n1(i)) = ds(i)%efficiency
     end do
     call collect (d%integral, d_integral)
     call collect (d%variance, d_variance)
     ! call collect (d%efficiency, d_efficiency)
     deallocate (d_x, d_integral, d_variance)
     ! deallocate (d_efficiency)
```

54c 〈*Declaration of* divisions *procedures* 38a〉+≡   (37a) ◁49c 56a▷
```
     private :: subdivide
     private :: distribute
```

54

```
      private :: collect
```

55a   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁50b 55b▷
```
      pure subroutine subdivide (x, x0)
        real(kind=default), dimension(0:), intent(inout) :: x
        real(kind=default), dimension(0:), intent(in) :: x0
        integer :: i, n, n0
        n0 = ubound (x0, dim=1)
        n = ubound (x, dim=1) / n0
        x(0) = x0(0)
        do i = 1, n
           x(i::n) = x0(0:n0-1) * real (n - i) / n + x0(1:n0) * real (i) / n
        end do
      end subroutine subdivide
```

55b   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁55a 55c▷
```
      pure subroutine distribute (x, x0)
        real(kind=default), dimension(:), intent(inout) :: x
        real(kind=default), dimension(:), intent(in) :: x0
        integer :: i, n
        n = ubound (x, dim=1) / ubound (x0, dim=1)
        do i = 1, n
           x(i::n) = x0 / n
        end do
      end subroutine distribute
```

55c   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁55b 55d▷
```
      pure subroutine collect (x0, x)
        real(kind=default), dimension(:), intent(inout) :: x0
        real(kind=default), dimension(:), intent(in) :: x
        integer :: i, n, n0
        n0 = ubound (x0, dim=1)
        n = ubound (x, dim=1) / n0
        do i = 1, n0
           x0(i) = sum (x((i-1)*n+1:i*n))
        end do
      end subroutine collect
```

Trivia

55d   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁55c 56b▷
```
      pure subroutine sum_division (d, ds)
        type(division_t), intent(inout) :: d
        type(division_t), dimension(:), intent(in) :: ds
        integer :: i
```

```
      d%integral = 0.0
      d%variance = 0.0
    ! d%efficiency = 0.0
      do i = 1, size (ds)
         d%integral = d%integral + ds(i)%integral
         d%variance = d%variance + ds(i)%variance
    !    d%efficiency = d%efficiency + ds(i)%efficiency
      end do
    end subroutine sum_division
```

56a ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁54c 57a▷
```
    public :: debug_division
    public :: dump_division
```

56b ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁55d 56c▷
```
    subroutine debug_division (d, prefix)
      type(division_t), intent(in) :: d
      character(len=*), intent(in) :: prefix
      print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%x: ", &
          lbound(d%x,dim=1), d%x(lbound(d%x,dim=1)), &
          " ... ", &
          ubound(d%x,dim=1), d%x(ubound(d%x,dim=1))
      print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%i: ", &
          lbound(d%integral,dim=1), d%integral(lbound(d%integral,dim=1)), &
          " ... ", &
          ubound(d%integral,dim=1), d%integral(ubound(d%integral,dim=1))
      print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%v: ", &
          lbound(d%variance,dim=1), d%variance(lbound(d%variance,dim=1)), &
          " ... ", &
          ubound(d%variance,dim=1), d%variance(ubound(d%variance,dim=1))
    ! print "(1x,a,2(a,1x,i3,1x,f10.7))", prefix, ": d%e: ", &
    !     lbound(d%efficiency,dim=1), d%efficiency(lbound(d%efficiency,dim=1)), &
    !     " ... ", &
    !     ubound(d%efficiency,dim=1), d%efficiency(ubound(d%efficiency,dim=1))
    end subroutine debug_division
```

56c ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁56b 57b▷
```
    subroutine dump_division (d, prefix)
      type(division_t), intent(in) :: d
      character(len=*), intent(in) :: prefix
    ! print "(2(1x,a),100(1x,f10.7))", prefix, ":x: ", d%x
      print "(2(1x,a),100(1x,f10.7))", prefix, ":x: ", d%x(1:)
      print "(2(1x,a),100(1x,e10.3))", prefix, ":i: ", d%integral
      print "(2(1x,a),100(1x,e10.3))", prefix, ":v: ", d%variance
    ! print "(2(1x,a),100(1x,e10.3))", prefix, ":e: ", d%efficiency
```

```
end subroutine dump_division
```

5.1.6   Inquiry

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

57a   ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁56a 58b▷
```
public :: inside_division, stratified_division
public :: volume_division, rigid_division, adaptive_division
```

57b   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁56c 57c▷
```
elemental function inside_division (d, x) result (theta)
  type(division_t), intent(in) :: d
  real(kind=default), intent(in) :: x
  logical :: theta
  theta = (x >= d%x_min_true) .and. (x <= d%x_max_true)
end function inside_division
```

57c   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁57b 57d▷
```
elemental function stratified_division (d) result (yorn)
  type(division_t), intent(in) :: d
  logical :: yorn
  yorn = d%stratified
end function stratified_division
```

57d   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁57c 57e▷
```
elemental function volume_division (d) result (vol)
  type(division_t), intent(in) :: d
  real(kind=default) :: vol
  vol = d%dx
end function volume_division
```

57e   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁57d 57f▷
```
elemental function rigid_division (d) result (n)
  type(division_t), intent(in) :: d
  integer :: n
  n = d%ng
end function rigid_division
```

57f   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁57e 58c▷
```
elemental function adaptive_division (d) result (n)
  type(division_t), intent(in) :: d
  integer :: n
  n = ubound (d%x, dim=1)
end function adaptive_division
```

5.1.7 Diagnostics

58a ⟨*Declaration of* divisions *types* 37b⟩+≡   (37a) ◁37b

```
type, public :: div_history
   private
   logical :: stratified
   integer :: ng, num_div
   real(kind=default) :: x_min, x_max, x_min_true, x_max_true
   real(kind=default) :: &
         spread_f_p, stddev_f_p, spread_p, stddev_p, spread_m, stddev_m
end type div_history
```

58b ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁57a 58d▷

```
public :: copy_history, summarize_division
```

58c ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁57f 58e▷

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

58d ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁58b 60b▷

```
private :: probabilities
```

58e ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁58c 59a▷

```
pure function probabilities (x) result (p)
   real(kind=default), dimension(0:), intent(in) :: x
   real(kind=default), dimension(ubound(x,dim=1)) :: p
```

```
      integer :: num_div
      num_div = ubound (x, dim=1)
      p = 1.0 / (x(1:num_div) - x(0:num_div-1))
      p = p / sum(p)
    end function probabilities
```

59a ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁58e 59b▷
```
    subroutine print_history (h, tag)
      type(div_history), dimension(:), intent(in) :: h
      character(len=*), intent(in), optional :: tag
      call write_history (output_unit, h, tag)
      flush (output_unit)
    end subroutine print_history
```

59b ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁59a 61c▷
```
    subroutine write_history (u, h, tag)
      integer, intent(in) :: u
      type(div_history), dimension(:), intent(in) :: h
      character(len=*), intent(in), optional :: tag
      character(len=BUFFER_SIZE) :: pfx
      character(len=1) :: s
      integer :: i
      if (present (tag)) then
         pfx = tag
      else
         pfx = "[vamp]"
      end if
      if ((minval (h%x_min) == maxval (h%x_min)) &
           .and. (minval (h%x_max) == maxval (h%x_max))) then
         write (u, "(1X,A11,1X,2X,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
              h(1)%x_min, " <= ", h(1)%x_min_true, &
              " < x < ", h(1)%x_max_true, " <= ", h(1)%x_max
      else
         do i = 1, size (h)
            write (u, "(1X,A11,1X,I2,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
                 i, h(i)%x_min, " <= ", h(i)%x_min_true, &
                 " < x < ", h(i)%x_max_true, " <= ", h(i)%x_max
         end do
      end if
      write (u, "(1X,A11,1X,A2,2(1X,A3),A1,6(1X,A8))") pfx, &
           "it", "nd", "ng", "", &
           "spr(f/p)", "dev(f/p)", "spr(m)", "dev(m)", "spr(p)", "dev(p)"
      iterations: do i = 1, size (h)
         if (h(i)%stratified) then
            s = "*"
```

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```
            else
               s = ""
            end if
            write (u, "(1X,A11,1X,I2,2(1X,I3),A1,6(1X,F7.2,A1))") pfx, &
                 i, h(i)%num_div, h(i)%ng, s, &
                 h(i)%spread_f_p, "%", h(i)%stddev_f_p, "%", &
                 h(i)%spread_m, "%", h(i)%stddev_m, "%", &
                 h(i)%spread_p, "%", h(i)%stddev_p, "%"
         end do iterations
         flush (u)
      end subroutine write_history
```

60a ⟨*Variables in* divisions 46a⟩+≡   (37a) ◁46a 62a▷
      ```
      integer, private, parameter :: BUFFER_SIZE = 50
      ```

60b ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁58d 61a▷
      ```
      public :: print_history, write_history
      ```

60c ⟨*Declaration of* divisions *procedures (removed from WHIZARD)* 60c⟩≡
      ```
      public :: division_x, division_integral
      public :: division_variance, division_efficiency
      ```

60d ⟨*Implementation of* divisions *procedures (removed from WHIZARD)* 45b⟩+≡   ◁45b 60e▷
      ```
      pure subroutine division_x (x, d)
        real(kind=default), dimension(:), pointer :: x
        type(division_t), intent(in) :: d
        call copy_array_pointer (x, d%x, 0)
      end subroutine division_x
      ```

60e ⟨*Implementation of* divisions *procedures (removed from WHIZARD)* 45b⟩+≡   ◁60d 60f▷
      ```
      pure subroutine division_integral (integral, d)
        real(kind=default), dimension(:), pointer :: integral
        type(division_t), intent(in) :: d
        call copy_array_pointer (integral, d%integral)
      end subroutine division_integral
      ```

60f ⟨*Implementation of* divisions *procedures (removed from WHIZARD)* 45b⟩+≡   ◁60e 60g▷
      ```
      pure subroutine division_variance (variance, d)
        real(kind=default), dimension(:), pointer :: variance
        type(division_t), intent(in) :: d
        call copy_array_pointer (variance, d%variance, 0)
      end subroutine division_variance
      ```

60g ⟨*Implementation of* divisions *procedures (removed from WHIZARD)* 45b⟩+≡   ◁60f
      ```
      pure subroutine division_efficiency (eff, d)
        real(kind=default), dimension(:), pointer :: eff
        type(division_t), intent(in) :: d
      ```

```
      call copy_array_pointer (eff, d%efficiency, 0)
    end subroutine division_efficiency
```

5.1.8   I/O

61a   ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁60b 66c▷
```
  public :: write_division
  private :: write_division_unit, write_division_name
  public :: read_division
  private :: read_division_unit, read_division_name
  public :: write_division_raw
  private :: write_division_raw_unit, write_division_raw_name
  public :: read_division_raw
  private :: read_division_raw_unit, read_division_raw_name
```

61b   ⟨*Interfaces of* divisions *procedures* 61b⟩≡   (37a)
```
  interface write_division
     module procedure write_division_unit, write_division_name
  end interface
  interface read_division
     module procedure read_division_unit, read_division_name
  end interface
  interface write_division_raw
     module procedure write_division_raw_unit, write_division_raw_name
  end interface
  interface read_division_raw
     module procedure read_division_raw_unit, read_division_raw_name
  end interface
```

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

61c   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁59b 62b▷
```
  subroutine write_division_unit (d, unit, write_integrals)
    type(division_t), intent(in) :: d
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    logical :: write_integrals0
    integer :: i
    write_integrals0 = .false.
    if (present(write_integrals)) write_integrals0 = write_integrals
    write (unit = unit, fmt = descr_fmt) "begin type(division_t) :: d"
    write (unit = unit, fmt = integer_fmt) "ubound(d%x,1) = ", ubound (d%x, dim=1)
    write (unit = unit, fmt = integer_fmt) "d%ng = ", d%ng
    write (unit = unit, fmt = logical_fmt) "d%stratified = ", d%stratified
```

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```
            write (unit = unit, fmt = double_fmt) "d%dx = ", d%dx
            write (unit = unit, fmt = double_fmt) "d%dxg = ", d%dxg
            write (unit = unit, fmt = double_fmt) "d%x_min = ", d%x_min
            write (unit = unit, fmt = double_fmt) "d%x_max = ", d%x_max
            write (unit = unit, fmt = double_fmt) "d%x_min_true = ", d%x_min_true
            write (unit = unit, fmt = double_fmt) "d%x_max_true = ", d%x_max_true
            write (unit = unit, fmt = descr_fmt) "begin d%x"
            do i = 0, ubound (d%x, dim=1)
               if (write_integrals0 .and. i/=0) then
                  write (unit = unit, fmt = double_array_fmt) &
                       i, d%x(i), d%integral(i), d%variance(i)
               else
                  write (unit = unit, fmt = double_array_fmt) i, d%x(i)
               end if
            end do
            write (unit = unit, fmt = descr_fmt) "end d%x"
            write (unit = unit, fmt = descr_fmt) "end type(division_t)"
         end subroutine write_division_unit
```

62a ⟨*Variables in* divisions 46a⟩+≡   (37a) ◁60a
```
         character(len=*), parameter, private :: &
              descr_fmt =        "(1x,a)", &
              integer_fmt =      "(1x,a15,1x,i15)", &
              logical_fmt =      "(1x,a15,1x,l1)", &
              double_fmt =       "(1x,a15,1x,e30.22)", &
              double_array_fmt = "(1x,i15,1x,3(e30.22))"
```

62b ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁61c 63b▷
```
         subroutine read_division_unit (d, unit, read_integrals)
           type(division_t), intent(inout) :: d
           integer, intent(in) :: unit
           logical, intent(in), optional :: read_integrals
           logical :: read_integrals0
           integer :: i, idum, num_div
           character(len=80) :: chdum
           read_integrals0 = .false.
           if (present(read_integrals)) read_integrals0 = read_integrals
           read (unit = unit, fmt = descr_fmt) chdum
           read (unit = unit, fmt = integer_fmt) chdum, num_div
```
           ⟨*Insure that* ubound (d%x, dim=1) == num_div 63a⟩
```
           read (unit = unit, fmt = integer_fmt) chdum, d%ng
           read (unit = unit, fmt = logical_fmt) chdum, d%stratified
           read (unit = unit, fmt = double_fmt) chdum, d%dx
           read (unit = unit, fmt = double_fmt) chdum, d%dxg
           read (unit = unit, fmt = double_fmt) chdum, d%x_min
```

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

⚠ What happened to `d%efficiency`?

63a ⟨*Insure that* `ubound (d%x, dim=1) == num_div` 63a⟩≡   (62b 65b 67b)
```
       if (associated (d%x)) then
          if (ubound (d%x, dim=1) /= num_div) then
             deallocate (d%x, d%integral, d%variance)
       !     deallocate (d%efficiency)
             allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
       !     allocate (d%efficiency(num_div))
          end if
       else
          allocate (d%x(0:num_div), d%integral(num_div), d%variance(num_div))
       !  allocate (d%efficiency(num_div))
       end if
```

63b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁62b 64a▷
```
       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)
```

```fortran
      call write_division_unit (d, unit, write_integrals)
      close (unit = unit)
    end subroutine write_division_name
```

64a   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁63b 64b▷
```fortran
    subroutine read_division_name (d, name, read_integrals)
      type(division_t), intent(inout) :: d
      character(len=*), intent(in) :: name
      logical, intent(in), optional :: read_integrals
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "read", status = "old", file = name)
      call read_division_unit (d, unit, read_integrals)
      close (unit = unit)
    end subroutine read_division_name
```

64b   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁64a 65b▷
```fortran
    subroutine write_division_raw_unit (d, unit, write_integrals)
      type(division_t), intent(in) :: d
      integer, intent(in) :: unit
      logical, intent(in), optional :: write_integrals
      logical :: write_integrals0
      integer :: i
      write_integrals0 = .false.
      if (present(write_integrals)) write_integrals0 = write_integrals
      write (unit = unit) MAGIC_DIVISION_BEGIN
      write (unit = unit) ubound (d%x, dim=1)
      write (unit = unit) d%ng
      write (unit = unit) d%stratified
      write (unit = unit) d%dx
      write (unit = unit) d%dxg
      write (unit = unit) d%x_min
      write (unit = unit) d%x_max
      write (unit = unit) d%x_min_true
      write (unit = unit) d%x_max_true
      do i = 0, ubound (d%x, dim=1)
         if (write_integrals0 .and. i/=0) then
            write (unit = unit) d%x(i), d%integral(i), d%variance(i)
         else
            write (unit = unit) d%x(i)
         end if
      end do
      write (unit = unit) MAGIC_DIVISION_END
    end subroutine write_division_raw_unit
```

65a   ⟨*Constants in* `divisions` 65a⟩≡   (37a)

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

65b   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁64b 66a▷

```fortran
subroutine read_division_raw_unit (d, unit, read_integrals)
  type(division_t), intent(inout) :: d
  integer, intent(in) :: unit
  logical, intent(in), optional :: read_integrals
  logical :: read_integrals0
  integer :: i, num_div, magic
  character(len=*), parameter :: FN = "read_division_raw_unit"
  read_integrals0 = .false.
  if (present(read_integrals)) read_integrals0 = read_integrals
  read (unit = unit) magic
  if (magic /= MAGIC_DIVISION_BEGIN) then
     print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_BEGIN, &
                  ", found ", magic
     stop
  end if
  read (unit = unit) num_div
  ⟨Insure that ubound (d%x, dim=1) == num_div 63a⟩
  read (unit = unit) d%ng
  read (unit = unit) d%stratified
  read (unit = unit) d%dx
  read (unit = unit) d%dxg
  read (unit = unit) d%x_min
  read (unit = unit) d%x_max
  read (unit = unit) d%x_min_true
  read (unit = unit) d%x_max_true
  do i = 0, ubound (d%x, dim=1)
     if (read_integrals0 .and. i/=0) then
        read (unit = unit) d%x(i), d%integral(i), d%variance(i)
     else
        read (unit = unit) d%x(i)
     end if
  end do
  if (.not.read_integrals0) then
     d%integral = 0.0
     d%variance = 0.0
!    d%efficiency = 0.0
  end if
  read (unit = unit) magic
```

```
        if (magic /= MAGIC_DIVISION_END) then
            print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_END, &
                        ", found ", magic
            stop
        end if
    end subroutine read_division_raw_unit
```

66a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁65b 66b▷
```
    subroutine write_division_raw_name (d, name, write_integrals)
        type(division_t), intent(in) :: d
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: write_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", &
              form = "unformatted", file = name)
        call write_division_unit (d, unit, write_integrals)
        close (unit = unit)
    end subroutine write_division_raw_name
```

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

5.1.9 Marshaling

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

66c ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡   (37a) ◁61a 68a▷
```
    public :: marshal_division_size, marshal_division, unmarshal_division
```

66d ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁66b 67a▷
```
    pure subroutine marshal_division (d, ibuf, dbuf)
        type(division_t), intent(in) :: d
```

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```
      integer, dimension(:), intent(inout) :: ibuf
      real(kind=default), dimension(:), intent(inout) :: dbuf
      integer :: num_div
      num_div = ubound (d%x, dim=1)
      ibuf(1) = d%ng
      ibuf(2) = num_div
      if (d%stratified) then
         ibuf(3) = 1
      else
         ibuf(3) = 0
      end if
      dbuf(1) = d%x_min
      dbuf(2) = d%x_max
      dbuf(3) = d%x_min_true
      dbuf(4) = d%x_max_true
      dbuf(5) = d%dx
      dbuf(6) = d%dxg
      dbuf(7:7+num_div) = d%x
      dbuf(8+  num_div:7+2*num_div) = d%integral
      dbuf(8+2*num_div:7+3*num_div) = d%variance
    ! dbuf(8+3*num_div:7+4*num_div) = d%efficiency
    end subroutine marshal_division
```

67a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁66d 67b▷

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

67b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁67a 68b▷

```
    pure subroutine unmarshal_division (d, ibuf, dbuf)
      type(division_t), intent(inout) :: d
      integer, dimension(:), intent(in) :: ibuf
      real(kind=default), dimension(:), intent(in) :: dbuf
      integer :: num_div
      d%ng = ibuf(1)
      num_div = ibuf(2)
      d%stratified = ibuf(3) /= 0
      d%x_min = dbuf(1)
      d%x_max = dbuf(2)
      d%x_min_true = dbuf(3)
      d%x_max_true = dbuf(4)
```

```
      d%dx = dbuf(5)
      d%dxg = dbuf(6)
      ⟨Insure that ubound (d%x, dim=1) == num_div 63a⟩
      d%x = dbuf(7:7+num_div)
      d%integral = dbuf(8+  num_div:7+2*num_div)
      d%variance = dbuf(8+2*num_div:7+3*num_div)
    ! d%efficiency = dbuf(8+3*num_div:7+4*num_div)
    end subroutine unmarshal_division
```

68a   ⟨*Declaration of* divisions *procedures* 38a⟩+≡   (37a) ◁66c
```
    public :: marshal_div_history_size, marshal_div_history, unmarshal_div_history
```

68b   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁67b 68c▷
```
    pure subroutine marshal_div_history (h, ibuf, dbuf)
      type(div_history), intent(in) :: h
      integer, dimension(:), intent(inout) :: ibuf
      real(kind=default), dimension(:), intent(inout) :: dbuf
      ibuf(1) = h%ng
      ibuf(2) = h%num_div
      if (h%stratified) then
         ibuf(3) = 1
      else
         ibuf(3) = 0
      end if
      dbuf(1) = h%x_min
      dbuf(2) = h%x_max
      dbuf(3) = h%x_min_true
      dbuf(4) = h%x_max_true
      dbuf(5) = h%spread_f_p
      dbuf(6) = h%stddev_f_p
      dbuf(7) = h%spread_p
      dbuf(8) = h%stddev_p
      dbuf(9) = h%spread_m
      dbuf(10) = h%stddev_m
    end subroutine marshal_div_history
```

68c   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁68b 68d▷
```
    pure subroutine marshal_div_history_size (h, iwords, dwords)
      type(div_history), intent(in) :: h
      integer, intent(out) :: iwords, dwords
      iwords = 3
      dwords = 10
    end subroutine marshal_div_history_size
```

68d   ⟨*Implementation of* divisions *procedures* 38b⟩+≡   (37a) ◁68c 69▷
```
    pure subroutine unmarshal_div_history (h, ibuf, dbuf)
```

```
      type(div_history), intent(inout) :: h
      integer, dimension(:), intent(in) :: ibuf
      real(kind=default), dimension(:), intent(in) :: dbuf
      h%ng = ibuf(1)
      h%num_div = ibuf(2)
      h%stratified = ibuf(3) /= 0
      h%x_min = dbuf(1)
      h%x_max = dbuf(2)
      h%x_min_true = dbuf(3)
      h%x_max_true = dbuf(4)
      h%spread_f_p = dbuf(5)
      h%stddev_f_p = dbuf(6)
      h%spread_p = dbuf(7)
      h%stddev_p = dbuf(8)
      h%spread_m = dbuf(9)
      h%stddev_m = dbuf(10)
    end subroutine unmarshal_div_history
```

5.1.10 Boring Copying and Deleting of Objects

69 ⟨Implementation of `divisions` procedures 38b⟩+≡   (37a) ◁68d 70a▷

```
    elemental subroutine copy_division (lhs, rhs)
      type(division_t), intent(inout) :: lhs
      type(division_t), intent(in) :: rhs
      if (associated (rhs%x)) then
         call copy_array_pointer (lhs%x, rhs%x, lb = 0)
      else if (associated (lhs%x)) then
         deallocate (lhs%x)
      end if
      if (associated (rhs%integral)) then
         call copy_array_pointer (lhs%integral, rhs%integral)
      else if (associated (lhs%integral)) then
         deallocate (lhs%integral)
      end if
      if (associated (rhs%variance)) then
         call copy_array_pointer (lhs%variance, rhs%variance)
      else if (associated (lhs%variance)) then
         deallocate (lhs%variance)
      end if
    ! if (associated (rhs%efficiency)) then
    !    call copy_array_pointer (lhs%efficiency, rhs%efficiency)
    ! else if (associated (lhs%efficiency)) then
    !    deallocate (lhs%efficiency)
```

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```
    ! 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   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁69 70b▷
```
    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   ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡   (37a) ◁70a
```
    elemental subroutine copy_history (lhs, rhs)
      type(div_history), intent(out) :: lhs
      type(div_history), intent(in) :: rhs
      lhs%stratified = rhs%stratified
      lhs%ng = rhs%ng
      lhs%num_div = rhs%num_div
      lhs%x_min = rhs%x_min
      lhs%x_max = rhs%x_max
      lhs%x_min_true = rhs%x_min_true
      lhs%x_max_true = rhs%x_max_true
      lhs%spread_f_p = rhs%spread_f_p
      lhs%stddev_f_p = rhs%stddev_f_p
      lhs%spread_p = rhs%spread_p
      lhs%stddev_p = rhs%stddev_p
      lhs%spread_m = rhs%spread_m
      lhs%stddev_m = rhs%stddev_m
    end subroutine copy_history
```

5.2   The Abstract Datatype $vamp\_grid$

70c   ⟨`vamp.f90` 70c⟩≡   71a▷

```
! 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 the expose the components of `vamp_grid`.

> **NB:** with the introduction of `vamp_equivalences`, this question has (probably) become academic.

71a ⟨`vamp.f90` 70c⟩+≡   ◁70c 71b▷
```
module vamp_grid_type
  use kinds
  use divisions
  private
  ⟨Declaration of vamp_grid_type types 76b⟩
end module vamp_grid_type
```

> By WK for WHIZARD.

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

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

72a　⟨*Declaration of* `vamp_equivalences` *types* 71c⟩+≡　　　　　　　　　　(71b)　◁71c
```
type, public :: vamp_equivalences_t
   type(vamp_equivalence_t), dimension(:), allocatable :: eq
   integer :: n_eq, n_ch
   integer, dimension(:), allocatable :: pointer
   logical, dimension(:), allocatable :: independent
   integer, dimension(:), allocatable :: equivalent_to_ch
   integer, dimension(:), allocatable :: multiplicity
   integer, dimension(:), allocatable :: symmetry
   logical, dimension(:,:), allocatable :: div_is_invariant
end type vamp_equivalences_t
```

72b　⟨*Constants in* `vamp_equivalences` 72b⟩≡　　　　　　　　　　　　　　(71b)
```
integer, parameter, public :: &
     VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3
```

72c　⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩≡　　　　(71b)　72e▷
```
subroutine vamp_equivalence_init (eq, n_dim)
   type(vamp_equivalence_t), intent(inout) :: eq
   integer, intent(in) :: n_dim
   allocate (eq%permutation(n_dim), eq%mode(n_dim))
end subroutine vamp_equivalence_init
```

72d　⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩≡　　　　　　(71b)　73b▷
```
public :: vamp_equivalences_init
```

72e　⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡　　(71b)　◁72c　73a▷
```
subroutine vamp_equivalences_init (eq, n_eq, n_ch, n_dim)
   type(vamp_equivalences_t), intent(inout) :: eq
   integer, intent(in) :: n_eq, n_ch, n_dim
   integer :: i
   eq%n_eq = n_eq
   eq%n_ch = n_ch
   allocate (eq%eq(n_eq))
   allocate (eq%pointer(n_ch+1))
   do i=1, n_eq
      call vamp_equivalence_init (eq%eq(i), n_dim)
   end do
   allocate (eq%independent(n_ch), eq%equivalent_to_ch(n_ch))
   allocate (eq%multiplicity(n_ch), eq%symmetry(n_ch))
   allocate (eq%div_is_invariant(n_ch, n_dim))
   eq%independent = .true.
   eq%equivalent_to_ch = 0
   eq%multiplicity = 0
   eq%symmetry = 0
   eq%div_is_invariant = .false.
```

```
         end subroutine vamp_equivalences_init
```

73a ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩+≡   (71b) ◁72e 73c▷
```
    subroutine vamp_equivalence_final (eq)
      type(vamp_equivalence_t), intent(inout) :: eq
      deallocate (eq%permutation, eq%mode)
    end subroutine vamp_equivalence_final
```

73b ⟨*Declaration of* vamp_equivalences *procedures* 72d⟩+≡   (71b) ◁72d 73e▷
```
    public :: vamp_equivalences_final
```

73c ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩+≡   (71b) ◁73a 73d▷
```
    subroutine vamp_equivalences_final (eq)
      type(vamp_equivalences_t), intent(inout) :: eq
    ! integer :: i
    ! do i=1, eq%n_eq
    !    call vamp_equivalence_final (eq%eq(i))
    ! end do
      if (allocated (eq%eq))  deallocate (eq%eq)
      if (allocated (eq%pointer))  deallocate (eq%pointer)
      if (allocated (eq%multiplicity))  deallocate (eq%multiplicity)
      if (allocated (eq%symmetry))  deallocate (eq%symmetry)
      if (allocated (eq%independent))  deallocate (eq%independent)
      if (allocated (eq%equivalent_to_ch))  deallocate (eq%equivalent_to_ch)
      if (allocated (eq%div_is_invariant))  deallocate (eq%div_is_invariant)
      eq%n_eq = 0
      eq%n_ch = 0
    end subroutine vamp_equivalences_final
```

73d ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩+≡   (71b) ◁73c 73f▷
```
    subroutine vamp_equivalence_write (eq, unit)
      integer, intent(in), optional :: unit
      integer :: u
      type(vamp_equivalence_t), intent(in) :: eq
      u = 6;  if (present (unit))  u = unit
      write (u, "(3x,A,2(1x,I0))") "Equivalent channels:", eq%left, eq%right
      write (u, "(5x,A,99(1x,I0))") "Permutation:", eq%permutation
      write (u, "(5x,A,99(1x,I0))") "Mode:        ", eq%mode
    end subroutine vamp_equivalence_write
```

73e ⟨*Declaration of* vamp_equivalences *procedures* 72d⟩+≡   (71b) ◁73b 74a▷
```
    public :: vamp_equivalences_write
```

73f ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩+≡   (71b) ◁73d 74b▷
```
    subroutine vamp_equivalences_write (eq, unit)
      type(vamp_equivalences_t), intent(in) :: eq
      integer, intent(in), optional :: unit
```

```
        integer :: u
        integer :: ch, i
        u = 6;  if (present (unit))  u = unit
        write (u, "(1x,A)") "Inequivalent channels:"
        if (allocated (eq%independent)) then
           do ch=1, eq%n_ch
              if (eq%independent(ch)) then
                 write (u, "(3x,A,1x,I0,A,4x,A,I0,4x,A,I0,4x,A,999(L1))") &
                       "Channel", ch, ":", &
                       "Mult. = ", eq%multiplicity(ch), &
                       "Symm. = ", eq%symmetry(ch), &
                       "Invar.: ", eq%div_is_invariant(ch,:)
              end if
           end do
        else
           write (u, "(3x,A)") "[not allocated]"
        end if
        write (u, "(1x,A)") "Equivalence list:"
        if (allocated (eq%eq)) then
           do i=1, size (eq%eq)
              call vamp_equivalence_write (eq%eq(i), u)
           end do
        else
           write (u, "(3x,A)") "[not allocated]"
        end if
      end subroutine vamp_equivalences_write
```

74a   ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡   (71b) ◁73e 74c▷
```
      public :: vamp_equivalence_set
```

74b   ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡   (71b) ◁73f 75a▷
```
      subroutine vamp_equivalence_set (eq, i, left, right, perm, mode)
        type(vamp_equivalences_t), intent(inout) :: eq
        integer, intent(in) :: i
        integer, intent(in) :: left, right
        integer, dimension(:), intent(in) :: perm, mode
        eq%eq(i)%left = left
        eq%eq(i)%right = right
        eq%eq(i)%permutation = perm
        eq%eq(i)%mode = mode
      end subroutine vamp_equivalence_set
```

74c   ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡   (71b) ◁74a
```
      public :: vamp_equivalences_complete
```

⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡   (71b) ◁74b

```fortran
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
```

⟨`vamp.f90` 70c⟩+≡   ◁71b 76a▷

```fortran
module vamp_rest
  use kinds
  use utils
```

```
    use exceptions
    use divisions
    use tao_random_numbers
    use vamp_stat
    use linalg
    use iso_fortran_env
    use vamp_grid_type !NODEP!
    use vamp_equivalences !NODEP!
    implicit none
    private
    ⟨Declaration of vamp procedures 77a⟩
    ⟨Interfaces of vamp procedures 96b⟩
    ⟨Constants in vamp 153a⟩
    ⟨Declaration of vamp types 77b⟩
    ⟨Variables in vamp 79a⟩
    character(len=*), public, parameter :: VAMP_RCS_ID = &
        "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
  contains
    ⟨Implementation of vamp procedures 78b⟩
  end module vamp_rest
```

76a ⟨vamp.f90 70c⟩+≡   ◁75b
```
  module vamp
    use vamp_grid_type    !NODEP!
    use vamp_rest         !NODEP!
    use vamp_equivalences !NODEP!
    public
  end module vamp
```

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

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

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

76b ⟨Declaration of vamp_grid_type types 76b⟩≡   (71a)

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

77a ⟨*Declaration of* vamp *procedures* 77a⟩≡   (75b) 78a▷
```
public :: vamp_copy_grid, vamp_delete_grid
```

5.2.1 Container for application data

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

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

77b ⟨*Declaration of* vamp *types* 77b⟩≡   (75b) 77c▷
```
type, public :: vamp_data_t
end type vamp_data_t
```

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

77c ⟨*Declaration of* vamp *types* 77b⟩+≡   (75b) ◁77b 106c▷
```
type(vamp_data_t), parameter, public :: NO_DATA = vamp_data_t ()
```

5.2.2 Initialization

78a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁77a 79b▷
```
  public :: vamp_create_grid, vamp_create_empty_grid
```

Create a fresh grid for the integration domain

$$\mathcal{D} = [D_{1,1}, D_{2,1}] \times [D_{1,2}, D_{2,2}] \times \ldots \times [D_{1,n}, D_{2,n}] \tag{5.9}$$

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

78b ⟨*Implementation of* `vamp` *procedures* 78b⟩≡   (75b) 79c▷
```
  pure subroutine vamp_create_grid &
      (g, domain, num_calls, num_div, &
       stratified, quadrupole, covariance, map, exc)
    type(vamp_grid), intent(inout) :: g
    real(kind=default), dimension(:,:), intent(in) :: domain
    integer, intent(in) :: num_calls
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole, covariance
    real(kind=default), dimension(:,:), intent(in), optional :: map
    type(exception), intent(inout), optional :: exc
    character(len=*), parameter :: FN = "vamp_create_grid"
    real(kind=default), dimension(size(domain,dim=2)) :: &
        x_min, x_max, x_min_true, x_max_true
    integer :: ndim
    ndim = size (domain, dim=2)
    allocate (g%div(ndim), g%num_div(ndim))
    x_min = domain(1,:)
    x_max = domain(2,:)
    if (present (map)) then
       allocate (g%map(ndim,ndim))
       g%map = map
       x_min_true = x_min
       x_max_true = x_max
       call map_domain (g%map, x_min_true, x_max_true, x_min, x_max)
       call create_division (g%div, x_min, x_max, x_min_true, x_max_true)
    else
       nullify (g%map)
       call create_division (g%div, x_min, x_max)
    end if
    g%num_calls = num_calls
```

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

Below, we assume that NUM_DIV_DEFAULT ≥ 6, but we will never go that low anyway.

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

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

$$\mathcal{D} \subset M\mathcal{D}_0 \tag{5.10}$$

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

$$\mathcal{D}_0^T = \overline{\mathcal{D}^T M} \tag{5.11}$$

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

79c $\langle$*Implementation of* vamp *procedures* 78b$\rangle+\equiv$ (75b) $\triangleleft$78b 80a$\triangleright$
```
    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,:) = &
```

79

```
                 merge (true_xmin, true_xmax, btest (perm-1, zero_to_n))
          end do
          corners = matmul (corners, map)
          xmin = minval (corners, dim=1)
          xmax = maxval (corners, dim=1)
        end subroutine map_domain
```

80a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁79c 80c▷
```
        elemental subroutine vamp_create_empty_grid (g)
          type(vamp_grid), intent(inout) :: g
          nullify (g%div, g%num_div, g%map, g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
        end subroutine vamp_create_empty_grid
```

80b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁79b 81a▷
```
        public :: vamp_discard_integral
```

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

80c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁80a 81b▷
```
        pure subroutine vamp_discard_integral &
             (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
              & independent, equivalent_to_ch, multiplicity)
          type(vamp_grid), intent(inout) :: g
          integer, intent(in), optional :: num_calls
          integer, dimension(:), intent(in), optional :: num_div
          logical, intent(in), optional :: stratified, quadrupole, covariance
          type(exception), intent(inout), optional :: exc
          logical, intent(in), optional :: independent
          integer, intent(in), optional :: equivalent_to_ch, multiplicity
          character(len=*), parameter :: FN = "vamp_discard_integral"
          g%mu = 0.0
          g%mu_plus = 0.0
          g%mu_minus = 0.0
          g%mu_gi = 0.0
          g%sum_integral = 0.0
          g%sum_weights = 0.0
          g%sum_chi2 = 0.0
          g%sum_mu_gi = 0.0
          if (associated (g%sum_mu_x)) then
             g%sum_mu_x = 0.0
             g%sum_mu_xx = 0.0
          end if
          call set_grid_options (g, num_calls, num_div, stratified, quadrupole, &
                                 independent, equivalent_to_ch, multiplicity)
```

```
    if ((present (num_calls)) &
         .or. (present (num_div)) &
         .or. (present (stratified)) &
         .or. (present (quadrupole)) &
         .or. (present (covariance))) then
       call vamp_reshape_grid &
            (g, g%num_calls, g%num_div, &
             g%stratified, g%quadrupole, covariance, exc)
    end if
  end subroutine vamp_discard_integral
```

81a   ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁80b 83a▷
```
  private :: set_grid_options
```

81b   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁80c 82▷
```
  pure subroutine set_grid_options &
       (g, num_calls, num_div, stratified, quadrupole, &
        independent, equivalent_to_ch, multiplicity)
    type(vamp_grid), intent(inout) :: g
    integer, intent(in), optional :: num_calls
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole
    logical, intent(in), optional :: independent
    integer, intent(in), optional :: equivalent_to_ch, multiplicity
    if (present (num_calls)) then
       g%num_calls = num_calls
    end if
    if (present (num_div)) then
       g%num_div = num_div
    end if
    if (present (stratified)) then
       g%stratified = stratified
    end if
    if (present (quadrupole)) then
       g%quadrupole = quadrupole
    end if
    if (present (independent)) then
       g%independent = independent
    end if
    if (present (equivalent_to_ch)) then
       g%equivalent_to_ch = equivalent_to_ch
    end if
    if (present (multiplicity)) then
       g%multiplicity = multiplicity
    end if
```

```
end subroutine set_grid_options
```

Setting Up the Initial Grid

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

82 ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁81b 83b▷
```
pure subroutine vamp_reshape_grid_internal &
     (g, num_calls, num_div, &
      stratified, quadrupole, covariance, exc, use_variance, &
      independent, equivalent_to_ch, multiplicity)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole, covariance
  type(exception), intent(inout), optional :: exc
  logical, intent(in), optional :: use_variance
  logical, intent(in), optional :: independent
  integer, intent(in), optional :: equivalent_to_ch, multiplicity
  integer :: ndim, num_cells
  integer, dimension(size(g%div)) :: ng
  character(len=*), parameter :: FN = "vamp_reshape_grid_internal"
  ndim = size (g%div)
  call set_grid_options &
       (g, num_calls, num_div, stratified, quadrupole, &
      & independent, equivalent_to_ch, multiplicity)
```
  ⟨*Adjust* `grid` *and other state for new* `num_calls` 84a⟩
```
  g%all_stratified = all (stratified_division (g%div))
  if (present (covariance)) then
     ndim = size (g%div)
     if (covariance .and. (.not. associated (g%mu_x))) then
        allocate (g%mu_x(ndim), g%mu_xx(ndim,ndim))
        allocate (g%sum_mu_x(ndim), g%sum_mu_xx(ndim,ndim))
        g%sum_mu_x = 0.0
        g%sum_mu_xx = 0.0
     else if ((.not. covariance) .and. (associated (g%mu_x))) then
        deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
     end if
  end if
end subroutine vamp_reshape_grid_internal
```
The `use_variance` argument is too dangerous for careless users, because the
`variance` in the divisions will contain garbage before sampling and after

reshaping. Build a fence with another routine.

83a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁81a 84d▷
```
private :: vamp_reshape_grid_internal
public :: vamp_reshape_grid
```

83b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁82 84e▷
```
pure subroutine vamp_reshape_grid &
     (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
      independent, equivalent_to_ch, multiplicity)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole, covariance
  type(exception), intent(inout), optional :: exc
  logical, intent(in), optional :: independent
  integer, intent(in), optional :: equivalent_to_ch, multiplicity
  call vamp_reshape_grid_internal &
       (g, num_calls, num_div, stratified, quadrupole, covariance, &
        exc, use_variance = .false., &
        independent=independent, equivalent_to_ch=equivalent_to_ch, &
        multiplicity=multiplicity)
end subroutine vamp_reshape_grid
```

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

The simplest case is when the user has overwritten the default of stratified sampling with the optional argument `stratified` in the call to `vamp_create_grid`. Then sample points will be choosen 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.

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

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

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

NB:

$$\prod_j n_{g,j} = \frac{N}{2} \tag{5.14}$$

84a   ⟨*Adjust* grid *and other state for new* num_calls 84a⟩≡   (82)   84b ▷

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

$$\texttt{jacobi} = J = \frac{\text{Volume}}{N_{\text{calls}}} \tag{5.15}$$

and

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

84b   ⟨*Adjust* grid *and other state for new* num_calls 84a⟩+≡   (82)   ◁84a   84c ▷

```
g%jacobi = product (volume_division (g%div)) / g%calls
g%dv2g = (g%calls / num_cells)**2 &
      / g%calls_per_cell / g%calls_per_cell / (g%calls_per_cell - 1.0)
```

84c   ⟨*Adjust* grid *and other state for new* num_calls 84a⟩+≡   (82)   ◁84b

```
call vamp_nullify_f_limits (g)
```

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

84d   ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b)   ◁83a   85a ▷

```
public :: vamp_nullify_f_limits
```

84e   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b)   ◁83b   85b ▷

```
elemental subroutine vamp_nullify_f_limits (g)
  type(vamp_grid), intent(inout) :: g
  g%f_min = 1.0
  g%f_max = 0.0
end subroutine vamp_nullify_f_limits
```

85a   ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁84d 86b▷

```
public :: vamp_rigid_divisions
public :: vamp_get_covariance, vamp_nullify_covariance
public :: vamp_get_variance, vamp_nullify_variance
```

85b   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁84e 85c▷

```
pure function vamp_rigid_divisions (g) result (ng)
  type(vamp_grid), intent(in) :: g
  integer, dimension(size(g%div)) :: ng
  ng = rigid_division (g%div)
end function vamp_rigid_divisions
```

85c   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁85b 85d▷

```
pure function vamp_get_covariance (g) result (cov)
  type(vamp_grid), intent(in) :: g
  real(kind=default), dimension(size(g%div),size(g%div)) :: cov
  if (associated (g%mu_x)) then
     if (abs (g%sum_weights) <= tiny (cov(1,1))) then
        where (g%sum_mu_xx == 0.0_default)
           cov = 0.0
        elsewhere
           cov = huge (cov(1,1))
        endwhere
     else
        cov = g%sum_mu_xx / g%sum_weights &
              - outer_product (g%sum_mu_x, g%sum_mu_x) / g%sum_weights**2
     end if
  else
     cov = 0.0
  end if
end function vamp_get_covariance
```

85d   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁85c 85e▷

```
elemental subroutine vamp_nullify_covariance (g)
  type(vamp_grid), intent(inout) :: g
  if (associated (g%mu_x)) then
     g%sum_mu_x = 0
     g%sum_mu_xx = 0
  end if
end subroutine vamp_nullify_covariance
```

85e   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁85d 86a▷

```
elemental function vamp_get_variance (g) result (v)
  type(vamp_grid), intent(in) :: g
  real(kind=default) :: v
  if (abs (g%sum_weights) <= tiny (v)) then
```

```
    if (g%sum_mu_gi == 0.0_default) then
        v = 0.0
    else
        v = huge (v)
    end if
else
    v = g%sum_mu_gi / g%sum_weights
end if
end function vamp_get_variance
```

86a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁85e 86c▷
```
elemental subroutine vamp_nullify_variance (g)
  type(vamp_grid), intent(inout) :: g
  g%sum_mu_gi = 0
end subroutine vamp_nullify_variance
```

5.2.3   Sampling

86b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁85a 92b▷
```
public :: vamp_sample_grid
public :: vamp_sample_grid0
public :: vamp_refine_grid
public :: vamp_refine_grids
```

Simple Non-Adaptive Sampling: S_0

86c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁86a 92c▷
```
subroutine vamp_sample_grid0 &
     (rng, g, func, data, channel, weights, grids, exc, &
      negative_weights)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  class(vamp_data_t), intent(in) :: data
  integer, intent(in), optional :: channel
  real(kind=default), dimension(:), intent(in), optional :: weights
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  type(exception), intent(inout), optional :: exc
```
  ⟨*Interface declaration for* `func` 22⟩
```
  character(len=*), parameter :: FN = "vamp_sample_grid0"
  logical, intent(in), optional :: negative_weights
```
  ⟨*Local variables in* `vamp_sample_grid0` 87c⟩
```
  integer :: ndim
  logical :: neg_w
```

```
        ndim = size (g%div)
        neg_w = .false.
        if (present (negative_weights)) neg_w = negative_weights
        ⟨Check optional arguments in vamp_sample_grid0 92a⟩
        ⟨Reset counters in vamp_sample_grid0 87b⟩
        loop_over_cells: do
            ⟨Sample calls_per_cell points in the current cell 88b⟩
            ⟨Collect integration and grid optimization data for current cell 90a⟩
            ⟨Count up cell, exit if done 87a⟩
        end do loop_over_cells
        ⟨Collect results of vamp_sample_grid0 90b⟩
    end subroutine vamp_sample_grid0
```

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

87a   ⟨Count up cell, exit if done 87a⟩≡   (86c)
```
      do j = ndim, 1, -1
          cell(j) = modulo (cell(j), rigid_division (g%div(j))) + 1
          if (cell(j) /= 1) then
              cycle loop_over_cells
          end if
      end do
      exit loop_over_cells
```

87b   ⟨Reset counters in vamp_sample_grid0 87b⟩≡   (86c)
```
      g%mu = 0.0
      g%mu_plus = 0.0
      g%mu_minus = 0.0
      cell = 1
      call clear_integral_and_variance (g%div)
      if (associated (g%mu_x)) then
          g%mu_x = 0.0
          g%mu_xx = 0.0
      end if
      if (present (channel)) then
          g%mu_gi = 0.0
      end if
```

87c   ⟨Local variables in vamp_sample_grid0 87c⟩≡   (86c) 88a ▷
```
      real(kind=default), parameter :: &
          eps =  tiny (1._default) / epsilon (1._default)
      character(len=6) :: buffer
```

88a ⟨*Local variables in* `vamp_sample_grid0` 87c⟩+≡   (86c) ◁87c 89c▷
```
integer :: j, k
integer, dimension(size(g%div)) :: cell
```

88b ⟨*Sample* `calls_per_cell` *points in the current* `cell` 88b⟩≡   (86c)
```
sum_f = 0.0
sum_f_plus = 0.0
sum_f_minus = 0.0
sum_f2 = 0.0
sum_f2_plus = 0.0
sum_f2_minus = 0.0
do k = 1, g%calls_per_cell
   ⟨Get x in the current cell 88c⟩
   ⟨f = wgt * func (x, weights, channel), iff x inside true_domain 88d⟩
   ⟨Collect integration and grid optimization data for x from f 89a⟩
end do
```

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

88c ⟨*Get* `x` *in the current* `cell` 88c⟩≡   (88b)
```
call tao_random_number (rng, r)
call inject_division (g%div, real (r, kind=default), &
                      cell, x, x_mid, ia, wgts)
wgt = g%jacobi * product (wgts)
if (associated (g%map)) then
   x = matmul (g%map, x)
end if
```

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

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

88d ⟨`f = wgt * func (x, weights, channel)`, *iff* `x` *inside* `true_domain` 88d⟩≡   (88b 136a)
```
if (associated (g%map)) then
```

```
            if (all (inside_division (g%div, x))) then
               f = wgt * func (x, data, weights, channel, grids)
            else
               f = 0.0
            end if
         else
            f = wgt * func (x, data, weights, channel, grids)
         end if
```

89a ⟨*Collect integration and grid optimization data for* x *from* f 89a⟩≡   (88b) 89b ▷
```
         if (g%f_min > g%f_max) then
            g%f_min = abs (f) * g%calls
            g%f_max = abs (f) * g%calls
         else if (abs (f) * g%calls < g%f_min) then
            g%f_min = abs (f) * g%calls
         else if (abs (f) * g%calls > g%f_max) then
            g%f_max = abs (f) * g%calls
         end if
```

89b ⟨*Collect integration and grid optimization data for* x *from* f 89a⟩+≡   (88b) ◁89a
```
         f2 = f * f
         sum_f = sum_f + f
         sum_f2 = sum_f2 + f2
         if (f > 0) then
            sum_f_plus = sum_f_plus + f
            sum_f2_plus = sum_f2_plus + f * f
         else if (f < 0) then
            sum_f_minus = sum_f_minus + f
            sum_f2_minus = sum_f2_minus + f * f
         end if
         call record_integral (g%div, ia, f)
         ! call record_efficiency (g%div, ia, f/g%f_max)
         if ((associated (g%mu_x)) .and. (.not. g%all_stratified)) then
            g%mu_x = g%mu_x + x * f
            g%mu_xx = g%mu_xx + outer_product (x, x) * f
         end if
         if (present (channel)) then
            g%mu_gi = g%mu_gi + f2
         end if
```

89c ⟨*Local variables in* vamp_sample_grid0 87c⟩+≡   (86c) ◁88a
```
         real(kind=default) :: wgt, f, f2
         real(kind=default) :: sum_f, sum_f2, var_f
         real(kind=default) :: sum_f_plus, sum_f2_plus, var_f_plus
         real(kind=default) :: sum_f_minus, sum_f2_minus, var_f_minus
```

```fortran
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
```

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

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

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

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

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

90b   〈*Collect results of* `vamp_sample_grid0` 90b〉≡   (86c) 91 ▷

```fortran
g%mu(2) = g%mu(2) * g%dv2g
if (g%mu(2) < eps * max (g%mu(1)**2, 1._default)) then
   g%mu(2) = eps * max (g%mu(1)**2, 1._default)
end if
```

```
       if (neg_w) then
          g%mu_plus(2) = g%mu_plus(2) * g%dv2g
          if (g%mu_plus(2) < eps * max (g%mu_plus(1)**2, 1._default)) then
             g%mu_plus(2) = eps * max (g%mu_plus(1)**2, 1._default)
          end if
          g%mu_minus(2) = g%mu_minus(2) * g%dv2g
          if (g%mu_minus(2) < eps * max (g%mu_minus(1)**2, 1._default)) then
             g%mu_minus(2) = eps * max (g%mu_minus(1)**2, 1._default)
          end if
       end if
```

91 ⟨*Collect results of* `vamp_sample_grid0` 90b⟩+≡   (86c) ◁90b

```
    if (g%mu(1)>0) then
       g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
       g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
       g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
       if (associated (g%mu_x)) then
          if (g%all_stratified) then
             g%mu_x = g%mu_x / g%mu(2)
             g%mu_xx = g%mu_xx / g%mu(2)
          else
             g%mu_x = g%mu_x / g%mu(1)
             g%mu_xx = g%mu_xx / g%mu(1)
          end if
          g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
          g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
       end if
       if (present (channel)) then
          g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
       end if
    else if (neg_w) then
       g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
       g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
       g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
       if (associated (g%mu_x)) then
          if (g%all_stratified) then
             g%mu_x = g%mu_x / g%mu(2)
             g%mu_xx = g%mu_xx / g%mu(2)
          else
             g%mu_x = g%mu_x / g%mu(1)
             g%mu_xx = g%mu_xx / g%mu(1)
          end if
          g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
          g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
```

```
        end if
        if (present (channel)) then
            g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
        end if
        else
        if (present(channel) .and. g%mu(1)==0) then
            write (buffer, "(I6)")  channel
            call raise_exception (exc, EXC_WARN, "! vamp", &
                "Function identically zero in channel " // buffer)
        else if (present(channel) .and. g%mu(1)<0) then
            write (buffer, "(I6)")  channel
            call raise_exception (exc, EXC_ERROR, "! vamp", &
                "Negative integral in channel " // buffer)
        end if
        g%sum_integral = 0
        g%sum_chi2 = 0
        g%sum_weights = 0
    end if
```

92a ⟨*Check optional arguments in* `vamp_sample_grid0` 92a⟩≡   (86c)
```
    if (present (channel) .neqv. present (weights)) then
        call raise_exception (exc, EXC_FATAL, FN, &
            "channel and weights required together")
        return
    end if
```

92b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁86b 96a▷
```
    public :: vamp_probability
```

92c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁86c 92d▷
```
    pure function vamp_probability (g, x) result (p)
      type(vamp_grid), intent(in) :: g
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default) :: p
      p = product (probability (g%div, x))
    end function vamp_probability
```

⚠ `%variance` should be private to `division`

92d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁92c 94a▷
```
    subroutine vamp_apply_equivalences (g, eq)
      type(vamp_grids), intent(inout) :: g
      type(vamp_equivalences_t), intent(in) :: eq
      integer :: n_ch, n_dim, nb, i, ch, ch_src, dim, dim_src
      integer, dimension(:,:), allocatable :: n_bin
      real(kind=default), dimension(:,:,:), allocatable :: var_tmp
```

92

```fortran
      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

$$n_{\mathrm{div},j} \to \frac{Q_j n_{\mathrm{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\mathrm{dim}}}} \tag{5.19}$$

where

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

94a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁92d 94b▷
```
pure subroutine vamp_refine_grid (g, exc)
  type(vamp_grid), intent(inout) :: g
  type(exception), intent(inout), optional :: exc
  real(kind=default), dimension(size(g%div)) :: quad
  integer :: ndim
  if (g%quadrupole) then
     ndim = size (g%div)
     quad = (quadrupole_division (g%div))**QUAD_POWER
     call vamp_reshape_grid_internal &
          (g, use_variance = .true., exc = exc, &
           num_div = int (quad / product (quad)**(1.0/ndim) * g%num_div))
  else
     call refine_division (g%div)
     call vamp_nullify_f_limits (g)
  end if
end subroutine vamp_refine_grid
```

94b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁94a 94d▷
```
subroutine vamp_refine_grids (g)
  type(vamp_grids), intent(inout) :: g
  integer :: ch
  do ch=1, size(g%grids)
     call refine_division (g%grids(ch)%div)
     call vamp_nullify_f_limits (g%grids(ch))
  end do
end subroutine vamp_refine_grids
```

94c ⟨*Variables in* `vamp` 79a⟩+≡   (75b) ◁79a 110a▷
```
real(kind=default), private, parameter :: QUAD_POWER = 0.5_default
```

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

94d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁94b 95▷
```
subroutine vamp_sample_grid &
     (rng, g, func, data, iterations, &
```

```
          integral, std_dev, avg_chi2, accuracy, &
          channel, weights, grids, exc, history)
     type(tao_random_state), intent(inout) :: rng
     type(vamp_grid), intent(inout) :: g
     class(vamp_data_t), intent(in) :: data
     integer, intent(in) :: iterations
     real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
     real(kind=default), intent(in), optional :: accuracy
     integer, intent(in), optional :: channel
     real(kind=default), dimension(:), intent(in), optional :: weights
     type(vamp_grid), dimension(:), intent(in), optional :: grids
     type(exception), intent(inout), optional :: exc
     type(vamp_history), dimension(:), intent(inout), optional :: history
     ⟨Interface declaration for func 22⟩
     character(len=*), parameter :: FN = "vamp_sample_grid"
     real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
     integer :: iteration, ndim
     ndim = size (g%div)
     iterate: do iteration = 1, iterations
        call vamp_sample_grid0 &
             (rng, g, func, data, channel, weights, grids, exc)
        call vamp_average_iterations &
             (g, iteration, local_integral, local_std_dev, local_avg_chi2)
        ⟨Trace results of vamp_sample_grid 107a⟩
        ⟨Exit iterate if accuracy has been reached 97a⟩
        if (iteration < iterations) call vamp_refine_grid (g)
     end do iterate
     ⟨Copy results of vamp_sample_grid to dummy variables 96c⟩
   end subroutine vamp_sample_grid
```

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

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

$$\frac{1}{\sigma_I^2} = \sum_i \frac{1}{\sigma_i^2} \tag{5.21b}$$

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

95 ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁94d 97d▷
```
     elemental subroutine vamp_average_iterations_grid &
          (g, iteration, integral, std_dev, avg_chi2)
```

```
      type(vamp_grid), intent(in) :: g
      integer, intent(in) :: iteration
      real(kind=default), intent(out) :: integral, std_dev, avg_chi2
      real(kind=default), parameter :: eps = 1000 * epsilon (1._default)
      if (g%sum_weights>0) then
         integral = g%sum_integral / g%sum_weights
         std_dev = sqrt (1.0 / g%sum_weights)
         avg_chi2 = &
              max ((g%sum_chi2 - g%sum_integral * integral) / (iteration-0.99), &
                   0.0_default)
         if (avg_chi2 < eps * g%sum_chi2)  avg_chi2 = 0
      else
         integral = 0
         std_dev = 0
         avg_chi2 = 0
      end if
   end subroutine vamp_average_iterations_grid
```

96a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁92b 97b▷

```
   public :: vamp_average_iterations
   private :: vamp_average_iterations_grid
```

96b ⟨*Interfaces of* `vamp` *procedures* 96b⟩≡   (75b) 97c▷

```
   interface vamp_average_iterations
      module procedure vamp_average_iterations_grid
   end interface
```

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

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

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

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

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

96c ⟨*Copy results of* `vamp_sample_grid` *to dummy variables* 96c⟩≡   (94d 104 120b)

```
   if (present (integral)) then
      integral = local_integral
   end if
   if (present (std_dev)) then
```

```
          std_dev = local_std_dev
      end if
      if (present (avg_chi2)) then
          avg_chi2 = local_avg_chi2
      end if
```

97a ⟨*Exit* `iterate` *if* `accuracy` *has been reached* 97a⟩≡   (94d 104 120b)
```
      if (present (accuracy)) then
          if (local_std_dev <= accuracy * local_integral) then
              call raise_exception (exc, EXC_INFO, FN, &
                  "requested accuracy reached")
              exit iterate
          end if
      end if
```


5.2.4   Forking and Joining

97b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁96a 102b▷
```
      public :: vamp_fork_grid
      private :: vamp_fork_grid_single, vamp_fork_grid_multi
      public :: vamp_join_grid
      private :: vamp_join_grid_single, vamp_join_grid_multi
```

97c ⟨*Interfaces of* `vamp` *procedures* 96b⟩+≡   (75b) ◁96b 107c▷
```
      interface vamp_fork_grid
         module procedure vamp_fork_grid_single, vamp_fork_grid_multi
      end interface
      interface vamp_join_grid
         module procedure vamp_join_grid_single, vamp_join_grid_multi
      end interface
```

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

97d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁95 100c▷
```
      pure subroutine vamp_fork_grid_single (g, gs, d, exc)
        type(vamp_grid), intent(in) :: g
        type(vamp_grid), dimension(:), intent(inout) :: gs
        integer, intent(in) :: d
        type(exception), intent(inout), optional :: exc
        character(len=*), parameter :: FN = "vamp_fork_grid_single"
        type(division_t), dimension(:), allocatable :: d_tmp
        integer :: i, j, num_grids, num_div, ndim, num_cells
        num_grids = size (gs)
```

97

```
         ndim = size (g%div)
         ⟨Allocate or resize the divisions 100b⟩
         do j = 1, ndim
            if (j == d) then
               ⟨call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 99c⟩
            else
               ⟨call copy_division (gs%div(j), g%div(j)) 100a⟩
            end if
         end do
         if (d == 0) then
            ⟨Handle g%calls_per_cell for d == 0 98a⟩
         end if
         ⟨Copy the rest of g to the gs 98b⟩
      end subroutine vamp_fork_grid_single
```

Divide the sampling points among identical grids

98a ⟨Handle g%calls_per_cell for d == 0 98a⟩≡   (97d)
```
      if (any (stratified_division (g%div))) then
         call raise_exception (exc, EXC_FATAL, FN, &
                              "d == 0 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
```

98b ⟨Copy the rest of g to the gs 98b⟩≡   (97d) 98c ▷
```
      do i = 1, num_grids
         call copy_array_pointer (gs(i)%num_div, g%num_div)
         if (associated (g%map)) then
            call copy_array_pointer (gs(i)%map, g%map)
         end if
         if (associated (g%mu_x)) then
            call create_array_pointer (gs(i)%mu_x, ndim)
            call create_array_pointer (gs(i)%sum_mu_x, ndim)
            call create_array_pointer (gs(i)%mu_xx, (/ ndim, ndim /))
            call create_array_pointer (gs(i)%sum_mu_xx, (/ ndim, ndim /))
         end if
      end do
```

Reset results

98c ⟨Copy the rest of g to the gs 98b⟩+≡   (97d) ◁98b 99a ▷
```
      gs%mu(1) = 0.0
      gs%mu(2) = 0.0
      gs%mu_plus(1) = 0.0
      gs%mu_plus(2) = 0.0
```

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

99a ⟨*Copy the rest of* g *to the* gs 98b⟩+≡   (97d) ◁98c 99b▷
```
    gs%stratified = g%stratified
    gs%all_stratified = g%all_stratified
    gs%quadrupole = g%quadrupole
```

99b ⟨*Copy the rest of* g *to the* gs 98b⟩+≡   (97d) ◁99a
```
    do i = 1, num_grids
       num_cells = product (rigid_division (gs(i)%div))
       gs(i)%calls = gs(i)%calls_per_cell * num_cells
       gs(i)%num_calls = gs(i)%calls
       gs(i)%jacobi = product (volume_division (gs(i)%div)) / gs(i)%calls
       gs(i)%dv2g = (gs(i)%calls / num_cells)**2 &
            / gs(i)%calls_per_cell / gs(i)%calls_per_cell / (gs(i)%calls_per_cell - 1.0)
    end do
    gs%f_min = g%f_min * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)
    gs%f_max = g%f_max * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)
```

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

99c ⟨call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 99c⟩≡   (97d)
```
    allocate (d_tmp(num_grids))
    do i = 1, num_grids
       d_tmp(i) = gs(i)%div(j)
    end do
    call fork_division (g%div(j), d_tmp, g%calls_per_cell, gs%calls_per_cell, exc)
    do i = 1, num_grids
       gs(i)%div(j) = d_tmp(i)
    end do
    deallocate (d_tmp)
```
    ⟨*Bail out if exception* exc *raised* 99d⟩

99d ⟨*Bail out if exception* exc *raised* 99d⟩≡   (99c 100d 104 140c 142c)
```
    if (present (exc)) then
       if (exc%level > EXC_WARN) then
          return
       end if
    end if
```

We have to do a deep copy (`gs(i)%div(j) = g%div(j)` does not suffice), because `copy_division` handles the memory management.

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

100b ⟨*Allocate or resize the divisions* 100b⟩≡   (97d)
```
num_div = size (g%div)
do i = 1, size (gs)
   if (associated (gs(i)%div)) then
      if (size (gs(i)%div) /= num_div) then
         allocate (gs(i)%div(num_div))
         call create_empty_division (gs(i)%div)
      end if
   else
      allocate (gs(i)%div(num_div))
      call create_empty_division (gs(i)%div)
   end if
end do
```

100c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁97d 102a▷
```
pure subroutine vamp_join_grid_single (g, gs, d, exc)
  type(vamp_grid), intent(inout) :: g
  type(vamp_grid), dimension(:), intent(inout) :: gs
  integer, intent(in) :: d
  type(exception), intent(inout), optional :: exc
  type(division_t), dimension(:), allocatable :: d_tmp
  integer :: i, j, num_grids
  num_grids = size (gs)
  do j = 1, size (g%div)
     if (j == d) then
        ⟨call join_division (g%div(j), gs%div(j)) 100d⟩
     else
        ⟨call sum_division (g%div(j), gs%div(j)) 101a⟩
     end if
  end do
  ⟨Combine the rest of gs onto g 101b⟩
end subroutine vamp_join_grid_single
```

100d ⟨call join_division (g%div(j), gs%div(j)) 100d⟩≡   (100c)
```
allocate (d_tmp(num_grids))
do i = 1, num_grids
   d_tmp(i) = gs(i)%div(j)
end do
```

```
      call join_division (g%div(j), d_tmp, exc)
      deallocate (d_tmp)
      ⟨Bail out if exception exc raised 99d⟩
```

101a ⟨call sum_division (g%div(j), gs%div(j)) 101a⟩≡   (100c)
```
      allocate (d_tmp(num_grids))
      do i = 1, num_grids
         d_tmp(i) = gs(i)%div(j)
      end do
      call sum_division (g%div(j), d_tmp)
      deallocate (d_tmp)
```

101b ⟨Combine the rest of gs onto g 101b⟩≡   (100c)
```
      g%f_min = minval (gs%f_min * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
      g%f_max = maxval (gs%f_max * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
      g%mu(1) = sum (gs%mu(1))
      g%mu(2) = sum (gs%mu(2))
      g%mu_plus(1) = sum (gs%mu_plus(1))
      g%mu_plus(2) = sum (gs%mu_plus(2))
      g%mu_minus(1) = sum (gs%mu_minus(1))
      g%mu_minus(2) = sum (gs%mu_minus(2))
      g%mu_gi = sum (gs%mu_gi)
      g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
      g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
      g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
      g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
      if (associated (g%mu_x)) then
         do i = 1, num_grids
            g%mu_x = g%mu_x + gs(i)%mu_x
            g%mu_xx = g%mu_xx + gs(i)%mu_xx
         end do
         g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
         g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
      end if
```

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

101c ⟨Idioms 101c⟩≡   250 ▷
```
      type(vamp_grid), dimension(:), allocatable :: gx
```

---

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

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

102a ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁100c 102c▷

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

102b ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁97b 103b▷

```
  public :: vamp_fork_grid_joints
```

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

102c ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁102a 103a▷

102

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

103a ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁102c 104▷
```
      pure recursive subroutine vamp_join_grid_multi (g, gs, gx, d, exc)
        type(vamp_grid), intent(inout) :: g
        type(vamp_grid), dimension(:), intent(inout) :: gs, gx
        integer, dimension(:,:), intent(in) :: d
        type(exception), intent(inout), optional :: exc
        character(len=*), parameter :: FN = "vamp_join_grid_multi"
        integer :: i, offset, stride, joints_offset, joints_stride
        select case (size (d, dim=2))
          case (0)
            return
          case (1)
            call vamp_join_grid_single (g, gs, d(1,1), exc)
          case default
            offset = 1
            stride = product (d(2,2:))
            joints_offset = 1 + d(2,1)
            joints_stride = vamp_fork_grid_joints (d(:,2:))
            do i = 1, d(2,1)
              call vamp_join_grid_multi &
                   (gx(i), gs(offset:offset+stride-1), &
                    gx(joints_offset:joints_offset+joints_stride-1), &
                    d(:,2:), exc)
              offset = offset + stride
              joints_offset = joints_offset + joints_stride
            end do
            call vamp_join_grid_single (g, gx(1:d(2,1)), d(1,1), exc)
            call vamp_delete_grid (gx(1:d(2,1)))
        end select
      end subroutine vamp_join_grid_multi
```

5.2.5   Parallel Execution

103b ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁102b 107b▷

```
      public :: vamp_sample_grid_parallel
      public :: vamp_distribute_work
```

HPF [10, 11, 15]:

104   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b)   ◁103a 105b▷

```
    subroutine vamp_sample_grid_parallel &
         (rng, g, func, data, iterations, &
          integral, std_dev, avg_chi2, accuracy, &
          channel, weights, grids, exc, history)
      type(tao_random_state), dimension(:), intent(inout) :: rng
      type(vamp_grid), intent(inout) :: g
      class(vamp_data_t), intent(in) :: data
      integer, intent(in) :: iterations
      real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
      real(kind=default), intent(in), optional :: accuracy
      integer, intent(in), optional :: channel
      real(kind=default), dimension(:), intent(in), optional :: weights
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      type(exception), intent(inout), optional :: exc
      type(vamp_history), dimension(:), intent(inout), optional :: history
```

⟨*Interface declaration for* `func` 22⟩

```
      character(len=*), parameter :: FN = "vamp_sample_grid_parallel"
      real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
      type(exception), dimension(size(rng)) :: excs
      type(vamp_grid), dimension(:), allocatable :: gs, gx
      !hpf$ processors p(number_of_processors())
      !hpf$ distribute gs(cyclic(1)) onto p
      integer, dimension(:,:), pointer :: d
      integer :: iteration, i
      integer :: num_workers
      nullify (d)
      call clear_exception (excs)
      iterate: do iteration = 1, iterations
         call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
         num_workers = max (1, product (d(2,:)))
         if (num_workers > 1) then
            allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
            call vamp_create_empty_grid (gs)
            ! vamp_fork_grid is certainly not local. Speed freaks might
            ! want to tune it to the processor topology, but the gain will be small.
            call vamp_fork_grid (g, gs, gx, d, exc)
            !hpf$ independent
            do i = 1, num_workers
               call vamp_sample_grid0 &
```

104

```
                        (rng(i), gs(i), func, data, &
                         channel, weights, grids, exc)
                  end do
                  ⟨Gather exceptions in vamp_sample_grid_parallel 105a⟩
                  call vamp_join_grid (g, gs, gx, d, exc)
                  call vamp_delete_grid (gs)
                  deallocate (gs, gx)
               else
                  call vamp_sample_grid0 &
                       (rng(1), g, func, data, channel, weights, grids, exc)
               end if
               ⟨Bail out if exception exc raised 99d⟩
               call vamp_average_iterations &
                    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
               ⟨Trace results of vamp_sample_grid 107a⟩
               ⟨Exit iterate if accuracy has been reached 97a⟩
               if (iteration < iterations) call vamp_refine_grid (g)
            end do iterate
            deallocate (d)
            ⟨Copy results of vamp_sample_grid to dummy variables 96c⟩
         end subroutine vamp_sample_grid_parallel
```

105a   ⟨*Gather exceptions in* vamp_sample_grid_parallel 105a⟩≡   (104)
```
         if ((present (exc)) .and. (any (excs(1:num_workers)%level > 0))) then
            call gather_exceptions (exc, excs(1:num_workers))
         end if
```

We could sort d such that (5.23) is minimized

$$d_1 \leq d_2 \leq \ldots \leq d_N \tag{5.24}$$

but the gain will be negligible.

105b   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁104 107d▷
```
         pure subroutine vamp_distribute_work (num_workers, ng, d)
            integer, intent(in) :: num_workers
            integer, dimension(:), intent(in) :: ng
            integer, dimension(:,:), pointer :: d
            integer, dimension(32) :: factors
            integer :: n, num_factors, i, j
            integer, dimension(size(ng)) :: num_forks
            integer :: nfork
            try: do n = num_workers, 1, -1
               call factorize (n, factors, num_factors)
               num_forks = 1
               do i = num_factors, 1, -1
```

```
                 j = sum (maxloc (ng / num_forks))
                 nfork = num_forks(j) * factors(i)
                 if (nfork <= ng(j)) then
                     num_forks(j) = nfork
                 else
                     cycle try
                 end if
             end do
             ⟨Accept distribution among n workers 106a⟩
         end do try
     end subroutine vamp_distribute_work
```

106a   ⟨*Accept distribution among* n *workers* 106a⟩≡   (105b) 106b▷
```
     j = count (num_forks > 1)
     if (associated (d)) then
       if (size (d, dim = 2) /= j) then
          deallocate (d)
          allocate (d(2,j))
       end if
     else
        allocate (d(2,j))
     end if
```

106b   ⟨*Accept distribution among* n *workers* 106a⟩+≡   (105b) ◁106a
```
     j = 1
     do i = 1, size (ng)
       if (num_forks(i) > 1) then
          d(:,j) = (/ i, num_forks(i) /)
          j = j + 1
       end if
     end do
     return
```

5.2.6 Diagnostics

106c   ⟨*Declaration of* vamp *types* 77b⟩+≡   (75b) ◁77c 113a▷
```
     type, public :: vamp_history
        private
        real(kind=default) :: &
             integral, std_dev, avg_integral, avg_std_dev, avg_chi2, f_min, f_max
        integer :: calls
        logical :: stratified
        logical :: verbose
        type(div_history), dimension(:), pointer :: div => null ()
```

```
          end type vamp_history
```

107a   ⟨*Trace results of* vamp_sample_grid 107a⟩≡   (94d 104)
```
       if (present (history)) then
          if (iteration <= size (history)) then
             call vamp_get_history &
                   (history(iteration), g, local_integral, local_std_dev, &
                    local_avg_chi2)
          else
             call raise_exception (exc, EXC_WARN, FN, "history too short")
          end if
          call vamp_terminate_history (history(iteration+1:))
       end if
```

107b   ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁103b 108c▷
```
       public :: vamp_create_history, vamp_copy_history, vamp_delete_history
       public :: vamp_terminate_history
       public :: vamp_get_history, vamp_get_history_single
```

107c   ⟨*Interfaces of* vamp *procedures* 96b⟩+≡   (75b) ◁97c 108d▷
```
       interface vamp_get_history
          module procedure vamp_get_history_single
       end interface
```

107d   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁105b 107e▷
```
       elemental subroutine vamp_create_history (h, ndim, verbose)
         type(vamp_history), intent(out) :: h
         integer, intent(in), optional :: ndim
         logical, intent(in), optional :: verbose
         if (present (verbose)) then
            h%verbose = verbose
         else
            h%verbose = .false.
         end if
         h%calls = 0.0
         if (h%verbose .and. (present (ndim))) then
            if (associated (h%div)) then
               deallocate (h%div)
            end if
            allocate (h%div(ndim))
         end if
       end subroutine vamp_create_history
```

107e   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁107d 108a▷
```
       elemental subroutine vamp_terminate_history (h)
         type(vamp_history), intent(inout) :: h
```

```
      h%calls = 0.0
    end subroutine vamp_terminate_history
```

108a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁107e 109▷
```
  pure subroutine vamp_get_history_single (h, g, integral, std_dev, avg_chi2)
    type(vamp_history), intent(inout) :: h
    type(vamp_grid), intent(in) :: g
    real(kind=default), intent(in) :: integral, std_dev, avg_chi2
    h%calls = g%calls
    h%stratified = g%all_stratified
    h%integral = g%mu(1)
    h%std_dev = sqrt (g%mu(2))
    h%avg_integral = integral
    h%avg_std_dev = std_dev
    h%avg_chi2 = avg_chi2
    h%f_min = g%f_min
    h%f_max = g%f_max
    if (h%verbose) then
      ⟨Adjust h%div iff necessary 108b⟩
      call copy_history (h%div, summarize_division (g%div))
    end if
  end subroutine vamp_get_history_single
```

108b ⟨*Adjust* `h%div` *iff necessary* 108b⟩≡   (108a)
```
  if (associated (h%div)) then
    if (size (h%div) /= size (g%div)) then
      deallocate (h%div)
      allocate (h%div(size(g%div)))
    end if
  else
    allocate (h%div(size(g%div)))
  end if
```

108c ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁107b 113b▷
```
  public :: vamp_print_history, vamp_write_history
  private :: vamp_print_one_history, vamp_print_histories
  ! private :: vamp_write_one_history, vamp_write_histories
```

108d ⟨*Interfaces of* `vamp` *procedures* 96b⟩+≡   (75b) ◁107c 124d▷
```
  interface vamp_print_history
    module procedure vamp_print_one_history, vamp_print_histories
  end interface
  interface vamp_write_history
    module procedure vamp_write_one_history_unit, vamp_write_histories_unit
  end interface
```

```
subroutine vamp_print_one_history (h, tag)
  type(vamp_history), dimension(:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  type(div_history), dimension(:), allocatable :: h_tmp
  character(len=BUFFER_SIZE) :: pfx
  character(len=1) :: s
  integer :: i, imax, j
  if (present (tag)) then
     pfx = tag
  else
     pfx = "[vamp]"
  end if
  print "(1X,A78)", repeat ("-", 78)
  print "(1X,A8,1X,A2,A9,A1,1X,A11,1X,8X,1X," &
                        // "1X,A13,1X,8X,1X,A5,1X,A5)", &
       pfx, "it", "#calls", "", "integral", "average", "chi2", "eff."
  imax = size (h)
  iterations: do i = 1, imax
     if (h(i)%calls <= 0) then
        imax = i - 1
        exit iterations
     end if
     ! *JR: Skip zero channel
     if (h(i)%f_max==0) cycle
     if (h(i)%stratified) then
        s = "*"
     else
        s = ""
     end if
     print "(1X,A8,1X,I2,I9,A1,1X,E11.4,A1,E8.2,A1," &
                        // "1X,E13.6,A1,E8.2,A1,F5.1,1X,F5.3)", pfx, &
          i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
          h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &
          h(i)%integral / h(i)%f_max
  end do iterations
  print "(1X,A78)", repeat ("-", 78)
  if (all (h%verbose) .and. (imax >= 1)) then
     if (associated (h(1)%div)) then
        allocate (h_tmp(imax))
        dimensions: do j = 1, size (h(1)%div)
           do i = 1, imax
              call copy_history (h_tmp(i), h(i)%div(j))
```

```
                    end do
                    if (present (tag)) then
                       write (unit = pfx, fmt = "(A,A1,I2.2)") &
                            trim (tag(1:min(len_trim(tag),8))), "#", j
                    else
                       write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
                    end if
                    call print_history (h_tmp, tag = pfx)
                    print "(1X,A78)", repeat ("-", 78)
                 end do dimensions
                 deallocate (h_tmp)
              end if
           end if
           flush (output_unit)
        end subroutine vamp_print_one_history
```

110a ⟨*Variables in* `vamp` 79a⟩+≡   (75b) ◁94c 146a▷
```
        integer, private, parameter :: BUFFER_SIZE = 50
```

110b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁109 110c▷
```
        subroutine vamp_print_histories (h, tag)
          type(vamp_history), dimension(:,:), intent(in) :: h
          character(len=*), intent(in), optional :: tag
          character(len=BUFFER_SIZE) :: pfx
          integer :: i
          print "(1X,A78)", repeat ("=", 78)
          channels: do i = 1, size (h, dim=2)
             if (present (tag)) then
                write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
             else
                write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
             end if
             call vamp_print_one_history (h(:,i), pfx)
          end do channels
          print "(1X,A78)", repeat ("=", 78)
          flush (output_unit)
        end subroutine vamp_print_histories
```

⬨ WK

110c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁110b 113c▷
```
        subroutine vamp_write_one_history_unit (u, h, tag)
          integer, intent(in) :: u
          type(vamp_history), dimension(:), intent(in) :: h
          character(len=*), intent(in), optional :: tag
```

```fortran
type(div_history), dimension(:), allocatable :: h_tmp
character(len=BUFFER_SIZE) :: pfx
character(len=1) :: s
integer :: i, imax, j
if (present (tag)) then
   pfx = tag
else
   pfx = "[vamp]"
end if
write (u, "(1X,A78)") repeat ("-", 78)
write (u, "(1X,A8,1X,A2,A9,A1,1X,A11,1X,8X,1X," &
     // "1X,A13,1X,8X,1X,A5,1X,A5)") &
     pfx, "it", "#calls", "", "integral", "average", "chi2", "eff."
imax = size (h)
iterations: do i = 1, imax
   if (h(i)%calls <= 0) then
      imax = i - 1
      exit iterations
   end if
   ! *WK: Skip zero channel
   if (h(i)%f_max==0) cycle
   if (h(i)%stratified) then
      s = "*"
   else
      s = ""
   end if
   write (u, "(1X,A8,1X,I2,I9,A1,1X,ES11.4,A1,ES8.2,A1," &
        // "1X,ES13.6,A1,ES8.2,A1,F5.1,1X,F5.3)") pfx, &
        i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
        h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &
        h(i)%integral / h(i)%f_max
end do iterations
write (u, "(1X,A78)") repeat ("-", 78)
if (all (h%verbose) .and. (imax >= 1)) then
   if (associated (h(1)%div)) then
      allocate (h_tmp(imax))
      dimensions: do j = 1, size (h(1)%div)
         do i = 1, imax
            call copy_history (h_tmp(i), h(i)%div(j))
         end do
         if (present (tag)) then
            write (unit = pfx, fmt = "(A,A1,I2.2)") &
                  trim (tag(1:min(len_trim(tag),8))), "#", j
```

```
             else
                write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
             end if
             call write_history (u, h_tmp, tag = pfx)
             print "(1X,A78)", repeat ("-", 78)
          end do dimensions
          deallocate (h_tmp)
        end if
    end if
    flush (u)
  end subroutine vamp_write_one_history_unit
  subroutine vamp_write_histories_unit (u, h, tag)
    integer, intent(in) :: u
    type(vamp_history), dimension(:,:), intent(in) :: h
    character(len=*), intent(in), optional :: tag
    character(len=BUFFER_SIZE) :: pfx
    integer :: i
    write (u, "(1X,A78)") repeat ("=", 78)
    channels: do i = 1, size (h, dim=2)
       if (present (tag)) then
          write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
       else
          write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
       end if
       call vamp_write_one_history_unit (u, h(:,i), pfx)
    end do channels
    write (u, "(1X,A78)") repeat ("=", 78)
    flush (u)
  end subroutine vamp_write_histories_unit
```

5.2.7   Multi Channel

[23]

$$g(x) = \sum_i \alpha_i g_i(x) \tag{5.25a}$$

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

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

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

112

Therefore. . .

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

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

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

113a ⟨*Declaration of* `vamp` *types* 77b⟩+≡ (75b) ◁106c

```
type, public :: vamp_grids
  !!! private ! used by vampi
  real(kind=default), dimension(:), pointer :: weights => null ()
  type(vamp_grid), dimension(:), pointer :: grids => null ()
  integer, dimension(:), pointer :: num_calls => null ()
  real(kind=default) :: sum_chi2, sum_integral, sum_weights
end type vamp_grids
```

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

113b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡ (75b) ◁108c 114b▷

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

113c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡ (75b) ◁110c 114a▷

```
function vamp_multi_channel &
     (func, data, phi, ihp, jacobian, x, weights, channel, grids) result (w_x)
  class(vamp_data_t), intent(in) :: data
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in) :: channel
  type(vamp_grid), dimension(:), intent(in) :: grids
  ⟨Interface declaration for func 22⟩
  ⟨Interface declaration for phi 31a⟩
  ⟨Interface declaration for ihp 31b⟩
  ⟨Interface declaration for jacobian 31c⟩
  real(kind=default) :: w_x
  integer :: i
```

```
        real(kind=default), dimension(size(x)) :: phi_x
        real(kind=default), dimension(size(weights)) :: g_phi_x, g_pi_x
        phi_x = phi (x, channel)
        do i = 1, size (weights)
           if (i == channel) then
              g_pi_x(i) = vamp_probability (grids(i), x)
           else
              g_pi_x(i) = vamp_probability (grids(i), ihp (phi_x, i))
           end if
        end do
        do i = 1, size (weights)
           g_phi_x(i) = g_pi_x(i) / g_pi_x(channel) * jacobian (phi_x, data, i)
        end do
        w_x = func (phi_x, data, weights, channel, grids) &
             / dot_product (weights, g_phi_x)
      end function vamp_multi_channel
```

114a   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁113c 114c▷

```
      function vamp_multi_channel0 &
           (func, data, phi, jacobian, x, weights, channel) result (w_x)
        class(vamp_data_t), intent(in) :: data
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), dimension(:), intent(in) :: weights
        integer, intent(in) :: channel
```
        ⟨*Interface declaration for* `func` 22⟩
        ⟨*Interface declaration for* `phi` 31a⟩
        ⟨*Interface declaration for* `jacobian` 31c⟩
```
        real(kind=default) :: w_x
        real(kind=default), dimension(size(x)) :: x_prime
        real(kind=default), dimension(size(weights)) :: g_phi_x
        integer :: i
        x_prime = phi (x, channel)
        do i = 1, size (weights)
           g_phi_x(i) = jacobian (x_prime, data, i)
        end do
        w_x = func (x_prime, data) / dot_product (weights, g_phi_x)
      end function vamp_multi_channel0
```

   ⚐ WK

114b   ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁113b 117a▷

```
      public :: vamp_jacobian, vamp_check_jacobian
```

114c   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁114a 115▷

```
      pure subroutine vamp_jacobian (phi, channel, x, region, jacobian, delta_x)
```

```
      integer, intent(in) :: channel
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default), dimension(:,:), intent(in) :: region
      real(kind=default), intent(out) :: jacobian
      real(kind=default), intent(in), optional :: delta_x
      interface
         pure function phi (xi, channel) result (x)
           use kinds
           real(kind=default), dimension(:), intent(in) :: xi
           integer, intent(in) :: channel
           real(kind=default), dimension(size(xi)) :: x
         end function phi
      end interface
      real(kind=default), dimension(size(x)) :: x_min, x_max
      real(kind=default), dimension(size(x)) :: x_plus, x_minus
      real(kind=default), dimension(size(x),size(x)) :: d_phi
      real(kind=default), parameter :: &
           dx_default = 10.0_default**(-precision(jacobian)/3)
      real(kind=default) :: dx
      integer :: j
      if (present (delta_x)) then
         dx = delta_x
      else
         dx = dx_default
      end if
      x_min = region(1,:)
      x_max = region(2,:)
      x_minus = max (x_min, x)
      x_plus = min (x_max, x)
      do j = 1, size (x)
         x_minus(j) = max (x_min(j), x(j) - dx)
         x_plus(j) = min (x_max(j), x(j) + dx)
         d_phi(:,j) = (phi (x_plus, channel) - phi (x_minus, channel)) &
              / (x_plus(j) - x_minus(j))
         x_minus(j) = max (x_min(j), x(j))
         x_plus(j) = min (x_max(j), x(j))
      end do
      call determinant (d_phi, jacobian)
      jacobian = abs (jacobian)
   end subroutine vamp_jacobian
```

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

115 ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁114c 117b▷

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

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

116a ⟨*Declaration of* `vamp` *procedures (removed from WHIZARD)* 116a⟩≡

```
private :: numeric_jacobian
```

116b ⟨*Implementation of* `vamp` *procedures (removed from WHIZARD)* 116b⟩≡

```
pure subroutine numeric_jacobian (phi, channel, x, region, jacobian, delta_x)
  integer, intent(in) :: channel
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:,:), intent(in) :: region
  real(kind=default), intent(out) :: jacobian
  real(kind=default), intent(in), optional :: delta_x
  ⟨Interface declaration for phi 31a⟩
```

```
real(kind=default), dimension(size(x)) :: x_min, x_max
real(kind=default), dimension(size(x)) :: x_plus, x_minus
real(kind=default), dimension(size(x),size(x)) :: d_phi
real(kind=default), parameter :: &
     dx_default = 10.0_default**(-precision(jacobian)/3)
real(kind=default) :: dx
integer :: j
if (present (delta_x)) then
   dx = delta_x
else
   dx = dx_default
end if
x_min = region(1,:)
x_max = region(2,:)
x_minus = max (x_min, x)
x_plus = min (x_max, x)
do j = 1, size (x)
   x_minus(j) = max (x_min(j), x(j) - dx)
   x_plus(j) = min (x_max(j), x(j) + dx)
   d_phi(:,j) = (phi (x_plus, channel) - phi (x_minus, channel)) &
                  / (x_plus(j) - x_minus(j))
   x_minus(j) = max (x_min(j), x(j))
   x_plus(j) = min (x_max(j), x(j))
end do
call determinant (d_phi, jacobian)
jacobian = abs (jacobian)
end subroutine numeric_jacobian
```

117a ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁114b 118b▷
```
public :: vamp_create_grids, vamp_create_empty_grids
public :: vamp_copy_grids, vamp_delete_grids
```

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

117b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁115 118a▷
```
pure subroutine vamp_create_grids &
     (g, domain, num_calls, weights, maps, num_div, &
      stratified, quadrupole, exc)
type(vamp_grids), intent(inout) :: g
real(kind=default), dimension(:,:), intent(in) :: domain
integer, intent(in) :: num_calls
real(kind=default), dimension(:), intent(in) :: weights
real(kind=default), dimension(:,:,:), intent(in), optional :: maps
```

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

118a ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁117b 118c▷
```
    pure subroutine vamp_create_empty_grids (g)
      type(vamp_grids), intent(inout) :: g
      nullify (g%grids, g%weights, g%num_calls)
    end subroutine vamp_create_empty_grids
```

118b ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁117a 119a▷
```
    public :: vamp_discard_integrals
```

118c ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁118a 119b▷
```
    pure subroutine vamp_discard_integrals &
         (g, num_calls, num_div, stratified, quadrupole, exc, eq)
      type(vamp_grids), intent(inout) :: g
      integer, intent(in), optional :: num_calls
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole
      type(exception), intent(inout), optional :: exc
      type(vamp_equivalences_t), intent(in), optional :: eq
      integer :: ch
      character(len=*), parameter :: FN = "vamp_discard_integrals"
```

```
      g%sum_integral = 0.0
      g%sum_weights = 0.0
      g%sum_chi2 = 0.0
      do ch = 1, size (g%grids)
         call vamp_discard_integral (g%grids(ch))
      end do
      if (present (num_calls)) then
         call vamp_reshape_grids &
              (g, num_calls, num_div, stratified, quadrupole, exc, eq)
      end if
   end subroutine vamp_discard_integrals
```

119a ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁118b 119c▷
```
   public :: vamp_update_weights
```

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

119b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁118c 119d▷
```
   pure subroutine vamp_update_weights &
        (g, weights, num_calls, num_div, stratified, quadrupole, exc)
      type(vamp_grids), intent(inout) :: g
      real(kind=default), dimension(:), intent(in) :: weights
      integer, intent(in), optional :: num_calls
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole
      type(exception), intent(inout), optional :: exc
      character(len=*), parameter :: FN = "vamp_update_weights"
      if (sum (weights) > 0) then
         g%weights = weights / sum (weights)
      else
         g%weights = 1._default / size(g%weights)
      end if
      if (present (num_calls)) then
         call vamp_discard_integrals (g, num_calls, num_div, &
                                      stratified, quadrupole, exc)
      else
         call vamp_discard_integrals (g, sum (g%num_calls), num_div, &
                                      stratified, quadrupole, exc)
      end if
   end subroutine vamp_update_weights
```

119c ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁119a 120a▷
```
   public :: vamp_reshape_grids
```

119d ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁119b 120b▷
```
   pure subroutine vamp_reshape_grids &
```

```fortran
      (g, num_calls, num_div, stratified, quadrupole, exc, eq)
  type(vamp_grids), intent(inout) :: g
  integer, intent(in) :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole
  type(exception), intent(inout), optional :: exc
  type(vamp_equivalences_t), intent(in), optional :: eq
  integer, dimension(size(g%grids(1)%num_div)) :: num_div_new
  integer :: ch
  character(len=*), parameter :: FN = "vamp_reshape_grids"
  g%num_calls = g%weights * num_calls
  do ch = 1, size (g%grids)
     if (g%num_calls(ch) >= 2) then
        if (present (eq)) then
           if (present (num_div)) then
              num_div_new = num_div
           else
              num_div_new = g%grids(ch)%num_div
           end if
           where (eq%div_is_invariant(ch,:))
              num_div_new = 1
           end where
           call vamp_reshape_grid (g%grids(ch), g%num_calls(ch), &
                   num_div_new, stratified, quadrupole, exc = exc, &
                   independent = eq%independent(ch), &
                   equivalent_to_ch = eq%equivalent_to_ch(ch), &
                   multiplicity = eq%multiplicity(ch))
        else
           call vamp_reshape_grid (g%grids(ch), g%num_calls(ch), &
                   num_div, stratified, quadrupole, exc = exc)
        end if
     else
        g%num_calls(ch) = 0
     end if
  end do
end subroutine vamp_reshape_grids
```

120a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁119c 123a▷
```fortran
  public :: vamp_sample_grids
```

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

120b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁119d 123b▷
```fortran
  subroutine vamp_sample_grids &
```

```
      (rng, g, func, data, iterations, integral, std_dev, avg_chi2, &
        accuracy, history, histories, exc, eq, warn_error, negative_weights)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids), intent(inout) :: g
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: iterations
    real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
    real(kind=default), intent(in), optional :: accuracy
    type(vamp_history), dimension(:), intent(inout), optional :: history
    type(vamp_history), dimension(:,:), intent(inout), optional :: histories
    type(exception), intent(inout), optional :: exc
    type(vamp_equivalences_t), intent(in), optional :: eq
    logical, intent(in), optional :: warn_error, negative_weights
    ⟨Interface declaration for func 22⟩
    integer :: ch, iteration
    logical :: neg_w
    type(exception), dimension(size(g%grids)) :: excs
    logical, dimension(size(g%grids)) :: active
    real(kind=default), dimension(size(g%grids)) :: weights, integrals, std_devs
    real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
    character(len=*), parameter :: FN = "vamp_sample_grids"
    integrals = 0
    std_devs = 0
    neg_w = .false.
    if (present (negative_weights)) neg_w = negative_weights
    active = (g%num_calls >= 2)
    where (active)
       weights = g%num_calls
    elsewhere
       weights = 0.0
    endwhere
    if (sum (weights) /= 0)  weights = weights / sum (weights)
    call clear_exception (excs)
    iterate: do iteration = 1, iterations
       do ch = 1, size (g%grids)
          if (active(ch)) then
             call vamp_discard_integral (g%grids(ch))
             ⟨Sample the grid g%grids(ch) 122⟩
          else
             call vamp_nullify_variance (g%grids(ch))
             call vamp_nullify_covariance (g%grids(ch))
          end if
       end do
```

```fortran
          if (present(eq))  call vamp_apply_equivalences (g, eq)
          if (iteration < iterations) then
             do ch = 1, size (g%grids)
                active(ch) = (integrals(ch) /= 0)
                if (active(ch)) then
                   call vamp_refine_grid (g%grids(ch))
                 end if
             end do
          end if
          if (present (exc) .and. (any (excs%level > 0))) then
             call gather_exceptions (exc, excs)
   !         return
          end if
          call vamp_reduce_channels (g, integrals, std_devs, active)
          call vamp_average_iterations &
               (g, iteration, local_integral, local_std_dev, local_avg_chi2)
          ⟨Trace results of vamp_sample_grids 125a⟩
          ⟨Exit iterate if accuracy has been reached 97a⟩
        end do iterate
        ⟨Copy results of vamp_sample_grid to dummy variables 96c⟩
      end subroutine vamp_sample_grids
```

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

122 ⟨*Sample the grid* g%grids(ch) 122⟩≡   (120b)

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

122

⟨*Declaration of* `vamp` *procedures* 77a⟩+≡ (75b) ◁120a 124a▷
```
public :: vamp_reduce_channels
```

$$I = \frac{1}{N} \sum_c N_c I_c \tag{5.30a}$$

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

$$N = \sum_c N_c \tag{5.30c}$$

where (5.30b) is actually

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

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

⟨*Implementation of* `vamp` *procedures* 78b⟩+≡ (75b) ◁120b 124b▷
```
pure subroutine vamp_reduce_channels (g, integrals, std_devs, active)
  type(vamp_grids), intent(inout) :: g
  real(kind=default), dimension(:), intent(in) :: integrals, std_devs
  logical, dimension(:), intent(in) :: active
  real(kind=default) :: this_integral, this_weight, total_calls
  real(kind=default) :: total_variance
  if (.not.any(active)) return
  total_calls = sum (g%num_calls, mask=active)
  if (total_calls > 0) then
     this_integral = sum (g%num_calls * integrals, mask=active) / total_calls
  else
     this_integral = 0
  end if
  total_variance = sum ((g%num_calls*std_devs)**2, mask=active)
  if (total_variance > 0) then
     this_weight = total_calls**2 / total_variance
  else
     this_weight = 0
  end if
  g%sum_weights = g%sum_weights + this_weight
  g%sum_integral = g%sum_integral + this_weight * this_integral
  g%sum_chi2 = g%sum_chi2 + this_weight * this_integral**2
end subroutine vamp_reduce_channels
```

124a   ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁123a 124c▷

```
public :: vamp_refine_weights
```

124b   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁123b 124e▷

```
elemental subroutine vamp_average_iterations_grids &
    (g, iteration, integral, std_dev, avg_chi2)
  type(vamp_grids), intent(in) :: g
  integer, intent(in) :: iteration
  real(kind=default), intent(out) :: integral, std_dev, avg_chi2
  real(kind=default), parameter :: eps = 1000 * epsilon (1._default)
  if (g%sum_weights>0) then
     integral = g%sum_integral / g%sum_weights
     std_dev = sqrt (1.0 / g%sum_weights)
     avg_chi2 = &
          max ((g%sum_chi2 - g%sum_integral * integral) / (iteration-0.99), &
               0.0_default)
     if (avg_chi2 < eps * g%sum_chi2)  avg_chi2 = 0
  else
     integral = 0
     std_dev = 0
     avg_chi2 = 0
  end if
end subroutine vamp_average_iterations_grids
```

124c   ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁124a 125b▷

```
private :: vamp_average_iterations_grids
```

124d   ⟨*Interfaces of* `vamp` *procedures* 96b⟩+≡   (75b) ◁108d 125c▷

```
interface vamp_average_iterations
   module procedure  vamp_average_iterations_grids
end interface
```

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

124e   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁124b 125d▷

```
pure subroutine vamp_refine_weights (g, power)
  type(vamp_grids), intent(inout) :: g
  real(kind=default), intent(in), optional :: power
  real(kind=default) :: local_power
  real(kind=default), parameter :: DEFAULT_POWER = 0.5_default
  if (present (power)) then
     local_power = power
  else
     local_power = DEFAULT_POWER
  end if
  call vamp_update_weights &
```

```
                    (g, g%weights * vamp_get_variance (g%grids) ** local_power)
          end subroutine vamp_refine_weights
```

125a ⟨*Trace results of* `vamp_sample_grids` 125a⟩≡   (120b)
```
          if (present (history)) then
            if (iteration <= size (history)) then
               call vamp_get_history &
                     (history(iteration), g, local_integral, local_std_dev, &
                      local_avg_chi2)
            else
               call raise_exception (exc, EXC_WARN, FN, "history too short")
            end if
            call vamp_terminate_history (history(iteration+1:))
          end if
```

125b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁124c 126a▷
```
          private :: vamp_get_history_multi
```

125c ⟨*Interfaces of* `vamp` *procedures* 96b⟩+≡   (75b) ◁124d 131b▷
```
          interface vamp_get_history
             module procedure vamp_get_history_multi
          end interface
```

125d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁124e 126b▷
```
          pure subroutine vamp_get_history_multi (h, g, integral, std_dev, avg_chi2)
            type(vamp_history), intent(inout) :: h
            type(vamp_grids), intent(in) :: g
            real(kind=default), intent(in) :: integral, std_dev, avg_chi2
            h%calls = sum (g%grids%calls)
            h%stratified = all (g%grids%all_stratified)
            h%integral = 0.0
            h%std_dev = 0.0
            h%avg_integral = integral
            h%avg_std_dev = std_dev
            h%avg_chi2 = avg_chi2
            h%f_min = 0.0
            h%f_max = huge (h%f_max)
            if (h%verbose) then
               h%verbose = .false.
               if (associated (h%div)) then
                  deallocate (h%div)
               end if
            end if
          end subroutine vamp_get_history_multi
```

⟨WK⟩
```
                                   125
```

```
public :: vamp_sum_channels
```

```
function vamp_sum_channels (x, weights, func, data, grids) result (g)
  real(kind=default), dimension(:), intent(in) :: x, weights
  class(vamp_data_t), intent(in) :: data
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  interface
     function func (xi, data, weights, channel, grids) result (f)
       use kinds
       use vamp_grid_type !NODEP!
       import vamp_data_t
       real(kind=default), dimension(:), intent(in) :: xi
       class(vamp_data_t), intent(in) :: data
       real(kind=default), dimension(:), intent(in), optional :: weights
       integer, intent(in), optional :: channel
       type(vamp_grid), dimension(:), intent(in), optional :: grids
       real(kind=default) :: f
     end function func
  end interface
  real(kind=default) :: g
  integer :: ch
  g = 0.0
  do ch = 1, size (weights)
     g = g + weights(ch) * func (x, data, weights, ch, grids)
  end do
end function vamp_sum_channels
```

5.2.8 Mapping

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

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

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

where

$$Cv_j = \lambda_j v_j \tag{5.33}$$

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

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

After `call diagonalize_real_symmetric (cov, evals, evecs)`, we have `evals`$(j) = \lambda_j$ and `evecs`$(:, j) = v_j$. This is equivalent with `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 isotripic in these directions. I 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 specfic axis, we can as well diagonalize in a subspace. Empirically, rotation around an axis is better than diagonalizing in a two-dimensional subspace, but diagonalizing in a three-dimensional subspace can be even better.

127a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁126a 128a▷
```
public :: select_rotation_axis
public :: select_rotation_subspace
```

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

127c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁126b 129d▷
```
subroutine more_pancake_than_cigar (eval, yes_or_no)
   real(kind=default), dimension(:), intent(in) :: eval
   logical, intent(out) :: yes_or_no
   integer, parameter :: N_CL = 2
```

```
      real(kind=default), dimension(size(eval)) :: evals
      real(kind=default), dimension(N_CL) :: cluster_pos
      integer, dimension(N_CL,2) :: clusters
      evals = eval
      call sort (evals)
      call condense (evals, cluster_pos, clusters)
      print *, clusters(1,2) - clusters(1,1) + 1, "small EVs: ", &
           evals(clusters(1,1):clusters(1,2))
      print *, clusters(2,2) - clusters(2,1) + 1, "large EVs: ", &
           evals(clusters(2,1):clusters(2,2))
      if ((clusters(1,2) - clusters(1,1)) &
           < (clusters(2,2) - clusters(2,1))) then
        print *, " => PANCAKE!"
        yes_or_no = .true.
      else
        print *, " => CIGAR!"
        yes_or_no = .false.
      end if
  end subroutine more_pancake_than_cigar
```

128a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁127a 131c▷
      `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

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

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

128b ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane* 128b⟩≡   (129d) 129a▷
      ```
      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 dgenerate eigenvalues:

128c ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane (broken!)* 128c⟩≡
      ```
      abs_evec = abs (evecs(:,iv))
      i(1) = sum (maxloc (abs_evec))
      i(2) = sum (maxloc (abs_evec, mask = abs_evec < abs_evec(i(1))))
      ```

---

[3]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.

129a ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane* 128b⟩+≡   (129d) ◁128b

```
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)
```

129b ⟨*Get* $\cos\theta$ *and* $\sin\theta$ *from* `evecs` 129b⟩≡   (129d)

```
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
```

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

129c ⟨*Construct* $\hat{R}(\theta;i,j)$ 129c⟩≡   (129d)

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

129d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁127c 130b▷

```
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
```
  ⟨*Handle optional* `pancake` *and* `cigar` 130a⟩
```
  call diagonalize_real_symmetric (cov, evals, evecs)
```
  ⟨*Set* `iv` *to the index of the optimal eigenvector* 127b⟩
  ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane* 128b⟩
  ⟨*Get* $\cos\theta$ *and* $\sin\theta$ *from* `evecs` 129b⟩
  ⟨*Construct* $\hat{R}(\theta;i,j)$ 129c⟩
```
end subroutine select_rotation_axis
```

130a ⟨*Handle optional* `pancake` *and* `cigar` 130a⟩≡   (129d 130c)

```
   if (present (pancake)) then
      num_pancake = pancake
   else
      num_pancake = -1
   endif
   if (present (cigar)) then
      num_cigar = cigar
   else
      num_cigar = -1
   endif
```

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

130b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁129d 130c▷

```
   subroutine select_subspace_explicit (cov, r, subspace)
     real(kind=default), dimension(:,:), intent(in) :: cov
     real(kind=default), dimension(:,:), intent(out) :: r
     integer, dimension(:), intent(in) :: subspace
     real(kind=default), dimension(size(subspace)) :: eval_sub
     real(kind=default), dimension(size(subspace),size(subspace)) :: &
         cov_sub, evec_sub
     cov_sub = cov(subspace,subspace)
     call diagonalize_real_symmetric (cov_sub, eval_sub, evec_sub)
     call unit (r)
     r(subspace,subspace) = evec_sub
   end subroutine select_subspace_explicit
```

130c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁130b 131e▷

```
   subroutine select_subspace_guess (cov, r, ndim, pancake, cigar)
     real(kind=default), dimension(:,:), intent(in) :: cov
     real(kind=default), dimension(:,:), intent(out) :: r
     integer, intent(in) :: ndim
     integer, intent(in), optional :: pancake, cigar
     integer :: num_pancake, num_cigar
     logical :: like_pancake
     real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evecs
     real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
     integer :: iv, i
     integer, dimension(ndim) :: subspace
```
     ⟨*Handle optional* `pancake` *and* `cigar` 130a⟩
```
     call diagonalize_real_symmetric (cov, evals, evecs)
```
     ⟨*Set* `iv` *to the index of the optimal eigenvector* 127b⟩
     ⟨*Set* `subspace` *to the axes of the optimal plane* 131a⟩

```
          call select_subspace_explicit (cov, r, subspace)
        end subroutine select_subspace_guess
```

131a ⟨*Set* subspace *to the axes of the optimal plane* 131a⟩≡   (130c)
```
        abs_evec = abs (evecs(:,iv))
        subspace(1) = sum (maxloc (abs_evec))
        do i = 2, ndim
          abs_evec(subspace(i-1)) = -1.0
          subspace(i) = sum (maxloc (abs_evec))
        end do
```

131b ⟨*Interfaces of* vamp *procedures* 96b⟩+≡   (75b) ◁125c 135b▷
```
        interface select_rotation_subspace
          module procedure select_subspace_explicit, select_subspace_guess
        end interface
```

131c ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁128a 131d▷
```
        private :: select_subspace_explicit
        private :: select_subspace_guess
```

131d ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁131c 132a▷
```
        public :: vamp_print_covariance
```

131e ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁130c 133c▷
```
        subroutine vamp_print_covariance (cov)
          real(kind=default), dimension(:,:), intent(in) :: cov
          real(kind=default), dimension(size(cov,dim=1)) :: &
               evals, abs_evals, tmp
          real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: &
               evecs, abs_evecs
          integer, dimension(size(cov,dim=1)) :: idx
          integer :: i, i_max, j
          i_max = size (evals)
          call diagonalize_real_symmetric (cov, evals, evecs)
          call sort (evals, evecs)
          abs_evals = abs (evals)
          abs_evecs = abs (evecs)
          print "(1X,A78)", repeat ("-", 78)
          print "(1X,A)", "Eigenvalues and eigenvectors:"
          print "(1X,A78)", repeat ("-", 78)
          do i = 1, i_max
            print "(1X,I2,A1,1X,E11.4,1X,A1,10(10(1X,F5.2)/,18X))", &
                 i, ":", evals(i), "|", evecs(:,i)
          end do
          print "(1X,A78)", repeat ("-", 78)
          print "(1X,A)", "Approximate subspaces:"
```

```
      print "(1X,A78)", repeat ("-", 78)
      do i = 1, i_max
         idx = (/ (j, j=1,i_max) /)
         tmp = abs_evecs(:,i)
         call sort (tmp, idx, reverse = .true.)
         print "(1X,I2,A1,1X,E11.4,1X,A1,10(1X,I5))", &
               i, ":", evals(i), "|", idx(1:min(10,size(idx)))
         print "(17X,A1,10(1X,F5.2))", &
                              "|", evecs(idx(1:min(10,size(idx))),i)
      end do
      print "(1X,A78)", repeat ("-", 78)
   end subroutine vamp_print_covariance
```

Condensing Eigenvalues

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

132a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁131d 134a▷
```
   ! private :: condense
   public :: condense
```

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

   ⟨⟩   If there's not a clean separation, this algorithm is certainly chaotic and we need to apply some form of damping!

132b ⟨*Initialize clusters* 132b⟩≡   (133c)
```
   cl_pos = x
   cl_num = size (cl_pos)
   cl = spread ((/ (i, i=1,cl_num) /), dim = 2, ncopies = 2)
```

It appears that the logarithmic metric

$$d_0(x,y) = \left| \log\left(\frac{x}{y}\right) \right| \tag{5.37a}$$

performs better than the linear metric

$$d_1(x,y) = |x - y| \tag{5.37b}$$

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since the latter won't separate very small eiegenvalues from the bulk. Another option is

$$d_\alpha(x,y) = |x^\alpha - y^\alpha| \qquad (5.37c)$$

with $\alpha \neq 1$, in particular $\alpha \approx -1$. I haven't studied it yet, though.

> but I should perform more empirical studies to determine whether the logarithmic or the linear metric is more appropriate in realistic cases.

133a ⟨*Join closest clusters* 133a⟩≡   (133c) 133b▷

```
if (linear_metric) then
   gap = sum (minloc (cl_pos(2:cl_num) - cl_pos(1:cl_num-1)))
else
   gap = sum (minloc (cl_pos(2:cl_num) / cl_pos(1:cl_num-1)))
end if
wgt0 = cl(gap,2) - cl(gap,1) + 1
wgt1 = cl(gap+1,2) - cl(gap+1,1) + 1
cl_pos(gap) = (wgt0 * cl_pos(gap) + wgt1 * cl_pos(gap+1)) / (wgt0 + wgt1)
cl(gap,2) = cl(gap+1,2)
```

133b ⟨*Join closest clusters* 133a⟩+≡   (133c) ◁133a

```
cl_pos(gap+1:cl_num-1) = cl_pos(gap+2:cl_num)
cl(gap+1:cl_num-1,:) = cl(gap+2:cl_num,:)
```

133c ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁131e 134b▷

```
subroutine condense (x, cluster_pos, clusters, linear)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(out) :: cluster_pos
  integer, dimension(:,:), intent(out) :: clusters
  logical, intent(in), optional :: linear
  logical :: linear_metric
  real(kind=default), dimension(size(x)) :: cl_pos
  real(kind=default) :: wgt0, wgt1
  integer :: cl_num
  integer, dimension(size(x),2) :: cl
  integer :: i, gap
  linear_metric = .false.
  if (present (linear)) then
     linear_metric = linear
  end if
  ⟨Initialize clusters 132b⟩
  do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
     ⟨Join closest clusters 133a⟩
     print *, cl_num, ": action = ", condense_action (x, cl)
```

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

134a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁132a 135a▷
```
  ! private :: condense_action
  public :: condense_action
```

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

134b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁133c 135d▷
```
  function condense_action (positions, clusters) result (s)
    real(kind=default), dimension(:), intent(in) :: positions
    integer, dimension(:,:), intent(in) :: clusters
    real(kind=default) :: s
    integer :: i
    integer, parameter :: POWER = 2
    s = 0
    do i = 1, size (clusters, dim = 1)
       s = s + standard_deviation (positions(clusters(i,1) &
                                    :clusters(i,2))) ** POWER
    end do
  end function condense_action
```

134c ⟨ctest.f90 134c⟩≡
```
  program ctest
    use kinds
    use utils
    use vamp_stat
    use tao_random_numbers
    use vamp
    implicit none
    integer, parameter :: N = 16, NC = 2
    real(kind=default), dimension(N) :: eval
    real(kind=default), dimension(NC) :: cluster_pos
    integer, dimension(NC,2) :: clusters
    integer :: i
    call tao_random_number (eval)
    call sort (eval)
    print *, eval
    eval(1:N/2) = 0.95*eval(1:N/2)
    eval(N/2+1:N) = 1.0 - 0.95*(1.0 - eval(N/2+1:N))
    print *, eval
    call condense (eval, cluster_pos, clusters, linear=.true.)
```

```
      do i = 1, NC
         print "(I2,A,F5.2,A,I2,A,I2,A,A,F5.2,A,F5.2,A,32F5.2)", &
              i, ": ", cluster_pos(i), &
              " [", clusters(i,1), "-", clusters(i,2), "]", &
              " [", eval(clusters(i,1)), " - ", eval(clusters(i,2)), "]", &
              eval(clusters(i,1)+1:clusters(i,2)) &
                 - eval(clusters(i,1):clusters(i,2)-1)
         print *, average (eval(clusters(i,1):clusters(i,2))), "+/-", &
                 standard_deviation (eval(clusters(i,1):clusters(i,2)))
      end do
   end program ctest
```

5.2.9   Event Generation

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

135a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁134a 135c▷
```
   public :: vamp_next_event
```

135b ⟨*Interfaces of* `vamp` *procedures* 96b⟩+≡   (75b) ◁131b 140b▷
```
   interface vamp_next_event
      module procedure vamp_next_event_single, vamp_next_event_multi
   end interface
```

135c ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁135a 139a▷
```
   private :: vamp_next_event_single, vamp_next_event_multi
```

Both event generation routines operate in two modes, depending on whether
the optional argument `weight` is present.

135d ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁134b 137▷
```
   subroutine vamp_next_event_single &
        (x, rng, g, func, data, &
         weight, channel, weights, grids, exc)
     real(kind=default), dimension(:), intent(out) :: x
     type(tao_random_state), intent(inout) :: rng
     type(vamp_grid), intent(inout) :: g
     real(kind=default), intent(out), optional :: weight
     class(vamp_data_t), intent(in) :: data
     integer, intent(in), optional :: channel
     real(kind=default), dimension(:), intent(in), optional :: weights
     type(vamp_grid), dimension(:), intent(in), optional :: grids
     type(exception), intent(inout), optional :: exc
```
⟨*Interface declaration for* `func` 22⟩
```
     character(len=*), parameter :: FN = "vamp_next_event_single"
```

```
      real(kind=default), dimension(size(g%div)):: wgts
      real(kind=default), dimension(size(g%div)):: r
      integer, dimension(size(g%div)):: ia
      real(kind=default) :: f, wgt
      real(kind=default) :: r0
      rejection: do
         ⟨Choose a x and calculate f(x) 136a⟩
         if (present (weight)) then
            ⟨Unconditionally accept weighted event 136b⟩
         else
            ⟨Maybe accept unweighted event 136c⟩
         end if
      end do rejection
   end subroutine vamp_next_event_single
```

136a   ⟨Choose a x and calculate f(x) 136a⟩≡   (135d)
```
      call tao_random_number (rng, r)
      call inject_division_short (g%div, real(r, kind=default), x, ia, wgts)
      wgt = g%jacobi * product (wgts)
      wgt = g%calls * wgt ! the calling procedure will divide by #calls
      if (associated (g%map)) then
         x = matmul (g%map, x)
      end if
```
      ⟨f = wgt * func (x, weights, channel), *iff* x *inside* true_domain 88d⟩
```
      ! call record_efficiency (g%div, ia, f/g%f_max)
```

136b   ⟨Unconditionally accept weighted event 136b⟩≡   (135d)
```
      weight = f
      exit rejection
```

136c   ⟨Maybe accept unweighted event 136c⟩≡   (135d)
```
      if (f > g%f_max) then
         g%f_max = f
         call raise_exception (exc, EXC_WARN, FN, "weight > 1")
         exit rejection
      end if
      call tao_random_number (rng, r0)
      if (r0 * g%f_max <= f) then
         exit rejection
      end if
```

We know that `g%weights` are normalized: `sum (g%weights) == 1.0`. The
basic formula for multi channel sampling is

$$f(x) = \sum_i \alpha_i g_i(x) w(x) \tag{5.39}$$

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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 poblem is that the adaptive grid is diferent in each channel, so we can't just reject on $w(x)$.

137 ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁135d 139b▷

```
 subroutine vamp_next_event_multi &
      (x, rng, g, func, data, phi, weight, excess, positive, exc)
   real(kind=default), dimension(:), intent(out) :: x
   type(tao_random_state), intent(inout) :: rng
   type(vamp_grids), intent(inout) :: g
   class(vamp_data_t), intent(in) :: data
   real(kind=default), intent(out), optional :: weight
   real(kind=default), intent(out), optional :: excess
   logical, intent(out), optional :: positive
   type(exception), intent(inout), optional :: exc
   ⟨Interface declaration for func 22⟩
   ⟨Interface declaration for phi 31a⟩
   character(len=*), parameter :: FN = "vamp_next_event_multi"
   real(kind=default), dimension(size(x)) :: xi
   real(kind=default) :: r, wgt
   real(kind=default), dimension(size(g%weights)) :: weights
   integer :: channel
   ⟨weights: αᵢ → w_max,i αᵢ 138a⟩
   rejection: do
      ⟨Select channel from weights 138b⟩
      call vamp_next_event_single &
           (xi, rng, g%grids(channel), func, data, wgt, &
            channel, g%weights, g%grids, exc)
      if (present (weight)) then
         ⟨Unconditionally accept weighted multi channel event 138c⟩
      else
         ⟨Maybe accept unweighted multi channel event 138d⟩
      end if
   end do rejection
   x = phi (xi, channel)
 end subroutine vamp_next_event_multi
```

We can either reject with the weights

$$\frac{w_i(x)}{\max_i \max_x w_i(x)} \tag{5.40}$$

after using the apriori weights α_i to select a channel i or we can reject with the weights

$$\frac{w_i(x)}{\max_x w_i(x)} \tag{5.41}$$

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after using the apriori weights $\alpha_i(\max_x w_i(x))/(\max_i \max_x w_i(x))$. The latter method is more efficient if the $\max_x w_i(x)$ have a wide spread.

138a ⟨weights: $\alpha_i \to w_{\max,i}\alpha_i$ 138a⟩≡   (137 138e)
```
  if (any (g%grids%f_max > 0)) then
     weights = g%weights * g%grids%f_max
  else
     weights = g%weights
  end if
  weights = weights / sum (weights)
```

138b ⟨*Select* channel *from* weights 138b⟩≡   (137)
```
  call tao_random_number (rng, r)
  select_channel: do channel = 1, size (g%weights)
     r = r - weights(channel)
     if (r <= 0.0) then
        exit select_channel
     end if
  end do select_channel
  channel = min (channel, size (g%weights)) ! for r = 1 and rounding errors
```

138c ⟨*Unconditionally accept weighted multi channel event* 138c⟩≡   (137)
```
  weight = wgt * g%weights(channel) / weights(channel)
  exit rejection
```

138d ⟨*Maybe accept unweighted multi channel event* 138d⟩≡   (137)
```
  if (abs (wgt) > g%grids(channel)%f_max) then
     if (present(excess)) then
        excess = abs (wgt) / g%grids(channel)%f_max - 1
     else
       call raise_exception (exc, EXC_WARN, FN, "weight > 1")
  !       print *, "weight > 1 (", wgt/g%grids(channel)%f_max, &
  !            & ") in channel ", channel

     end if
  !  exit rejection
  else
     if (present(excess)) excess = 0
  end if
  call tao_random_number (rng, r)
  if (r * g%grids(channel)%f_max <= abs (wgt)) then
     if (present (positive))  positive = wgt >= 0
     exit rejection
  end if
```

138e ⟨*Maybe accept unweighted multi channel event (old version)* 138e⟩≡

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```
      if (wgt > g%grids(channel)%f_max) then
         g%grids(channel)%f_max = wgt
         ⟨weights: αᵢ → w_max,i αᵢ 138a⟩
         call raise_exception (exc, EXC_WARN, FN, "weight > 1")
         exit rejection
      end if
   call tao_random_number (rng, r)
   if (r * g%grids(channel)%f_max <= wgt) then
      exit rejection
   end if
```

Using `vamp_sample_grid` (`g`, ...) to warm up the grid `g` has a somewhat subtle problem: the minimum and maximum weights `g%f_min` and `g%f_max` refer to the grid *before* the final refinement. One could require an additional `vamp_sample_grid0` (`g`, ...), but users are likely to forget such technical details. A better solution is a wrapper `vamp_warmup_grid` (`g`, ...) that drops the final refinement transparently.

139a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡   (75b) ◁135c 140a▷
```
   public :: vamp_warmup_grid, vamp_warmup_grids
```

139b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁137 139c▷
```
   subroutine vamp_warmup_grid &
        (rng, g, func, data, iterations, exc, history)
     type(tao_random_state), intent(inout) :: rng
     type(vamp_grid), intent(inout) :: g
     class(vamp_data_t), intent(in) :: data
     integer, intent(in) :: iterations
     type(exception), intent(inout), optional :: exc
     type(vamp_history), dimension(:), intent(inout), optional :: history
     ⟨Interface declaration for func 22⟩
     call vamp_sample_grid &
        (rng, g, func, data, &
          iterations - 1, exc = exc, history = history)
     call vamp_sample_grid0 (rng, g, func, data, exc = exc)
   end subroutine vamp_warmup_grid
```

⬙ WHERE ... END WHERE alert!

139c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁139b 140c▷
```
   subroutine vamp_warmup_grids &
        (rng, g, func, data, iterations, history, histories, exc)
     type(tao_random_state), intent(inout) :: rng
     type(vamp_grids), intent(inout) :: g
     class(vamp_data_t), intent(in) :: data
     integer, intent(in) :: iterations
```

```fortran
    type(vamp_history), dimension(:), intent(inout), optional :: history
    type(vamp_history), dimension(:,:), intent(inout), optional :: histories
    type(exception), intent(inout), optional :: exc
    ⟨Interface declaration for func 22⟩
    integer :: ch
    logical, dimension(size(g%grids)) :: active
    real(kind=default), dimension(size(g%grids)) :: weights
    active = (g%num_calls >= 2)
    where (active)
       weights = g%num_calls
    elsewhere
       weights = 0.0
    end where
    weights = weights / sum (weights)
    call vamp_sample_grids (rng, g, func, data, iterations - 1, &
                            exc = exc, history = history, histories = histories)
    do ch = 1, size (g%grids)
       if (g%grids(ch)%num_calls >= 2) then
          call vamp_sample_grid0 &
               (rng, g%grids(ch), func, data, &
                ch, weights, g%grids, exc = exc)
       end if
    end do
 end subroutine vamp_warmup_grids
```

5.2.10   Convenience Routines

140a   ⟨Declaration of vamp procedures 77a⟩+≡   (75b) ◁139a 142a▷
```fortran
    public :: vamp_integrate
    private :: vamp_integrate_grid, vamp_integrate_region
```

140b   ⟨Interfaces of vamp procedures 96b⟩+≡   (75b) ◁135b 142b▷
```fortran
    interface vamp_integrate
       module procedure vamp_integrate_grid, vamp_integrate_region
    end interface
```

140c   ⟨Implementation of vamp procedures 78b⟩+≡   (75b) ◁139c 141▷
```fortran
    subroutine vamp_integrate_grid &
        (rng, g, func, data, calls, integral, std_dev, avg_chi2, num_div, &
         stratified, quadrupole, accuracy, exc, history)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    class(vamp_data_t), intent(in) :: data
    integer, dimension(:,:), intent(in) :: calls
```

```
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
⟨Interface declaration for func 22⟩
character(len=*), parameter :: FN = "vamp_integrate_grid"
integer :: step, last_step, it
last_step = size (calls, dim = 2)
it = 1
do step = 1, last_step - 1
   call vamp_discard_integral (g, calls(2,step), num_div, &
                                 stratified, quadrupole, exc = exc)
   call vamp_sample_grid (rng, g, func, data, calls(1,step), &
                           exc = exc, history = history(it:))
   ⟨Bail out if exception exc raised 99d⟩
   it = it + calls(1,step)
end do
call vamp_discard_integral (g, calls(2,last_step), exc = exc)
call vamp_sample_grid (rng, g, func, data, calls(1,last_step), &
                        integral, std_dev, avg_chi2, accuracy, exc = exc, &
                        history = history(it:))
end subroutine vamp_integrate_grid
```

141   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁140c 142c▷

```
subroutine vamp_integrate_region &
     (rng, region, func, data, calls, &
      integral, std_dev, avg_chi2, num_div, &
      stratified, quadrupole, accuracy, map, covariance, exc, history)
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), dimension(:,:), intent(in) :: region
  class(vamp_data_t), intent(in) :: data
  integer, dimension(:,:), intent(in) :: calls
  real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole
  real(kind=default), intent(in), optional :: accuracy
  real(kind=default), dimension(:,:), intent(in), optional :: map
  real(kind=default), dimension(:,:), intent(out), optional :: covariance
  type(exception), intent(inout), optional :: exc
  type(vamp_history), dimension(:), intent(inout), optional :: history
  ⟨Interface declaration for func 22⟩
  character(len=*), parameter :: FN = "vamp_integrate_region"
```

```
      type(vamp_grid) :: g
      call vamp_create_grid &
           (g, region, calls(2,1), num_div, &
            stratified, quadrupole, present (covariance), map, exc)
      call vamp_integrate_grid &
           (rng, g, func, data, calls, &
            integral, std_dev, avg_chi2, num_div, &
            accuracy = accuracy, exc = exc, history = history)
      if (present (covariance)) then
         covariance = vamp_get_covariance (g)
      end if
      call vamp_delete_grid (g)
    end subroutine vamp_integrate_region
```

142a ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁140a 143▷
```
      public :: vamp_integratex
      private :: vamp_integratex_region
```

142b ⟨*Interfaces of* vamp *procedures* 96b⟩+≡   (75b) ◁140b 144b▷
```
      interface vamp_integratex
        module procedure vamp_integratex_region
      end interface
```

142c ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁141 144d▷
```
    subroutine vamp_integratex_region &
         (rng, region, func, data, calls, integral, std_dev, avg_chi2, &
          num_div, stratified, quadrupole, accuracy, pancake, cigar, &
          exc, history)
      type(tao_random_state), intent(inout) :: rng
      real(kind=default), dimension(:,:), intent(in) :: region
      class(vamp_data_t), intent(in) :: data
      integer, dimension(:,:,:), intent(in) :: calls
      real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole
      real(kind=default), intent(in), optional :: accuracy
      integer, intent(in), optional :: pancake, cigar
      type(exception), intent(inout), optional :: exc
      type(vamp_history), dimension(:), intent(inout), optional :: history
```
⟨*Interface declaration for* func 22⟩
```
      real(kind=default), dimension(size(region,dim=2)) :: eval
      real(kind=default), dimension(size(region,dim=2),size(region,dim=2)) :: evec
      type(vamp_grid) :: g
      integer :: step, last_step, it
      it = 1
```

```fortran
      call vamp_create_grid &
           (g, region, calls(2,1,1), num_div, &
            stratified, quadrupole, covariance = .true., exc = exc)
      call vamp_integrate_grid &
           (rng, g, func, data, calls(:,:,1), num_div = num_div, &
            exc = exc, history = history(it:))
```
⟨*Bail out if exception* exc *raised* 99d⟩
```fortran
      it = it + sum (calls(1,:,1))
      last_step = size (calls, dim = 3)
      do step = 2, last_step - 1
         call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
         call sort (eval, evec)
         call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
         call vamp_delete_grid (g)
         call vamp_create_grid &
              (g, region, calls(2,1,step), num_div, stratified, quadrupole, &
               covariance = .true., map = evec, exc = exc)
         call vamp_integrate_grid &
              (rng, g, func, data, calls(:,:,step), num_div = num_div, &
               exc = exc, history = history(it:))
```
         ⟨*Bail out if exception* exc *raised* 99d⟩
```fortran
         it = it + sum (calls(1,:,step))
      end do
      call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
      call sort (eval, evec)
      call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
      call vamp_delete_grid (g)
      call vamp_create_grid &
           (g, region, calls(2,1,last_step), num_div, stratified, quadrupole, &
            covariance = .true., map = evec, exc = exc)
      call vamp_integrate_grid &
           (rng, g, func, data, calls(:,:,last_step), &
            integral, std_dev, avg_chi2, &
            num_div = num_div, exc = exc, history = history(it:))
      call vamp_delete_grid (g)
   end subroutine vamp_integratex_region
```

5.2.11   I/O

143   ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁142a 144a▷
```fortran
      public :: vamp_write_grid
      private :: write_grid_unit, write_grid_name
      public :: vamp_read_grid
```

```
      private :: read_grid_unit, read_grid_name
      public :: vamp_write_grids
      private :: write_grids_unit, write_grids_name
      public :: vamp_read_grids
      private :: read_grids_unit, read_grids_name
```

144a ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁143 158a▷
```
      public :: vamp_read_grids_raw
      private :: read_grids_raw_unit, read_grids_raw_name
      public :: vamp_read_grid_raw
      private :: read_grid_raw_unit, read_grid_raw_name
      public :: vamp_write_grids_raw
      private :: write_grids_raw_unit, write_grids_raw_name
      public :: vamp_write_grid_raw
      private :: write_grid_raw_unit, write_grid_raw_name
```

144b ⟨*Interfaces of* vamp *procedures* 96b⟩+≡   (75b) ◁142b 144c▷
```
      interface vamp_write_grid
         module procedure write_grid_unit, write_grid_name
      end interface
      interface vamp_read_grid
         module procedure read_grid_unit, read_grid_name
      end interface
      interface vamp_write_grids
         module procedure write_grids_unit, write_grids_name
      end interface
      interface vamp_read_grids
         module procedure read_grids_unit, read_grids_name
      end interface
```

144c ⟨*Interfaces of* vamp *procedures* 96b⟩+≡   (75b) ◁144b
```
      interface vamp_write_grid_raw
         module procedure write_grid_raw_unit, write_grid_raw_name
      end interface
      interface vamp_read_grid_raw
         module procedure read_grid_raw_unit, read_grid_raw_name
      end interface
      interface vamp_write_grids_raw
         module procedure write_grids_raw_unit, write_grids_raw_name
      end interface
      interface vamp_read_grids_raw
         module procedure read_grids_raw_unit, read_grids_raw_name
      end interface
```

144d ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁142c 146b▷
```
      subroutine write_grid_unit (g, unit, write_integrals)
```

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```fortran
    type(vamp_grid), intent(in) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    integer :: i, j
    write (unit = unit, fmt = descr_fmt) "begin type(vamp_grid) :: g"
    write (unit = unit, fmt = integer_fmt) "size (g%div) = ", size (g%div)
    write (unit = unit, fmt = integer_fmt) "num_calls = ", g%num_calls
    write (unit = unit, fmt = integer_fmt) "calls_per_cell = ", g%calls_per_cell
    write (unit = unit, fmt = logical_fmt) "stratified = ", g%stratified
    write (unit = unit, fmt = logical_fmt) "all_stratified = ", g%all_stratified
    write (unit = unit, fmt = logical_fmt) "quadrupole = ", g%quadrupole
    write (unit = unit, fmt = double_fmt) "mu(1) = ", g%mu(1)
    write (unit = unit, fmt = double_fmt) "mu(2) = ", g%mu(2)
    write (unit = unit, fmt = double_fmt) "mu_plus(1) = ", g%mu_plus(1)
    write (unit = unit, fmt = double_fmt) "mu_plus(2) = ", g%mu_plus(2)
    write (unit = unit, fmt = double_fmt) "mu_minus(1) = ", g%mu_minus(1)
    write (unit = unit, fmt = double_fmt) "mu_minus(2) = ", g%mu_minus(2)
    write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
    write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
    write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
    write (unit = unit, fmt = double_fmt) "calls = ", g%calls
    write (unit = unit, fmt = double_fmt) "dv2g = ", g%dv2g
    write (unit = unit, fmt = double_fmt) "jacobi = ", g%jacobi
    write (unit = unit, fmt = double_fmt) "f_min = ", g%f_min
    write (unit = unit, fmt = double_fmt) "f_max = ", g%f_max
    write (unit = unit, fmt = double_fmt) "mu_gi = ", g%mu_gi
    write (unit = unit, fmt = double_fmt) "sum_mu_gi = ", g%sum_mu_gi
    write (unit = unit, fmt = descr_fmt) "begin g%num_div"
    do i = 1, size (g%div)
       write (unit = unit, fmt = integer_array_fmt) i, g%num_div(i)
    end do
    write (unit = unit, fmt = descr_fmt) "end g%num_div"
    write (unit = unit, fmt = descr_fmt) "begin g%div"
    do i = 1, size (g%div)
       call write_division (g%div(i), unit, write_integrals)
    end do
    write (unit = unit, fmt = descr_fmt) "end g%div"
    if (associated (g%map)) then
       write (unit = unit, fmt = descr_fmt) "begin g%map"
       do i = 1, size (g%div)
          do j = 1, size (g%div)
             write (unit = unit, fmt = double_array2_fmt) i, j, g%map(i,j)
          end do
```

```fortran
      end do
      write (unit = unit, fmt = descr_fmt) "end g%map"
   else
      write (unit = unit, fmt = descr_fmt) "empty g%map"
   end if
   if (associated (g%mu_x)) then
      write (unit = unit, fmt = descr_fmt) "begin g%mu_x"
      do i = 1, size (g%div)
         write (unit = unit, fmt = double_array_fmt) i, g%mu_x(i)
         write (unit = unit, fmt = double_array_fmt) i, g%sum_mu_x(i)
         do j = 1, size (g%div)
            write (unit = unit, fmt = double_array2_fmt) i, j, g%mu_xx(i,j)
            write (unit = unit, fmt = double_array2_fmt) i, j, g%sum_mu_xx(i,j)
         end do
      end do
      write (unit = unit, fmt = descr_fmt) "end g%mu_x"
   else
      write (unit = unit, fmt = descr_fmt) "empty g%mu_x"
   end if
   write (unit = unit, fmt = descr_fmt) "end type(vamp_grid)"
end subroutine write_grid_unit
```

146a ⟨*Variables in* vamp 79a⟩+≡   (75b) ◁110a
```fortran
character(len=*), parameter, private :: &
    descr_fmt =         "(1x,a)", &
    integer_fmt =       "(1x,a17,1x,i15)", &
    integer_array_fmt = "(1x,i17,1x,i15)", &
    logical_fmt =       "(1x,a17,1x,l1)", &
    double_fmt =        "(1x,a17,1x,e30.22e4)", &
    double_array_fmt =  "(1x,i17,1x,e30.22e4)", &
    double_array2_fmt =  "(2(1x,i8),1x,e30.22e4)"
```

146b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁144d 149a▷
```fortran
subroutine read_grid_unit (g, unit, read_integrals)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: unit
  logical, intent(in), optional :: read_integrals
  character(len=*), parameter :: FN = "vamp_read_grid"
  character(len=80) :: chdum
  integer :: ndim, i, j, idum, jdum
  read (unit = unit, fmt = descr_fmt) chdum
  read (unit = unit, fmt = integer_fmt) chdum, ndim
  ⟨Insure that size (g%div) == ndim 148a⟩
  call create_array_pointer (g%num_div, ndim)
  read (unit = unit, fmt = integer_fmt) chdum, g%num_calls
```

```fortran
read (unit = unit, fmt = integer_fmt) chdum, g%calls_per_cell
read (unit = unit, fmt = logical_fmt) chdum, g%stratified
read (unit = unit, fmt = logical_fmt) chdum, g%all_stratified
read (unit = unit, fmt = logical_fmt) chdum, g%quadrupole
read (unit = unit, fmt = double_fmt) chdum, g%mu(1)
read (unit = unit, fmt = double_fmt) chdum, g%mu(2)
read (unit = unit, fmt = double_fmt) chdum, g%mu_plus(1)
read (unit = unit, fmt = double_fmt) chdum, g%mu_plus(2)
read (unit = unit, fmt = double_fmt) chdum, g%mu_minus(1)
read (unit = unit, fmt = double_fmt) chdum, g%mu_minus(2)
read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
read (unit = unit, fmt = double_fmt) chdum, g%calls
read (unit = unit, fmt = double_fmt) chdum, g%dv2g
read (unit = unit, fmt = double_fmt) chdum, g%jacobi
read (unit = unit, fmt = double_fmt) chdum, g%f_min
read (unit = unit, fmt = double_fmt) chdum, g%f_max
read (unit = unit, fmt = double_fmt) chdum, g%mu_gi
read (unit = unit, fmt = double_fmt) chdum, g%sum_mu_gi
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
   read (unit = unit, fmt = integer_array_fmt) idum, g%num_div(i)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
   call read_division (g%div(i), unit, read_integrals)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
if (chdum == "begin g%map") then
   call create_array_pointer (g%map, (/ ndim, ndim /))
   do i = 1, size (g%div)
      do j = 1, size (g%div)
         read (unit = unit, fmt = double_array2_fmt) idum, jdum, g%map(i,j)
      end do
   end do
   read (unit = unit, fmt = descr_fmt) chdum
else
   ⟨*Insure that* associated (g%map) == .false. 148b⟩
end if
read (unit = unit, fmt = descr_fmt) chdum
```

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```
      if (chdum == "begin g%mu_x") then
          call create_array_pointer (g%mu_x, ndim )
          call create_array_pointer (g%sum_mu_x, ndim)
          call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
          call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
          do i = 1, size (g%div)
             read (unit = unit, fmt = double_array_fmt) idum, jdum, g%mu_x(i)
             read (unit = unit, fmt = double_array_fmt) idum, jdum, g%sum_mu_x(i)
             do j = 1, size (g%div)
                read (unit = unit, fmt = double_array2_fmt) &
                     idum, jdum, g%mu_xx(i,j)
                read (unit = unit, fmt = double_array2_fmt) &
                     idum, jdum, g%sum_mu_xx(i,j)
             end do
          end do
          read (unit = unit, fmt = descr_fmt) chdum
        else
          ⟨Insure that associated (g%mu_x) == .false. 148c⟩
        end if
        read (unit = unit, fmt = descr_fmt) chdum
      end subroutine read_grid_unit
```

148a ⟨*Insure that* `size (g%div) == ndim` 148a⟩≡   (146b 153b 160b)
```
      if (associated (g%div)) then
        if (size (g%div) /= ndim) then
          call delete_division (g%div)
          deallocate (g%div)
          allocate (g%div(ndim))
          call create_empty_division (g%div)
        end if
      else
        allocate (g%div(ndim))
        call create_empty_division (g%div)
      end if
```

148b ⟨*Insure that* `associated (g%map) == .false.` 148b⟩≡   (146b 153b 160b)
```
      if (associated (g%map)) then
        deallocate (g%map)
      end if
```

148c ⟨*Insure that* `associated (g%mu_x) == .false.` 148c⟩≡   (146b 153b 160b)
```
      if (associated (g%mu_x)) then
        deallocate (g%mu_x)
      end if
      if (associated (g%mu_xx)) then
```

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```
          deallocate (g%mu_xx)
        end if
        if (associated (g%sum_mu_x)) then
           deallocate (g%sum_mu_x)
        end if
        if (associated (g%sum_mu_xx)) then
           deallocate (g%sum_mu_xx)
        end if
```

149a   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁146b 149b▷
```
      subroutine write_grid_name (g, name, write_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: write_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", file = name)
        call write_grid_unit (g, unit, write_integrals)
        close (unit = unit)
      end subroutine write_grid_name
```

149b   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁149a 149c▷
```
      subroutine read_grid_name (g, name, read_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: read_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", file = name)
        call read_grid_unit (g, unit, read_integrals)
        close (unit = unit)
      end subroutine read_grid_name
```

149c   ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁149b 150▷
```
      subroutine write_grids_unit (g, unit, write_integrals)
        type(vamp_grids), intent(in) :: g
        integer, intent(in) :: unit
        logical, intent(in), optional :: write_integrals
        integer :: i
        write (unit = unit, fmt = descr_fmt) "begin type(vamp_grids) :: g"
        write (unit = unit, fmt = integer_fmt) "size (g%grids) = ", size (g%grids)
        write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
        write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
        write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
        write (unit = unit, fmt = descr_fmt) "begin g%weights"
```

```
          do i = 1, size (g%grids)
             write (unit = unit, fmt = double_array_fmt) i, g%weights(i)
          end do
          write (unit = unit, fmt = descr_fmt) "end g%weights"
          write (unit = unit, fmt = descr_fmt) "begin g%num_calls"
          do i = 1, size (g%grids)
             write (unit = unit, fmt = integer_array_fmt) i, g%num_calls(i)
          end do
          write (unit = unit, fmt = descr_fmt) "end g%num_calls"
          write (unit = unit, fmt = descr_fmt) "begin g%grids"
          do i = 1, size (g%grids)
             call write_grid_unit (g%grids(i), unit, write_integrals)
          end do
          write (unit = unit, fmt = descr_fmt) "end g%grids"
          write (unit = unit, fmt = descr_fmt) "end type(vamp_grids)"
       end subroutine write_grids_unit
```

150 ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁149c 151a▷

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

```
      end do
      read (unit = unit, fmt = descr_fmt) chdum
      read (unit = unit, fmt = descr_fmt) chdum
      do i = 1, nch
         read (unit = unit, fmt = integer_array_fmt) idum, g%num_calls(i)
      end do
      read (unit = unit, fmt = descr_fmt) chdum
      read (unit = unit, fmt = descr_fmt) chdum
      do i = 1, nch
         call read_grid_unit (g%grids(i), unit, read_integrals)
      end do
      read (unit = unit, fmt = descr_fmt) chdum
      read (unit = unit, fmt = descr_fmt) chdum
    end subroutine read_grids_unit
```

151a ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁150 151b▷
```
    subroutine write_grids_name (g, name, write_integrals)
      type(vamp_grids), intent(inout) :: g
      character(len=*), intent(in) :: name
      logical, intent(in), optional :: write_integrals
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "write", status = "replace", file = name)
      call write_grids_unit (g, unit, write_integrals)
      close (unit = unit)
    end subroutine write_grids_name
```

151b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁151a 151c▷
```
    subroutine read_grids_name (g, name, read_integrals)
      type(vamp_grids), intent(inout) :: g
      character(len=*), intent(in) :: name
      logical, intent(in), optional :: read_integrals
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "read", status = "old", file = name)
      call read_grids_unit (g, unit, read_integrals)
      close (unit = unit)
    end subroutine read_grids_name
```

151c ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁151b 153b▷
```
    subroutine write_grid_raw_unit (g, unit, write_integrals)
      type(vamp_grid), intent(in) :: g
      integer, intent(in) :: unit
      logical, intent(in), optional :: write_integrals
      integer :: i, j
```

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```fortran
write (unit = unit) MAGIC_GRID_BEGIN
write (unit = unit) size (g%div)
write (unit = unit) g%num_calls
write (unit = unit) g%calls_per_cell
write (unit = unit) g%stratified
write (unit = unit) g%all_stratified
write (unit = unit) g%quadrupole
write (unit = unit) g%mu(1)
write (unit = unit) g%mu(2)
write (unit = unit) g%mu_plus(1)
write (unit = unit) g%mu_plus(2)
write (unit = unit) g%mu_minus(1)
write (unit = unit) g%mu_minus(2)
write (unit = unit) g%sum_integral
write (unit = unit) g%sum_weights
write (unit = unit) g%sum_chi2
write (unit = unit) g%calls
write (unit = unit) g%dv2g
write (unit = unit) g%jacobi
write (unit = unit) g%f_min
write (unit = unit) g%f_max
write (unit = unit) g%mu_gi
write (unit = unit) g%sum_mu_gi
do i = 1, size (g%div)
   write (unit = unit) g%num_div(i)
end do
do i = 1, size (g%div)
   call write_division_raw (g%div(i), unit, write_integrals)
end do
if (associated (g%map)) then
   write (unit = unit) MAGIC_GRID_MAP
   do i = 1, size (g%div)
      do j = 1, size (g%div)
         write (unit = unit) g%map(i,j)
      end do
   end do
else
   write (unit = unit) MAGIC_GRID_EMPTY
end if
if (associated (g%mu_x)) then
   write (unit = unit) MAGIC_GRID_MU_X
   do i = 1, size (g%div)
      write (unit = unit) g%mu_x(i)
```

```
          write (unit = unit) g%sum_mu_x(i)
          do j = 1, size (g%div)
              write (unit = unit) g%mu_xx(i,j)
              write (unit = unit) g%sum_mu_xx(i,j)
          end do
        end do
      else
        write (unit = unit) MAGIC_GRID_EMPTY
      end if
      write (unit = unit) MAGIC_GRID_END
    end subroutine write_grid_raw_unit
```

153a ⟨*Constants in* vamp 153a⟩≡   (75b) 156b▷
```
    integer, parameter, private :: MAGIC_GRID = 22222222
    integer, parameter, private :: MAGIC_GRID_BEGIN = MAGIC_GRID + 1
    integer, parameter, private :: MAGIC_GRID_END = MAGIC_GRID + 2
    integer, parameter, private :: MAGIC_GRID_EMPTY = MAGIC_GRID + 3
    integer, parameter, private :: MAGIC_GRID_MAP = MAGIC_GRID + 4
    integer, parameter, private :: MAGIC_GRID_MU_X = MAGIC_GRID + 5
```

153b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁151c 155a▷
```
    subroutine read_grid_raw_unit (g, unit, read_integrals)
      type(vamp_grid), intent(inout) :: g
      integer, intent(in) :: unit
      logical, intent(in), optional :: read_integrals
      character(len=*), parameter :: FN = "vamp_read_raw_grid"
      integer :: ndim, i, j, magic
      read (unit = unit) magic
      if (magic /= MAGIC_GRID_BEGIN) then
        print *, FN, " fatal: expecting magic ", MAGIC_GRID_BEGIN, &
                    ", found ", magic
        stop
      end if
      read (unit = unit) ndim
```
      ⟨*Insure that* size (g%div) == ndim 148a⟩
```
      call create_array_pointer (g%num_div, ndim)
      read (unit = unit) g%num_calls
      read (unit = unit) g%calls_per_cell
      read (unit = unit) g%stratified
      read (unit = unit) g%all_stratified
      read (unit = unit) g%quadrupole
      read (unit = unit) g%mu(1)
      read (unit = unit) g%mu(2)
      read (unit = unit) g%mu_plus(1)
      read (unit = unit) g%mu_plus(2)
```

```
read (unit = unit) g%mu_minus(1)
read (unit = unit) g%mu_minus(2)
read (unit = unit) g%sum_integral
read (unit = unit) g%sum_weights
read (unit = unit) g%sum_chi2
read (unit = unit) g%calls
read (unit = unit) g%dv2g
read (unit = unit) g%jacobi
read (unit = unit) g%f_min
read (unit = unit) g%f_max
read (unit = unit) g%mu_gi
read (unit = unit) g%sum_mu_gi
do i = 1, size (g%div)
   read (unit = unit) g%num_div(i)
end do
do i = 1, size (g%div)
   call read_division_raw (g%div(i), unit, read_integrals)
end do
read (unit = unit) magic
if (magic == MAGIC_GRID_MAP) then
   call create_array_pointer (g%map, (/ ndim, ndim /))
   do i = 1, size (g%div)
      do j = 1, size (g%div)
         read (unit = unit) g%map(i,j)
      end do
   end do
else if (magic == MAGIC_GRID_EMPTY) then
   ⟨Insure that associated (g%map) == .false. 148b⟩
else
   print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
               " or ", MAGIC_GRID_MAP, ", found ", magic
   stop
end if
read (unit = unit) magic
if (magic == MAGIC_GRID_MU_X) then
   call create_array_pointer (g%mu_x, ndim )
   call create_array_pointer (g%sum_mu_x, ndim)
   call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
   call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
   do i = 1, size (g%div)
      read (unit = unit) g%mu_x(i)
      read (unit = unit) g%sum_mu_x(i)
      do j = 1, size (g%div)
```

```
                  read (unit = unit) g%mu_xx(i,j)
                  read (unit = unit) g%sum_mu_xx(i,j)
               end do
            end do
         else if (magic == MAGIC_GRID_EMPTY) then
            ⟨Insure that associated (g%mu_x) == .false. 148c⟩
         else
            print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
                         " or ", MAGIC_GRID_MU_X, ", found ", magic
            stop
         end if
         read (unit = unit) magic
         if (magic /= MAGIC_GRID_END) then
            print *, FN, " fatal: expecting magic ", MAGIC_GRID_END, &
                         " found ", magic
            stop
         end if
      end subroutine read_grid_raw_unit
```

155a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁153b 155b▷
```
      subroutine write_grid_raw_name (g, name, write_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: write_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", &
              form = "unformatted", file = name)
        call write_grid_raw_unit (g, unit, write_integrals)
        close (unit = unit)
      end subroutine write_grid_raw_name
```

155b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁155a 156a▷
```
      subroutine read_grid_raw_name (g, name, read_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: read_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", &
              form = "unformatted",  file = name)
        call read_grid_raw_unit (g, unit, read_integrals)
        close (unit = unit)
      end subroutine read_grid_raw_name
```

156a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁155b 156c▷
```
  subroutine write_grids_raw_unit (g, unit, write_integrals)
    type(vamp_grids), intent(in) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    integer :: i
    write (unit = unit) MAGIC_GRIDS_BEGIN
    write (unit = unit) size (g%grids)
    write (unit = unit) g%sum_integral
    write (unit = unit) g%sum_weights
    write (unit = unit) g%sum_chi2
    do i = 1, size (g%grids)
       write (unit = unit) g%weights(i)
    end do
    do i = 1, size (g%grids)
       write (unit = unit) g%num_calls(i)
    end do
    do i = 1, size (g%grids)
       call write_grid_raw_unit (g%grids(i), unit, write_integrals)
    end do
    write (unit = unit) MAGIC_GRIDS_END
  end subroutine write_grids_raw_unit
```

156b ⟨*Constants in* `vamp` 153a⟩+≡   (75b) ◁153a
```
  integer, parameter, private :: MAGIC_GRIDS = 33333333
  integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1
  integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2
```

156c ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁156a 157a▷
```
  subroutine read_grids_raw_unit (g, unit, read_integrals)
    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: read_integrals
    character(len=*), parameter :: FN = "vamp_read_grids_raw"
    integer :: i, nch, magic
    read (unit = unit) magic
    if (magic /= MAGIC_GRIDS_BEGIN) then
       print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_BEGIN, &
                    " found ", magic
       stop
    end if
    read (unit = unit) nch
    if (associated (g%grids)) then
       if (size (g%grids) /= nch) then
          call vamp_delete_grid (g%grids)
```

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```
            deallocate (g%grids, g%weights, g%num_calls)
            allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
            call vamp_create_empty_grid (g%grids)
        end if
    else
        allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
        call vamp_create_empty_grid (g%grids)
    end if
    read (unit = unit) g%sum_integral
    read (unit = unit) g%sum_weights
    read (unit = unit) g%sum_chi2
    do i = 1, nch
        read (unit = unit) g%weights(i)
    end do
    do i = 1, nch
        read (unit = unit) g%num_calls(i)
    end do
    do i = 1, nch
        call read_grid_raw_unit (g%grids(i), unit, read_integrals)
    end do
    read (unit = unit) magic
    if (magic /= MAGIC_GRIDS_END) then
        print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_END, &
                    " found ", magic
        stop
    end if
end subroutine read_grids_raw_unit
```

157a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁156c 157b▷

```
subroutine write_grids_raw_name (g, name, write_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: write_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "write", status = "replace", &
            form = "unformatted", file = name)
    call write_grids_raw_unit (g, unit, write_integrals)
    close (unit = unit)
end subroutine write_grids_raw_name
```

157b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁157a 158b▷

```
subroutine read_grids_raw_name (g, name, read_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name
```

```
    logical, intent(in), optional :: read_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "read", status = "old", &
          form = "unformatted", file = name)
    call read_grids_raw_unit (g, unit, read_integrals)
    close (unit = unit)
  end subroutine read_grids_raw_name
```

5.2.12 Marshaling

[WK] Note: mu_plus and mu_minus not transferred (hard-coded buffer indices)!

158a ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁144a 161▷
```
    public :: vamp_marshal_grid_size, vamp_marshal_grid, vamp_unmarshal_grid
```

158b ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁157b 160a▷
```
    pure subroutine vamp_marshal_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
```

```fortran
      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_marshal_grid
```

160a   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁158b 160b▷

```
      pure subroutine vamp_marshal_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_marshal_grid_size
```

160b   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁160a 162a▷

```
      pure subroutine vamp_unmarshal_grid (g, ibuf, dbuf)
        type(vamp_grid), intent(inout) :: g
        integer, dimension(:), intent(in) :: ibuf
        real(kind=default), dimension(:), intent(in) :: dbuf
        integer :: i, iwords, dwords, iidx, didx, ndim
        g%num_calls = ibuf(1)
        g%calls_per_cell = ibuf(2)
        ndim = ibuf(3)
        g%stratified = ibuf(4) /= 0
        g%all_stratified = ibuf(5) /= 0
        g%quadrupole = ibuf(6) /= 0
        g%mu = dbuf(1:2)
        g%sum_integral = dbuf(3)
        g%sum_weights = dbuf(4)
        g%sum_chi2 = dbuf(5)
        g%calls = dbuf(6)
        g%dv2g = dbuf(7)
        g%jacobi = dbuf(8)
```

```
      g%f_min = dbuf(9)
      g%f_max = dbuf(10)
      g%mu_gi = dbuf(11)
      g%sum_mu_gi = dbuf(12)
      call copy_array_pointer (g%num_div, ibuf(7:6+ndim))
      ⟨Insure that size (g%div) == ndim 148a⟩
      iidx = 7 + ndim
      didx = 13
      do i = 1, ndim
         iwords = ibuf(iidx)
         dwords = ibuf(iidx+1)
         iidx = iidx + 2
         call unmarshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
                                  dbuf(didx:didx-1+dwords))
         iidx = iidx + iwords
         didx = didx + dwords
      end do
      if (ibuf(iidx) > 0) then
         call copy_array_pointer &
              (g%map, reshape (dbuf(didx:didx-1+ibuf(iidx)), (/ ndim, ndim /)))
         didx = didx + ibuf(iidx)
      else
         ⟨Insure that associated (g%map) == .false. 148b⟩
      end if
      iidx = iidx + 1
      if (ibuf(iidx) > 0) then
         call copy_array_pointer (g%mu_x, dbuf(didx:didx-1+ndim))
         didx = didx + ndim
         call copy_array_pointer (g%sum_mu_x, dbuf(didx:didx-1+ndim))
         didx = didx + ndim
         call copy_array_pointer &
              (g%mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
         didx = didx + ndim**2
         call copy_array_pointer &
              (g%sum_mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
         didx = didx + ndim**2
      else
         ⟨Insure that associated (g%mu_x) == .false. 148c⟩
      end if
      iidx = iidx + 1
    end subroutine vamp_unmarshal_grid
```

161 ⟨*Declaration of* vamp *procedures* 77a⟩+≡   (75b) ◁158a
```
      public :: vamp_marshal_history_size, vamp_marshal_history
```

```
          public :: vamp_unmarshal_history
```

162a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁160b 162b▷

```
        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
```

162b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁162a 163▷

```
        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
```

163 ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁162b 164▷

```
   pure subroutine vamp_unmarshal_history (h, ibuf, dbuf)
     type(vamp_history), intent(inout) :: h
     integer, dimension(:), intent(in) :: ibuf
     real(kind=default), dimension(:), intent(in) :: dbuf
     integer :: j, ndim, iidx, didx, iwords, dwords
     ndim = ibuf(1)
     h%calls = ibuf(2)
     h%stratified = ibuf(3) /= 0
     h%integral = dbuf(1)
     h%std_dev = dbuf(2)
     h%avg_integral = dbuf(3)
     h%avg_std_dev = dbuf(4)
     h%avg_chi2 = dbuf(5)
     h%f_min = dbuf(6)
     h%f_max = dbuf(7)
     if (ndim > 0) then
        if (associated (h%div)) then
           if (size (h%div) /= ndim) then
              deallocate (h%div)
              allocate (h%div(ndim))
           end if
        else
           allocate (h%div(ndim))
        end if
        iidx = 4
        didx = 8
        do j = 1, ndim
           iwords = ibuf(iidx)
```

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```
        dwords = ibuf(iidx+1)
        iidx = iidx + 2
        call unmarshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                                    dbuf(didx:didx-1+dwords))
        iidx = iidx + iwords
        didx = didx + dwords
      end do
    end if
  end subroutine vamp_unmarshal_history
```

5.2.13   Boring Copying and Deleting of Objects

164   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁163 165a▷

```
elemental subroutine vamp_copy_grid (lhs, rhs)
  type(vamp_grid), intent(inout) :: lhs
  type(vamp_grid), intent(in) :: rhs
  integer :: ndim
  ndim = size (rhs%div)
  lhs%mu = rhs%mu
  lhs%mu_plus = rhs%mu_plus
  lhs%mu_minus = rhs%mu_minus
  lhs%sum_integral = rhs%sum_integral
  lhs%sum_weights = rhs%sum_weights
  lhs%sum_chi2 = rhs%sum_chi2
  lhs%calls = rhs%calls
  lhs%num_calls = rhs%num_calls
  call copy_array_pointer (lhs%num_div, rhs%num_div)
  lhs%dv2g = rhs%dv2g
  lhs%jacobi = rhs%jacobi
  lhs%f_min = rhs%f_min
  lhs%f_max = rhs%f_max
  lhs%mu_gi = rhs%mu_gi
  lhs%sum_mu_gi = rhs%sum_mu_gi
  lhs%calls_per_cell = rhs%calls_per_cell
  lhs%stratified = rhs%stratified
  lhs%all_stratified = rhs%all_stratified
  lhs%quadrupole = rhs%quadrupole
  if (associated (lhs%div)) then
    if (size (lhs%div) /= ndim) then
      call delete_division (lhs%div)
      deallocate (lhs%div)
      allocate (lhs%div(ndim))
    end if
```

```
      else
         allocate (lhs%div(ndim))
      end if
      call copy_division (lhs%div, rhs%div)
      if (associated (rhs%map)) then
         call copy_array_pointer (lhs%map, rhs%map)
      else if (associated (lhs%map)) then
         deallocate (lhs%map)
      end if
      if (associated (rhs%mu_x)) then
         call copy_array_pointer (lhs%mu_x, rhs%mu_x)
         call copy_array_pointer (lhs%mu_xx, rhs%mu_xx)
         call copy_array_pointer (lhs%sum_mu_x, rhs%sum_mu_x)
         call copy_array_pointer (lhs%sum_mu_xx, rhs%sum_mu_xx)
      else if (associated (lhs%mu_x)) then
         deallocate (lhs%mu_x, lhs%mu_xx, lhs%sum_mu_x, lhs%sum_mu_xx)
      end if
    end subroutine vamp_copy_grid
```

165a   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁164 165b▷
```
    elemental subroutine vamp_delete_grid (g)
      type(vamp_grid), intent(inout) :: g
      if (associated (g%div)) then
         call delete_division (g%div)
         deallocate (g%div, g%num_div)
      end if
      if (associated (g%map)) then
         deallocate (g%map)
      end if
      if (associated (g%mu_x)) then
         deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
      end if
    end subroutine vamp_delete_grid
```

165b   ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁165a 166a▷
```
    elemental subroutine vamp_copy_grids (lhs, rhs)
      type(vamp_grids), intent(inout) :: lhs
      type(vamp_grids), intent(in) :: rhs
      integer :: nch
      nch = size (rhs%grids)
      lhs%sum_integral = rhs%sum_integral
      lhs%sum_chi2 = rhs%sum_chi2
      lhs%sum_weights = rhs%sum_weights
      if (associated (lhs%grids)) then
```

```
      if (size (lhs%grids) /= nch) then
         deallocate (lhs%grids)
         allocate (lhs%grids(nch))
         call vamp_create_empty_grid (lhs%grids(nch))
      end if
   else
      allocate (lhs%grids(nch))
      call vamp_create_empty_grid (lhs%grids(nch))
   end if
   call vamp_copy_grid (lhs%grids, rhs%grids)
   call copy_array_pointer (lhs%weights, rhs%weights)
   call copy_array_pointer (lhs%num_calls, rhs%num_calls)
end subroutine vamp_copy_grids
```

166a ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁165b 166b▷

```
elemental subroutine vamp_delete_grids (g)
  type(vamp_grids), intent(inout) :: g
  if (associated (g%grids)) then
     call vamp_delete_grid (g%grids)
     deallocate (g%weights, g%grids, g%num_calls)
  end if
end subroutine vamp_delete_grids
```

166b ⟨*Implementation of* `vamp` *procedures* 78b⟩+≡   (75b) ◁166a 167a▷

```
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
```

167a ⟨*Implementation of* vamp *procedures* 78b⟩+≡   (75b) ◁166b
```
          elemental subroutine vamp_delete_history (h)
            type(vamp_history), intent(inout) :: h
            if (associated (h%div)) then
               deallocate (h%div)
            end if
          end subroutine vamp_delete_history
```

5.3 Interface to MPI

The module vamp makes no specific assumptions about the hardware and
software supporting parallel execution. In this section, we present a specific
example of a parallel implementation of multi channel sampling using the
message passing paradigm.

The modules vamp_serial_mpi and vamp_parallel_mpi are not intended
to be used directly by application programs. For this purpose, the module
vampi is provided. vamp_serial_mpi is identical to vamp, but some types,
procedures and variables are renamed so that vamp_parallel_mpi can rede-
fine them:

167b ⟨vampi.f90 167b⟩≡   167c ▷
```
        ! vampi.f90 --
        ⟨Copyleft notice 1⟩
        module vamp_serial_mpi
          use vamp, &
              ⟨vamp0_* => vamp_* 168c⟩
              VAMP0_RCS_ID => VAMP_RCS_ID
          public
        end module vamp_serial_mpi
```

vamp_parallel_mpi contains the non trival MPI code and will be discussed
in detail below.

167c ⟨vampi.f90 167b⟩+≡   ◁167b 168a ▷
```
        module vamp_parallel_mpi
          use kinds
          use utils
```

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```
          use tao_random_numbers
          use exceptions
          use mpi90
          use divisions
          use vamp_serial_mpi !NODEP!
          use iso_fortran_env
          implicit none
          private
          ⟨Declaration of vampi procedures 168b⟩
          ⟨Interfaces of vampi procedures 173a⟩
          ⟨Parameters in vampi 169b⟩
          ⟨Declaration of vampi types 173d⟩
          character(len=*), public, parameter :: VAMPI_RCS_ID = &
               "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
        contains
          ⟨Implementation of vampi procedures 169a⟩
        end module vamp_parallel_mpi
```

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

168a   ⟨vampi.f90 167b⟩+≡   ◁167c
```
        module vampi
          use vamp_serial_mpi !NODEP!
          use vamp_parallel_mpi !NODEP!
          public
        end module vampi
```

5.3.1 Parallel Execution

Single Channel

168b   ⟨Declaration of vampi procedures 168b⟩≡   (167c) 172b▷
```
          public :: vamp_create_grid
          public :: vamp_discard_integral
          public :: vamp_reshape_grid
          public :: vamp_sample_grid
          public :: vamp_delete_grid
```

168c   ⟨vamp0_* => vamp_* 168c⟩≡   (167b) 172c▷
```
          vamp0_create_grid => vamp_create_grid, &
          vamp0_discard_integral => vamp_discard_integral, &
          vamp0_reshape_grid => vamp_reshape_grid, &
          vamp0_sample_grid => vamp_sample_grid, &
```

```
         vamp0_delete_grid => vamp_delete_grid, &
```

169a ⟨*Implementation of* `vampi` *procedures* 169a⟩≡   (167c) 169c ▷
```
      subroutine vamp_create_grid &
           (g, domain, num_calls, num_div, &
            stratified, quadrupole, covariance, map, exc)
        type(vamp_grid), intent(inout) :: g
        real(kind=default), dimension(:,:), intent(in) :: domain
        integer, intent(in) :: num_calls
        integer, dimension(:), intent(in), optional :: num_div
        logical, intent(in), optional :: stratified, quadrupole, covariance
        real(kind=default), dimension(:,:), intent(in), optional :: map
        type(exception), intent(inout), optional :: exc
        integer :: proc_id
        call mpi90_rank (proc_id)
        if (proc_id == VAMP_ROOT) then
           call vamp0_create_grid &
                (g, domain, num_calls, num_div, &
                 stratified, quadrupole, covariance, map, exc)
        else
           call vamp_create_empty_grid (g)
        end if
      end subroutine vamp_create_grid
```

169b ⟨*Parameters in* `vampi` 169b⟩≡   (167c) 177a ▷
```
      integer, public, parameter :: VAMP_ROOT = 0
```

169c ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁ 169a 169d ▷
```
      subroutine vamp_discard_integral &
           (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
        type(vamp_grid), intent(inout) :: g
        integer, intent(in), optional :: num_calls
        integer, dimension(:), intent(in), optional :: num_div
        logical, intent(in), optional :: stratified, quadrupole, covariance
        type(exception), intent(inout), optional :: exc
        integer :: proc_id
        call mpi90_rank (proc_id)
        if (proc_id == VAMP_ROOT) then
           call vamp0_discard_integral &
                (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
        end if
      end subroutine vamp_discard_integral
```

169d ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁ 169c 170 ▷
```
      subroutine vamp_reshape_grid &
           (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
```

```
      type(vamp_grid), intent(inout) :: g
      integer, intent(in), optional :: num_calls
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole, covariance
      type(exception), intent(inout), optional :: exc
      integer :: proc_id
      call mpi90_rank (proc_id)
      if (proc_id == VAMP_ROOT) then
         call vamp0_reshape_grid &
              (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
      end if
    end subroutine vamp_reshape_grid
```

NB: `grids` has to have `intent(inout)` because we will call `vamp_broadcast_grid` on it.

170 ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁169d 172a▷

```
    subroutine vamp_sample_grid &
         (rng, g, func, iterations, integral, std_dev, avg_chi2, accuracy, &
          channel, weights, grids, exc, history)
      type(tao_random_state), intent(inout) :: rng
      type(vamp_grid), intent(inout) :: g
      integer, intent(in) :: iterations
      real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
      real(kind=default), intent(in), optional :: accuracy
      integer, intent(in), optional :: channel
      real(kind=default), dimension(:), intent(in), optional :: weights
      type(vamp_grid), dimension(:), intent(inout), optional :: grids
      type(exception), intent(inout), optional :: exc
      type(vamp_history), dimension(:), intent(inout), optional :: history
      ⟨Interface declaration for func 22⟩
      character(len=*), parameter :: FN = "vamp_sample_grid"
      real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
      type(vamp_grid), dimension(:), allocatable :: gs, gx
      integer, dimension(:,:), pointer :: d
      integer :: iteration, i
      integer :: num_proc, proc_id, num_workers
      nullify (d)
      call mpi90_size (num_proc)
      call mpi90_rank (proc_id)
      iterate: do iteration = 1, iterations
         if (proc_id == VAMP_ROOT) then
            call vamp_distribute_work (num_proc, vamp_rigid_divisions (g), d)
            num_workers = max (1, product (d(2,:)))
         end if
```

```fortran
call mpi90_broadcast (num_workers, VAMP_ROOT)
if ((present (grids)) .and. (num_workers > 1)) then
   call vamp_broadcast_grid (grids, VAMP_ROOT)
end if
if (proc_id == VAMP_ROOT) then
   allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
   call vamp_create_empty_grid (gs)
   call vamp_fork_grid (g, gs, gx, d, exc)
   do i = 2, num_workers
      call vamp_send_grid (gs(i), i-1, 0)
   end do
else if (proc_id < num_workers) then
   call vamp_receive_grid (g, VAMP_ROOT, 0)
end if
if (proc_id == VAMP_ROOT) then
   if (num_workers > 1) then
      call vamp_sample_grid0 &
           (rng, gs(1), func, channel, weights, grids, exc)
   else
      call vamp_sample_grid0 &
           (rng, g, func, channel, weights, grids, exc)
   end if
else if (proc_id < num_workers) then
   call vamp_sample_grid0 &
        (rng, g, func, channel, weights, grids, exc)
end if
if (proc_id == VAMP_ROOT) then
   do i = 2, num_workers
      call vamp_receive_grid (gs(i), i-1, 0)
   end do
   call vamp_join_grid (g, gs, gx, d, exc)
   call vamp0_delete_grid (gs)
   deallocate (gs, gx)
   call vamp_refine_grid (g)
   call vamp_average_iterations &
        (g, iteration, local_integral, local_std_dev, local_avg_chi2)
   if (present (history)) then
      if (iteration <= size (history)) then
         call vamp_get_history &
              (history(iteration), g, &
               local_integral, local_std_dev, local_avg_chi2)
      else
         call raise_exception (exc, EXC_WARN, FN, "history too short")
```

```
                    end if
                    call vamp_terminate_history (history(iteration+1:))
                end if
                if (present (accuracy)) then
                    if (local_std_dev <= accuracy * local_integral) then
                        call raise_exception (exc, EXC_INFO, FN, &
                            "requested accuracy reached")
                        exit iterate
                    end if
                end if
            else if (proc_id < num_workers) then
                call vamp_send_grid (g, VAMP_ROOT, 0)
            end if
        end do iterate
        if (proc_id == VAMP_ROOT) then
            deallocate (d)
            if (present (integral)) then
                integral = local_integral
            end if
            if (present (std_dev)) then
                std_dev = local_std_dev
            end if
            if (present (avg_chi2)) then
                avg_chi2 = local_avg_chi2
            end if
        end if
    end subroutine vamp_sample_grid
```

172a   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁170 173b▷

```
    subroutine vamp_delete_grid (g)
        type(vamp_grid), intent(inout) :: g
        integer :: proc_id
        call mpi90_rank (proc_id)
        if (proc_id == VAMP_ROOT) then
            call vamp0_reshape_grid (g)
        end if
    end subroutine vamp_delete_grid
```

172b   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c) ◁168b 173f▷

```
    public :: vamp_print_history
    private :: vamp_print_one_history, vamp_print_histories
```

172c   ⟨`vamp0_* => vamp_*` 168c⟩+≡   (167b) ◁168c 173e▷

```
    vamp0_print_history => vamp_print_history, &
```

173a   ⟨*Interfaces of* `vampi` *procedures* 173a⟩≡   (167c)   182c ▷

```
interface vamp_print_history
   module procedure vamp_print_one_history, vamp_print_histories
end interface
```

173b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c)   ◁172a   173c ▷

```
subroutine vamp_print_one_history (h, tag)
  type(vamp_history), dimension(:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_print_history (h, tag)
  end if
end subroutine vamp_print_one_history
```

173c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c)   ◁173b   174b ▷

```
subroutine vamp_print_histories (h, tag)
  type(vamp_history), dimension(:,:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_print_history (h, tag)
  end if
end subroutine vamp_print_histories
```

Multi Channel

173d   ⟨*Declaration of* `vampi` *types* 173d⟩≡   (167c)

```
type, public :: vamp_grids
   !!! private
   type(vamp0_grids) :: g0
   logical, dimension(:), pointer :: active
   integer, dimension(:), pointer :: proc
   real(kind=default), dimension(:), pointer :: integrals, std_devs
end type vamp_grids
```

173e   ⟨`vamp0_*` => `vamp_*` 168c⟩+≡   (167b)   ◁172c   174a ▷

```
vamp0_grids => vamp_grids, &
```

Partially duplicate the API of `vamp`:

173f   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c)   ◁172b   179c ▷

```
public :: vamp_create_grids
public :: vamp_discard_integrals
```

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

174a   ⟨vamp0_* => vamp_* 168c⟩+≡   (167b) ◁173e 182b▷
```
          vamp0_create_grids => vamp_create_grids, &
          vamp0_discard_integrals => vamp_discard_integrals, &
          vamp0_update_weights => vamp_update_weights, &
          vamp0_refine_weights => vamp_refine_weights, &
          vamp0_delete_grids => vamp_delete_grids, &
          vamp0_sample_grids => vamp_sample_grids, &
```

Call `vamp_create_grids` just like the serial version. It will create the actual
grids on the root processor and create stubs on the other processors

174b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁173c 174c▷
```
          subroutine vamp_create_grids (g, domain, num_calls, weights, maps, &
                                      num_div, stratified, quadrupole, exc)
            type(vamp_grids), intent(inout) :: g
            real(kind=default), dimension(:,:), intent(in) :: domain
            integer, intent(in) :: num_calls
            real(kind=default), dimension(:), intent(in) :: weights
            real(kind=default), dimension(:,:,:), intent(in), optional :: maps
            integer, dimension(:), intent(in), optional :: num_div
            logical, intent(in), optional :: stratified, quadrupole
            type(exception), intent(inout), optional :: exc
            integer :: proc_id, nch
            call mpi90_rank (proc_id)
            nch = size (weights)
            allocate (g%active(nch), g%proc(nch), g%integrals(nch), g%std_devs(nch))
            if (proc_id == VAMP_ROOT) then
               call vamp0_create_grids (g%g0, domain, num_calls, weights, maps, &
                                      num_div, stratified, quadrupole, exc)
            else
               allocate (g%g0%grids(nch), g%g0%weights(nch), g%g0%num_calls(nch))
               call vamp_create_empty_grid (g%g0%grids)
            end if
          end subroutine vamp_create_grids
```

174c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁174b 175a▷
```
          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
```

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```
      logical, intent(in), optional :: stratified, quadrupole
      type(exception), intent(inout), optional :: exc
      integer :: proc_id
      call mpi90_rank (proc_id)
      if (proc_id == VAMP_ROOT) then
         call vamp0_discard_integrals &
              (g%g0, num_calls, num_div, stratified, quadrupole, exc)
      end if
   end subroutine vamp_discard_integrals
```

175a   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁174c 175b▷
```
   subroutine vamp_update_weights &
        (g, weights, num_calls, num_div, stratified, quadrupole, exc)
      type(vamp_grids), intent(inout) :: g
      real(kind=default), dimension(:), intent(in) :: weights
      integer, intent(in), optional :: num_calls
      integer, dimension(:), intent(in), optional :: num_div
      logical, intent(in), optional :: stratified, quadrupole
      type(exception), intent(inout), optional :: exc
      integer :: proc_id
      call mpi90_rank (proc_id)
      if (proc_id == VAMP_ROOT) then
         call vamp0_update_weights &
              (g%g0, weights, num_calls, num_div, stratified, quadrupole, exc)
      end if
   end subroutine vamp_update_weights
```

175b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁175a 175c▷
```
   subroutine vamp_refine_weights (g, power)
      type(vamp_grids), intent(inout) :: g
      real(kind=default), intent(in), optional :: power
      integer :: proc_id
      call mpi90_rank (proc_id)
      if (proc_id == VAMP_ROOT) then
         call vamp0_refine_weights (g%g0, power)
      end if
   end subroutine vamp_refine_weights
```

175c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁175b 176▷
```
   subroutine vamp_delete_grids (g)
      type(vamp_grids), intent(inout) :: g
      character(len=*), parameter :: FN = "vamp_delete_grids"
      deallocate (g%active, g%proc, g%integrals, g%std_devs)
      call vamp0_delete_grids (g%g0)
   end subroutine vamp_delete_grids
```

Call `vamp_sample_grids` just like `vamp0_sample_grids`.

176 ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁175c 179d▷

```
subroutine vamp_sample_grids &
     (rng, g, func, iterations, integral, std_dev, avg_chi2, &
      accuracy, history, histories, exc)
type(tao_random_state), intent(inout) :: rng
type(vamp_grids), intent(inout) :: g
integer, intent(in) :: iterations
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
real(kind=default), intent(in), optional :: accuracy
type(vamp_history), dimension(:), intent(inout), optional :: history
type(vamp_history), dimension(:,:), intent(inout), optional :: histories
type(exception), intent(inout), optional :: exc
```
⟨*Interface declaration for* `func` 22⟩
```
character(len=*), parameter :: FN = "vamp_sample_grids"
integer :: num_proc, proc_id, nch, ch, iteration
real(kind=default), dimension(size(g%g0%weights)) :: weights
real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
real(kind=default) :: current_accuracy, waste
logical :: distribute_complete_grids
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
nch = size (g%g0%weights)
if (proc_id == VAMP_ROOT) then
   g%active = (g%g0%num_calls >= 2)
   where (g%active)
      weights = g%g0%num_calls
   elsewhere
      weights = 0.0
   endwhere
   weights = weights / sum (weights)
   call schedule (weights, num_proc, g%proc, waste)
   distribute_complete_grids = (waste <= VAMP_MAX_WASTE)
end if
call mpi90_broadcast (weights, VAMP_ROOT)
call mpi90_broadcast (g%active, VAMP_ROOT)
call mpi90_broadcast (distribute_complete_grids, VAMP_ROOT)
if (distribute_complete_grids) then
   call mpi90_broadcast (g%proc, VAMP_ROOT)
end if
iterate: do iteration = 1, iterations
   if (distribute_complete_grids) then
      call vamp_broadcast_grid (g%g0%grids, VAMP_ROOT)
```

```
        ⟨Distribute complete grids among processes 177b⟩
        else
            ⟨Distribute each grid among processes 181b⟩
        end if
        ⟨Exit iterate if accuracy has been reached (MPI) 180a⟩
    end do iterate
    ⟨Copy results of vamp_sample_grids to dummy variables 179f⟩
  end subroutine vamp_sample_grids
```

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

177a ⟨*Parameters in* `vampi` 169b⟩+≡   (167c) ◁169b 179e▷
```
  real(kind=default), private, parameter :: VAMP_MAX_WASTE = 1.0
  ! real(kind=default), private, parameter :: VAMP_MAX_WASTE = 0.3
```

177b ⟨*Distribute complete grids among processes* 177b⟩≡   (176) 177c▷
```
  do ch = 1, nch
     if (g%active(ch)) then
        if (proc_id == g%proc(ch)) then
           call vamp0_discard_integral (g%g0%grids(ch))
           ⟨Sample g%g0%grids(ch) 177d⟩
        end if
     else
        call vamp_nullify_variance (g%g0%grids(ch))
        call vamp_nullify_covariance (g%g0%grids(ch))
     end if
  end do
```

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

177c ⟨*Distribute complete grids among processes* 177b⟩+≡   (176) ◁177b 178a▷
```
  do ch = 1, nch
     if (g%active(ch) .and. (proc_id == g%proc(ch))) then
        call vamp_refine_grid (g%g0%grids(ch))
        if (proc_id /= VAMP_ROOT) then
           ⟨Ship the result for channel #ch back to the root 179a⟩
        end if
     end if
  end do
```

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

177d ⟨*Sample* `g%g0%grids(ch)` 177d⟩≡   (177b)
```
  call vamp_sample_grid0 &
       (rng, g%g0%grids(ch), func, ch, weights, g%g0%grids, exc)
  call vamp_average_iterations &
       (g%g0%grids(ch), iteration, g%integrals(ch), g%std_devs(ch), local_avg_chi2)
```

```
      if (present (histories)) then
         if (iteration <= ubound (histories, dim=1)) then
            call vamp_get_history &
                 (histories(iteration,ch), g%g0%grids(ch), &
                  g%integrals(ch), g%std_devs(ch), local_avg_chi2)
         else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
         end if
         call vamp_terminate_history (histories(iteration+1:,ch))
      end if
```

178a   ⟨*Distribute complete grids among processes* 177b⟩+≡   (176) ◁177c
```
   if (proc_id == VAMP_ROOT) then
      do ch = 1, nch
         if (g%active(ch) .and. (g%proc(ch) /= proc_id)) then
            ⟨Receive the result for channel #ch at the root 179b⟩
         end if
      end do
      call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
      call vamp_average_iterations &
           (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
      if (present (history)) then
         if (iteration <= size (history)) then
            call vamp_get_history &
                 (history(iteration), g%g0, local_integral, local_std_dev, &
                  local_avg_chi2)
         else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
         end if
         call vamp_terminate_history (history(iteration+1:))
      end if
   end if
```

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

178b   ⟨*Ship* g%g0%grids *from the root to the assigned processor* 178b⟩≡
```
   do ch = 1, nch
      if (g%active(ch) .and. (g%proc(ch) /= VAMP_ROOT)) then
         if (proc_id == VAMP_ROOT) then
            call vamp_send_grid &
                 (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
         else if (proc_id == g%proc(ch)) then
            call vamp_receive_grid &
                 (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
```

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```

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

179a ⟨*Ship the result for channel #*ch *back to the root* 179a⟩≡   (177c)
```
      call mpi90_send (g%integrals(ch), VAMP_ROOT, object (ch, TAG_INTEGRAL))
      call mpi90_send (g%std_devs(ch), VAMP_ROOT, object (ch, TAG_STD_DEV))
      call vamp_send_grid (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
      if (present (histories)) then
        call vamp_send_history &
             (histories(iteration,ch), VAMP_ROOT, object (ch, TAG_HISTORY))
      end if
```

179b ⟨*Receive the result for channel #*ch *at the root* 179b⟩≡   (178a)
```
      call mpi90_receive (g%integrals(ch), g%proc(ch), object (ch, TAG_INTEGRAL))
      call mpi90_receive (g%std_devs(ch), g%proc(ch), object (ch, TAG_STD_DEV))
      call vamp_receive_grid (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
      if (present (histories)) then
        call vamp_receive_history &
             (histories(iteration,ch), g%proc(ch), object (ch, TAG_HISTORY))
      end if
```

179c ⟨*Declaration of* vampi *procedures* 168b⟩+≡   (167c) ◁173f 180b▷
```
      private :: object
```

179d ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁176 180c▷
```
      pure function object (ch, obj) result (tag)
        integer, intent(in) :: ch, obj
        integer :: tag
        tag = 100 * ch + obj
      end function object
```

179e ⟨*Parameters in* vampi 169b⟩+≡   (167c) ◁177a
```
      integer, public, parameter :: &
           TAG_INTEGRAL = 1, &
           TAG_STD_DEV = 2, &
           TAG_GRID = 3, &
           TAG_HISTORY = 6, &
           TAG_NEXT_FREE = 9
```

179f ⟨*Copy results of* vamp_sample_grids *to dummy variables* 179f⟩≡   (176)
```
      if (present (integral)) then
        call mpi90_broadcast (local_integral, VAMP_ROOT)
        integral = local_integral
      end if
      if (present (std_dev)) then
        call mpi90_broadcast (local_std_dev, VAMP_ROOT)
```

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```
          std_dev = local_std_dev
       end if
       if (present (avg_chi2)) then
          call mpi90_broadcast (local_avg_chi2, VAMP_ROOT)
          avg_chi2 = local_avg_chi2
       end if
```

180a   ⟨*Exit* `iterate` *if* `accuracy` *has been reached (MPI)* 180a⟩≡   (176)
```
       if (present (accuracy)) then
          if (proc_id == VAMP_ROOT) then
             current_accuracy = local_std_dev / local_integral
          end if
          call mpi90_broadcast (current_accuracy, VAMP_ROOT)
          if (current_accuracy <= accuracy) then
             call raise_exception (exc, EXC_INFO, FN, &
                   "requested accuracy reached")
             exit iterate
          end if
       end if
```

A very simple minded scheduler: maximizes processor utilization and, does
not pay attention to communication costs.

180b   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c) ◁179c 182a▷
```
       private :: schedule
```

We disfavor the root process a little bit (by starting up with a fake filling
ratio of 10%) so that it is likely to be ready to answer all communication
requests.

180c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁179d 182d▷
```
       pure subroutine schedule (jobs, num_procs, assign, waste)
         real(kind=default), dimension(:), intent(in) :: jobs
         integer, intent(in) :: num_procs
         integer, dimension(:), intent(out) :: assign
         real(kind=default), intent(out), optional :: waste
         integer, dimension(size(jobs)) :: idx
         real(kind=default), dimension(size(jobs)) :: sjobs
         real(kind=default), dimension(num_procs) :: fill
         integer :: job, proc
         sjobs = jobs / sum (jobs) * num_procs
         idx = (/ (job, job = 1, size(jobs)) /)
         call sort (sjobs, idx, reverse = .true.)
         fill = 0.0
         fill(VAMP_ROOT+1) = 0.1
         do job = 1, size (sjobs)
            proc = sum (minloc (fill))
```

```
         fill(proc) = fill(proc) + sjobs(job)
         assign(idx(job)) = proc - 1
      end do
      ⟨Estimate waste of processor time 181a⟩
   end subroutine schedule
```

Assuming equivalent processors and uniform computation costs, the waste is given by the fraction of the time that it spent by the other processors waiting for the processor with the biggest assigment:

181a ⟨*Estimate* `waste` *of processor time* 181a⟩≡   (180c)
```
   if (present (waste)) then
      waste = 1.0 - sum (fill) / (num_procs * maxval (fill))
   end if
```

Accordingly, if the waste caused by distributing only complete grids, we switch to splitting the grids, just like in single channel sampling. This is *not* the default, because the communication costs are measurably higher for many grids and many processors.

This version is broken!

181b ⟨*Distribute each grid among processes* 181b⟩≡   (176)
```
   do ch = 1, size (g%g0%grids)
      if (g%active(ch)) then
         call vamp_discard_integral (g%g0%grids(ch))
         if (present (histories)) then
            call vamp_sample_grid &
                  (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
                   channel = ch, weights = weights, grids = g%g0%grids, &
                   history = histories(iteration:iteration,ch))
         else
            call vamp_sample_grid &
                  (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
                   channel = ch, weights = weights, grids = g%g0%grids)
         end if
      else
         if (proc_id == VAMP_ROOT) then
            call vamp_nullify_variance (g%g0%grids(ch))
            call vamp_nullify_covariance (g%g0%grids(ch))
         end if
      end if
   end do
   if (proc_id == VAMP_ROOT) then
      call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
      call vamp_average_iterations &
```

```
                (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
        if (present (history)) then
           if (iteration <= size (history)) then
              call vamp_get_history &
                    (history(iteration), g%g0, local_integral, local_std_dev, &
                     local_avg_chi2)
           else
              call raise_exception (exc, EXC_WARN, FN, "history too short")
           end if
           call vamp_terminate_history (history(iteration+1:))
        end if
     end if
```

5.3.2   Event Generation

This is currently only a syntacical translation . . .

182a   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c)   ◁180b 184a▷
```
  public :: vamp_warmup_grid
  public :: vamp_warmup_grids
  public :: vamp_next_event
  private :: vamp_next_event_single, vamp_next_event_multi
```

182b   ⟨`vamp0_* => vamp_*` 168c⟩+≡   (167b)   ◁174a 184b▷
```
  vamp0_warmup_grid => vamp_warmup_grid, &
  vamp0_warmup_grids => vamp_warmup_grids, &
  vamp0_next_event => vamp_next_event, &
```

182c   ⟨*Interfaces of* `vampi` *procedures* 173a⟩+≡   (167c)   ◁173a 184c▷
```
  interface vamp_next_event
     module procedure vamp_next_event_single, vamp_next_event_multi
  end interface
```

182d   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c)   ◁180c 183a▷
```
  subroutine vamp_next_event_single &
       (x, rng, g, func, weight, channel, weights, grids, exc)
    real(kind=default), dimension(:), intent(out) :: x
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    real(kind=default), intent(out), optional :: weight
    integer, intent(in), optional :: channel
    real(kind=default), dimension(:), intent(in), optional :: weights
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    type(exception), intent(inout), optional :: exc
```
⟨*Interface declaration for* `func` 22⟩

```
          integer :: proc_id
          call mpi90_rank (proc_id)
          if (proc_id == VAMP_ROOT) then
             call vamp0_next_event &
                    (x, rng, g, func, weight, channel, weights, grids, exc)
          end if
        end subroutine vamp_next_event_single
```

183a ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁182d 183b▷
```
        subroutine vamp_next_event_multi (x, rng, g, func, phi, weight, exc)
          real(kind=default), dimension(:), intent(out) :: x
          type(tao_random_state), intent(inout) :: rng
          type(vamp_grids), intent(inout) :: g
          real(kind=default), intent(out), optional :: weight
          type(exception), intent(inout), optional :: exc
```
          ⟨*Interface declaration for* func 22⟩
          ⟨*Interface declaration for* phi 31a⟩
```
          integer :: proc_id
          call mpi90_rank (proc_id)
          if (proc_id == VAMP_ROOT) then
             call vamp0_next_event (x, rng, g%g0, func, phi, weight, exc)
          end if
        end subroutine vamp_next_event_multi
```

183b ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁183a 183c▷
```
        subroutine vamp_warmup_grid (rng, g, func, iterations, exc, history)
          type(tao_random_state), intent(inout) :: rng
          type(vamp_grid), intent(inout) :: g
          integer, intent(in) :: iterations
          type(exception), intent(inout), optional :: exc
          type(vamp_history), dimension(:), intent(inout), optional :: history
```
          ⟨*Interface declaration for* func 22⟩
```
          call vamp_sample_grid &
             (rng, g, func, iterations - 1, exc = exc, history = history)
          call vamp_sample_grid0 (rng, g, func, exc = exc)
        end subroutine vamp_warmup_grid
```

183c ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁183b 184d▷
```
        subroutine vamp_warmup_grids &
             (rng, g, func, iterations, history, histories, exc)
          type(tao_random_state), intent(inout) :: rng
          type(vamp_grids), intent(inout) :: g
          integer, intent(in) :: iterations
          type(vamp_history), dimension(:), intent(inout), optional :: history
          type(vamp_history), dimension(:,:), intent(inout), optional :: histories
```

```
       type(exception), intent(inout), optional :: exc
       ⟨Interface declaration for func 22⟩
       integer :: ch
       call vamp0_sample_grids (rng, g%g0, func, iterations - 1, exc = exc, &
                                history = history, histories = histories)
       do ch = 1, size (g%g0%grids)
          ! if (g%g0%grids(ch)%num_calls >= 2) then
             call vamp_sample_grid0 (rng, g%g0%grids(ch), func, exc = exc)
          ! end if
       end do
     end subroutine vamp_warmup_grids
```

5.3.3   I/O

184a   ⟨*Declaration of* vampi *procedures* 168b⟩+≡   (167c) ◁182a 185c▷
```
       public :: vamp_write_grid, vamp_read_grid
       private :: write_grid_unit, write_grid_name
       private :: read_grid_unit, read_grid_name
```

184b   ⟨vamp0_* => vamp_* 168c⟩+≡   (167b) ◁182b 185d▷
```
       vamp0_write_grid => vamp_write_grid, &
       vamp0_read_grid => vamp_read_grid, &
```

184c   ⟨*Interfaces of* vampi *procedures* 173a⟩+≡   (167c) ◁182c 185e▷
```
       interface vamp_write_grid
          module procedure write_grid_unit, write_grid_name
       end interface
       interface vamp_read_grid
          module procedure read_grid_unit, read_grid_name
       end interface
```

184d   ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁183c 184e▷
```
       subroutine write_grid_unit (g, unit)
         type(vamp_grid), intent(in) :: g
         integer, intent(in) :: unit
         integer :: proc_id
         call mpi90_rank (proc_id)
         if (proc_id == VAMP_ROOT) then
            call vamp0_write_grid (g, unit)
         end if
       end subroutine write_grid_unit
```

184e   ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁184d 185a▷
```
       subroutine read_grid_unit (g, unit)
         type(vamp_grid), intent(inout) :: g
```

```
            integer, intent(in) :: unit
            integer :: proc_id
            call mpi90_rank (proc_id)
            if (proc_id == VAMP_ROOT) then
               call vamp0_read_grid (g, unit)
            end if
          end subroutine read_grid_unit
```

185a ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁184e 185b▷
```
          subroutine write_grid_name (g, name)
            type(vamp_grid), intent(inout) :: g
            character(len=*), intent(in) :: name
            integer :: proc_id
            call mpi90_rank (proc_id)
            if (proc_id == VAMP_ROOT) then
               call vamp0_write_grid (g, name)
            end if
          end subroutine write_grid_name
```

185b ⟨*Implementation of* vampi *procedures* 169a⟩+≡   (167c) ◁185a 186a▷
```
          subroutine read_grid_name (g, name)
            type(vamp_grid), intent(inout) :: g
            character(len=*), intent(in) :: name
            integer :: proc_id
            call mpi90_rank (proc_id)
            if (proc_id == VAMP_ROOT) then
               call vamp0_read_grid (g, name)
            end if
          end subroutine read_grid_name
```

185c ⟨*Declaration of* vampi *procedures* 168b⟩+≡   (167c) ◁184a 187a▷
```
          public :: vamp_write_grids, vamp_read_grids
          private :: write_grids_unit, write_grids_name
          private :: read_grids_unit, read_grids_name
```

185d ⟨vamp0_* => vamp_* 168c⟩+≡   (167b) ◁184b
```
          vamp0_write_grids => vamp_write_grids, &
          vamp0_read_grids => vamp_read_grids, &
```

185e ⟨*Interfaces of* vampi *procedures* 173a⟩+≡   (167c) ◁184c 189a▷
```
          interface vamp_write_grids
             module procedure write_grids_unit, write_grids_name
          end interface
          interface vamp_read_grids
             module procedure read_grids_unit, read_grids_name
          end interface
```

186a   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁185b 186b▷

```fortran
subroutine write_grids_unit (g, unit)
  type(vamp_grids), intent(in) :: g
  integer, intent(in) :: unit
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_write_grids (g%g0, unit)
  end if
end subroutine write_grids_unit
```

186b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁186a 186c▷

```fortran
subroutine read_grids_unit (g, unit)
  type(vamp_grids), intent(inout) :: g
  integer, intent(in) :: unit
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_read_grids (g%g0, unit)
  end if
end subroutine read_grids_unit
```

186c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁186b 186d▷

```fortran
subroutine write_grids_name (g, name)
  type(vamp_grids), intent(inout) :: g
  character(len=*), intent(in) :: name
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_write_grids (g%g0, name)
  end if
end subroutine write_grids_name
```

186d   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁186c 187b▷

```fortran
subroutine read_grids_name (g, name)
  type(vamp_grids), intent(inout) :: g
  character(len=*), intent(in) :: name
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
     call vamp0_read_grids (g%g0, name)
  end if
```

```
      end subroutine read_grids_name
```

5.3.4   Communicating Grids

187a   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c) ◁185c 191a▷
```
      public :: vamp_send_grid
      public :: vamp_receive_grid
      public :: vamp_broadcast_grid
      public :: vamp_broadcast_grids
```

⟨⚠⟩ The next two are still kludged. Nicer implementations with one message
less per call below, but MPICH does funny things during `mpi_get_count`,
which is called by `mpi90_receive_pointer`.

Caveat: this `vamp_send_grid` uses *three* tags: `tag`, `tag+1` and `tag+2`:

187b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁186d 187c▷
```
      subroutine vamp_send_grid (g, target, tag, domain, error)
        type(vamp_grid), intent(in) :: g
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(2) :: words
        integer, dimension(:), allocatable :: ibuf
        real(kind=default), dimension(:), allocatable :: dbuf
        call vamp_marshal_grid_size (g, words(1), words(2))
        allocate (ibuf(words(1)), dbuf(words(2)))
        call vamp_marshal_grid (g, ibuf, dbuf)
        call mpi90_send (words, target, tag, domain, error)
        call mpi90_send (ibuf, target, tag+1, domain, error)
        call mpi90_send (dbuf, target, tag+2, domain, error)
        deallocate (ibuf, dbuf)
      end subroutine vamp_send_grid
```

187c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁187b 189b▷
```
      subroutine vamp_receive_grid (g, source, tag, domain, status, error)
        type(vamp_grid), intent(inout) :: g
        integer, intent(in) :: source, tag
        integer, intent(in), optional :: domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        integer, dimension(2) :: words
        integer, dimension(:), allocatable :: ibuf
```

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```
              real(kind=default), dimension(:), allocatable :: dbuf
              call mpi90_receive (words, source, tag, domain, status, error)
              allocate (ibuf(words(1)), dbuf(words(2)))
              call mpi90_receive (ibuf, source, tag+1, domain, status, error)
              call mpi90_receive (dbuf, source, tag+2, domain, status, error)
              call vamp_unmarshal_grid (g, ibuf, dbuf)
              deallocate (ibuf, dbuf)
            end subroutine vamp_receive_grid
```

Caveat: the real `vamp_send_grid` uses *two* tags: `tag` and `tag+1`:

188a   ⟨*Implementation of* `vampi` *procedures (doesn't work with MPICH yet)* 188a⟩≡   188b ▷

```
            subroutine vamp_send_grid (g, target, tag, domain, error)
              type(vamp_grid), intent(in) :: g
              integer, intent(in) :: target, tag
              integer, intent(in), optional :: domain
              integer, intent(out), optional :: error
              integer :: iwords, dwords
              integer, dimension(:), allocatable :: ibuf
              real(kind=default), dimension(:), allocatable :: dbuf
              call vamp_marshal_grid_size (g, iwords, dwords)
              allocate (ibuf(iwords), dbuf(dwords))
              call vamp_marshal_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 wrone with MPICH: if I call `mpi90_receive_pointer`
  in the opposite order, the low level call to `mpi_get_count` bombs for no
  apparent reason!

⚠ There are also funky things going on with `tag`: `mpi90_receive_pointer`
  should leave it alone, but . . .

188b   ⟨*Implementation of* `vampi` *procedures (doesn't work with MPICH yet)* 188a⟩+≡   ◁188a

```
            subroutine vamp_receive_grid (g, source, tag, domain, status, error)
              type(vamp_grid), intent(inout) :: g
              integer, intent(in) :: source, tag
              integer, intent(in), optional :: domain
              type(mpi90_status), intent(out), optional :: status
              integer, intent(out), optional :: error
              integer, dimension(:), pointer :: ibuf
```

```
      real(kind=default), dimension(:), pointer :: dbuf
      nullify (ibuf, dbuf)
      call mpi90_receive_pointer (dbuf, source, tag+1, domain, status, error)
      call mpi90_receive_pointer (ibuf, source, tag, domain, status, error)
      call vamp_unmarshal_grid (g, ibuf, dbuf)
      deallocate (ibuf, dbuf)
    end subroutine vamp_receive_grid
```

This if not a good idea, with respect to communication costs. For SMP
machines, it appears to be negligible however.

189a ⟨*Interfaces of* `vampi` *procedures* 173a⟩+≡   (167c) ◁185e
```
    interface vamp_broadcast_grid
       module procedure &
            vamp_broadcast_one_grid, vamp_broadcast_many_grids
    end interface
```

189b ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁187c 189c▷
```
    subroutine vamp_broadcast_one_grid (g, root, domain, error)
      type(vamp_grid), intent(inout) :: g
      integer, intent(in) :: root
      integer, intent(in), optional :: domain
      integer, intent(out), optional :: error
      integer, dimension(:), allocatable :: ibuf
      real(kind=default), dimension(:), allocatable :: dbuf
      integer :: iwords, dwords, me
      call mpi90_rank (me)
      if (me == root) then
         call vamp_marshal_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_marshal_grid (g, ibuf, dbuf)
      end if
      call mpi90_broadcast (ibuf, root, domain, error)
      call mpi90_broadcast (dbuf, root, domain, error)
      if (me /= root) then
         call vamp_unmarshal_grid (g, ibuf, dbuf)
      end if
      deallocate (ibuf, dbuf)
    end subroutine vamp_broadcast_one_grid
```

189c ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁189b 190▷

```
subroutine vamp_broadcast_many_grids (g, root, domain, error)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: i
  do i = 1, size(g)
     call vamp_broadcast_one_grid (g(i), root, domain, error)
  end do
end subroutine vamp_broadcast_many_grids
```

190 ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁189c 191b▷

```
subroutine vamp_broadcast_grids (g, root, domain, error)
  type(vamp0_grids), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: nch, me
  call mpi90_broadcast (g%sum_chi2, root, domain, error)
  call mpi90_broadcast (g%sum_integral, root, domain, error)
  call mpi90_broadcast (g%sum_weights, root, domain, error)
  call mpi90_rank (me)
  if (me == root) then
     nch = size (g%grids)
  end if
  call mpi90_broadcast (nch, root, domain, error)
  if (me /= root) then
     if (associated (g%grids)) then
        if (size (g%grids) /= nch) then
           call vamp0_delete_grid (g%grids)
           deallocate (g%grids, g%weights, g%num_calls)
           allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
           call vamp_create_empty_grid (g%grids)
        end if
     else
        allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
        call vamp_create_empty_grid (g%grids)
     end if
  end if
  call vamp_broadcast_grid (g%grids, root, domain, error)
  call mpi90_broadcast (g%weights, root, domain, error)
  call mpi90_broadcast (g%num_calls, root, domain, error)
end subroutine vamp_broadcast_grids
```

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191a   ⟨*Declaration of* `vampi` *procedures* 168b⟩+≡   (167c) ◁187a

```
public :: vamp_send_history
public :: vamp_receive_history
```

191b   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁190 191c▷

```
subroutine vamp_send_history (g, target, tag, domain, error)
  type(vamp_history), intent(in) :: g
  integer, intent(in) :: target, tag
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call vamp_marshal_history_size (g, words(1), words(2))
  allocate (ibuf(words(1)), dbuf(words(2)))
  call vamp_marshal_history (g, ibuf, dbuf)
  call mpi90_send (words, target, tag, domain, error)
  call mpi90_send (ibuf, target, tag+1, domain, error)
  call mpi90_send (dbuf, target, tag+2, domain, error)
  deallocate (ibuf, dbuf)
end subroutine vamp_send_history
```

191c   ⟨*Implementation of* `vampi` *procedures* 169a⟩+≡   (167c) ◁191b

```
subroutine vamp_receive_history (g, source, tag, domain, status, error)
  type(vamp_history), intent(inout) :: g
  integer, intent(in) :: source, tag
  integer, intent(in), optional :: domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call mpi90_receive (words, source, tag, domain, status, error)
  allocate (ibuf(words(1)), dbuf(words(2)))
  call mpi90_receive (ibuf, source, tag+1, domain, status, error)
  call mpi90_receive (dbuf, source, tag+2, domain, status, error)
  call vamp_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 perfom 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 reslet and error estimate.

6.1.1   Serial Test

192a   ⟨vamp_test.f90 192a⟩≡   200c ▷
   ! vamp_test.f90 --
   ⟨*Copyleft notice* 1⟩
   ⟨*Module* vamp_test_functions 192b⟩
   ⟨*Module* vamp_tests 196b⟩

192b   ⟨*Module* vamp_test_functions 192b⟩≡   (192a 202a)

```
module vamp_test_functions
  use kinds
  use constants, only: PI
  use coordinates
  use vamp, only: vamp_grid, vamp_multi_channel
  use vamp, only: vamp_data_t
  implicit none
  private
  public :: f, j, phi, ihp, w
  public :: lorentzian
  private :: lorentzian_normalized
  real(kind=default), public :: width
contains
```
   ⟨*Implementation of* vamp_test_functions *procedures* 193a⟩

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```
end module vamp_test_functions
```

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

193a   ⟨*Implementation of* vamp_test_functions *procedures* 193a⟩≡   (192b) 193b ▷

```
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
```

$$\int \mathrm{d}^n x \, f(x) = \int \mathrm{d}\Omega_n \, r^{n-1} \mathrm{d}r \, f(x) = 1 \tag{6.2}$$

193b   ⟨*Implementation of* vamp_test_functions *procedures* 193a⟩+≡   (192b) ◁193a 193c ▷

```
pure function lorentzian (x, x0, x1, x2, r0, a) result (f)
  real(kind=default), dimension(:), intent(in) :: x, x0, x1, x2
  real(kind=default), intent(in) :: r0, a
  real(kind=default) :: f
  real(kind=default) :: r, r1, r2
  integer :: n
  n = size (x)
  if (n > 1) then
     r = sqrt (dot_product (x-x0, x-x0))
     r1 = 0.4_default
     r2 = min (minval (x2-x0), minval (x0-x1))
     if (r1 <= r .and. r <= r2) then
        f = lorentzian_normalized (r, r0, r1, r2, a) * r**(1-n) / surface (n)
     else
        f = 0
     end if
  else
     f = lorentzian_normalized (x(1), x0(1), x1(1), x2(1), a)
  endif
end function lorentzian
```

193c   ⟨*Implementation of* vamp_test_functions *procedures* 193a⟩+≡   (192b) ◁193b 194 ▷

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

```
      real(kind=default), dimension(:), intent(in), optional :: weights
      integer, intent(in), optional :: channel
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: f_x
      real(kind=default), dimension(size(x)) :: minus_one, plus_one, zero, w_i, f_i
      integer :: n, i
      n = size(x)
      minus_one = -1
      zero = 0
      plus_one = 1
      w_i = 1
      do i = 1, n
         if (all (abs (x(i+1:)) <= 1)) then
            f_i = lorentzian (x(1:i), zero(1:i), minus_one(1:i), plus_one(1:i), &
                              0.7_default, width) &
                  / 2.0_default**(n-i)
         else
            f_i = 0
         end if
      end do
      f_x = dot_product (w_i, f_i) / sum (w_i)
    end function f
```

194 ⟨*Implementation of* vamp_test_functions *procedures* 193a⟩+≡   (192b) ◁193c 195a▷

```
    pure function phi (xi, channel) result (x)
      real(kind=default), dimension(:), intent(in) :: xi
      integer, intent(in) :: channel
      real(kind=default), dimension(size(xi)) :: x
      real(kind=default) :: r
      real(kind=default), dimension(0) :: dummy
      integer :: n
      n = size(x)
      if (channel == 1) then
         x = xi
      else if (channel == 2) then
         r = (xi(1) + 1) / 2 * sqrt (2.0_default)
         x(1:2) = spherical_cos_to_cartesian (r, PI * xi(2), dummy)
         x(3:) = xi(3:)
      else if (channel < n) then
         r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))
         x(1:channel) = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:channel))
         x(channel+1:) = xi(channel+1:)
      else if (channel == n) then
         r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))
```

```
          x = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:))
        else
          x = 0
        end if
      end function phi
```

195a ⟨*Implementation of* `vamp_test_functions` *procedures* 193a⟩+≡   (192b) ◁194 195b▷

```
      pure function ihp (x, channel) result (xi)
        real(kind=default), dimension(:), intent(in) :: x
        integer, intent(in) :: channel
        real(kind=default), dimension(size(x)) :: xi
        real(kind=default) :: r, phi
        integer :: n
        n = size(x)
        if (channel == 1) then
          xi = x
        else if (channel == 2) then
          call cartesian_to_spherical_cos (x(1:2), r, phi)
          xi(1) = 2 * r / sqrt (2.0_default) - 1
          xi(2) = phi / PI
          xi(3:) = x(3:)
        else if (channel < n) then
          call cartesian_to_spherical_cos (x(1:channel), r, phi, xi(3:channel))
          xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
          xi(2) = phi / PI
          xi(channel+1:) = x(channel+1:)
        else if (channel == n) then
          call cartesian_to_spherical_cos (x, r, phi, xi(3:))
          xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
          xi(2) = phi / PI
        else
          xi = 0
        end if
      end function ihp
```

195b ⟨*Implementation of* `vamp_test_functions` *procedures* 193a⟩+≡   (192b) ◁195a 196a▷

```
      pure function j (x, data, channel) result (j_x)
        real(kind=default), dimension(:), intent(in) :: x
        class(vamp_data_t), intent(in) :: data
        integer, intent(in) :: channel
        real(kind=default) :: j_x
        if (channel == 1) then
          j_x = 1
        else if (channel > 1) then
          j_x = 2 / sqrt (real (channel, kind=default)) ! $1/|\mathrm{d}r/\mathrm{d}\xi_1|$
```

```
          j_x = j_x / PI                              ! 1/|dφ/dξ₂|
          j_x = j_x * cartesian_to_spherical_cos_j (x(1:channel))
        else
          j_x = 0
        end if
      end function j
```

196a ⟨*Implementation of* `vamp_test_functions` *procedures* 193a⟩+≡   (192b) ◁195b
```
      function w (x, data, weights, channel, grids) result (w_x)
        real(kind=default), dimension(:), intent(in) :: x
        class(vamp_data_t), intent(in) :: data
        real(kind=default), dimension(:), intent(in), optional :: weights
        integer, intent(in), optional :: channel
        type(vamp_grid), dimension(:), intent(in), optional :: grids
        real(kind=default) :: w_x
        w_x = vamp_multi_channel (f, data, phi, ihp, j, x, weights, channel, grids)
      end function w
```

196b ⟨*Module* `vamp_tests` 196b⟩≡   (192a)
```
      module vamp_tests
        use kinds
        use exceptions
        use histograms
        use tao_random_numbers
        use coordinates
        use vamp
        use vamp_test_functions !NODEP!
        implicit none
        private
```
        ⟨*Declaration of procedures in* `vamp_tests` 196c⟩
```
      contains
```
        ⟨*Implementation of procedures in* `vamp_tests` 197a⟩
```
      end module vamp_tests
```

Verification

196c ⟨*Declaration of procedures in* `vamp_tests` 196c⟩≡   (196b 202b) 198a ▷
```
        ! public :: check_jacobians, check_inverses, check_inverses3
        public :: check_inverses, check_inverses3
```

196d ⟨*Implementation of procedures in* `vamp_tests` *(broken?)* 196d⟩≡
```
        subroutine check_jacobians (rng, region, weights, samples)
          type(tao_random_state), intent(inout) :: rng
          real(kind=default), dimension(:,:), intent(in) :: region
          real(kind=default), dimension(:), intent(in) :: weights
```

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

197a ⟨*Implementation of procedures in* vamp_tests 197a⟩≡   (196b 202b) 197b ▷
```
     subroutine check_inverses (rng, region, weights, samples)
        type(tao_random_state), intent(inout) :: rng
        real(kind=default), dimension(:,:), intent(in) :: region
        real(kind=default), dimension(:), intent(in) :: weights
        integer, intent(in) :: samples
        real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx
        real(kind=default) :: dx, dx_max
        integer :: ch, i
        dx_max = 0
        x_dx = 0
        do ch = 1, size(weights)
           do i = 1, samples
              call tao_random_number (rng, x1)
              x2 = ihp (phi (x1, ch), ch)
              dx = sqrt (dot_product (x1-x2, x1-x2))
              if (dx > dx_max) then
                 dx_max = dx
                 x_dx = x1
              end if
           end do
           print *, "channel", ch, ": |x-x|=", real(dx), ", @x=", real (x_dx)
        end do
     end subroutine check_inverses
```

197b ⟨*Implementation of procedures in* vamp_tests 197a⟩+≡   (196b 202b) ◁197a 198b ▷
```
     subroutine check_inverses3 (rng, region, samples)
        type(tao_random_state), intent(inout) :: rng
        real(kind=default), dimension(:,:), intent(in) :: region
        integer, intent(in) :: samples
        real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx, x_dj
        real(kind=default) :: r, phi, jac, caj, dx, dx_max, dj, dj_max
        real(kind=default), dimension(size(x1)-2) :: cos_theta
        integer :: i
        dx_max = 0
```

197

```
      x_dx = 0
      dj_max = 0
      x_dj = 0
      do i = 1, samples
         call tao_random_number (rng, x1)
         call cartesian_to_spherical_cos_2 (x1, r, phi, cos_theta, jac)
         call spherical_cos_to_cartesian_2 (r, phi, cos_theta, x2, caj)
         dx = sqrt (dot_product (x1-x2, x1-x2))
         dj = jac*caj - 1
         if (dx > dx_max) then
            dx_max = dx
            x_dx = x1
         end if
         if (dj > dj_max) then
            dj_max = dj
            x_dj = x1
         end if
      end do
      print *, "channel 3 : j*j-1=", real(dj), ", @x=", real (x_dj)
      print *, "channel 3 : |x-x|=", real(dx), ", @x=", real (x_dx)
   end subroutine check_inverses3
```

Integration

198a ⟨*Declaration of procedures in* vamp_tests 196c⟩+≡   (196b 202b) ◁196c 200a▷
 public :: single_channel, multi_channel

198b ⟨*Implementation of procedures in* vamp_tests 197a⟩+≡   (196b 202b) ◁197b 199a▷
```
   subroutine single_channel (rng, region, samples, iterations, &
         integral, standard_dev, chi_squared)
   type(tao_random_state), intent(inout) :: rng
   real(kind=default), dimension(:,:), intent(in) :: region
   integer, dimension(:), intent(in) :: samples, iterations
   real(kind=default), intent(out) :: integral, standard_dev, chi_squared
   type(vamp_grid) :: gr
   type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
   call vamp_create_history (history)
   call vamp_create_grid (gr, region, samples(1))
   call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
   call vamp_discard_integral (gr, samples(2))
   call vamp_sample_grid &
         (rng, gr, f, NO_DATA, iterations(2), &
          integral, standard_dev, chi_squared, &
          history = history(iterations(1)+1:))
```

```
        call vamp_write_grid (gr, "vamp_test.grid")
        call vamp_delete_grid (gr)
        call vamp_print_history (history, "single")
        call vamp_delete_history (history)
      end subroutine single_channel
```

199a ⟨*Implementation of procedures in* vamp_tests 197a⟩+≡   (196b 202b) ◁198b 200b▷
```
      subroutine multi_channel (rng, region, weights, samples, iterations, powers, &
          integral, standard_dev, chi_squared)
      type(tao_random_state), intent(inout) :: rng
      real(kind=default), dimension(:,:), intent(in) :: region
      real(kind=default), dimension(:), intent(inout) :: weights
      integer, dimension(:), intent(in) :: samples, iterations
      real(kind=default), dimension(:), intent(in) :: powers
      real(kind=default), intent(out) :: integral, standard_dev, chi_squared
      type(vamp_grids) :: grs
```
      ⟨*Body of* multi_channel 199b⟩
```
      end subroutine multi_channel
```

199b ⟨*Body of* multi_channel 199b⟩≡   (199a 213a) 213b▷
```
      type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
          history
      type(vamp_history), dimension(size(history),size(weights)) :: histories
      integer :: it, nit
      nit = size (powers)
      call vamp_create_history (history)
      call vamp_create_history (histories)
      call vamp_create_grids (grs, region, samples(1), weights)
      call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
                            history = history, histories = histories)
      call vamp_print_history (history, "multi")
      call vamp_print_history (histories, "multi")
      do it = 1, nit
         call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
                               history = history(iterations(1)+it-1:), &
                               histories = histories(iterations(1)+it-1:,:))
         call vamp_print_history (history(iterations(1)+it-1:), "multi")
         call vamp_print_history (histories(iterations(1)+it-1:,:), "multi")
         call vamp_refine_weights (grs, powers(it))
      end do
      call vamp_discard_integrals (grs, samples(2))
      call vamp_sample_grids &
          (rng, grs, w, NO_DATA, iterations(2), &
           integral, standard_dev, chi_squared, &
           history = history(iterations(1)+nit:), &
```

```
         histories = histories(iterations(1)+nit:,:))
    call vamp_print_history (history(iterations(1)+nit:), "multi")
    call vamp_print_history (histories(iterations(1)+nit:,:), "multi")
    call vamp_write_grids (grs, "vamp_test.grids")
    call vamp_delete_grids (grs)
    call vamp_print_history (history, "multi")
    call vamp_print_history (histories, "multi")
    call vamp_delete_history (history)
    call vamp_delete_history (histories)
```

Input/Output

200a ⟨*Declaration of procedures in* vamp_tests 196c⟩+≡   (196b 202b) ◁198a
```
  public :: print_results
```

200b ⟨*Implementation of procedures in* vamp_tests 197a⟩+≡   (196b 202b) ◁199a
```
  subroutine print_results (prefix, prev_ticks, &
       integral, std_dev, chi2, acceptable, failures)
    character(len=*), intent(in) :: prefix
    integer, intent(in) :: prev_ticks
    real(kind=default), intent(in) :: integral, std_dev, chi2, acceptable
    integer, intent(inout) :: failures
    integer :: ticks, ticks_per_second
    real(kind=default) :: pull
    call system_clock (ticks, ticks_per_second)
    pull = (integral - 1) / std_dev
    print "(1X,A,A,F6.2,A)", prefix, &
         ": time = ", real (ticks - prev_ticks) / ticks_per_second, " secs"
    print *, prefix, ":     int, err, chi2: ", &
         real (integral), real (std_dev), real (chi2)
    if (abs (pull) > acceptable) then
       failures = failures + 1
       print *, prefix, ": inacceptable pull:", real (pull)
    else
       print *, prefix, ":   acceptable pull:", real (pull)
    end if
  end subroutine print_results
```

Main Program

200c ⟨vamp_test.f90 192a⟩+≡   ◁192a
```
  program vamp_test
    use kinds
    use tao_random_numbers
```

200

```fortran
use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp
use vamp_test_functions !NODEP!
use vamp_tests !NODEP!
implicit none
integer :: start_ticks, status
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
failures = 0
call tao_random_create (rng, 0)
call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
if (status == 0) then
   call system_clock (start_ticks)
else
   start_ticks = 42
end if
call tao_random_seed (rng, start_ticks)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
region(1,:)  = -1.0
region(2,:)  =  1.0
width = 0.0001
print *, "Starting VAMP 1.0 self test..."
print *, "serial code"
print *, VAMP_RCS_ID
print *, DIVISIONS_RCS_ID
call system_clock (start_ticks)
call single_channel (rng, region, samples, iterations, &
        single_integral, single_standard_dev, single_chi_squared)
call print_results ("SINGLE", start_ticks, &
        single_integral, single_standard_dev, single_chi_squared, &
        10*ACCEPTABLE, failures)
weight_vector = 1
powers = 0.25_default
call system_clock (start_ticks)
```

```
        call multi_channel (rng, region, weight_vector, samples, iterations, &
                powers, multi_integral, multi_standard_dev, multi_chi_squared)
        call print_results ("MULTI", start_ticks, &
                 multi_integral, multi_standard_dev, multi_chi_squared, &
                ACCEPTABLE, failures)
        call system_clock (start_ticks)
      ! call check_jacobians (rng, region, weight_vector, samples(1))
        call check_inverses (rng, region, weight_vector, samples(1))
        call check_inverses3 (rng, region, samples(1))
        if (failures == 0) then
           stop 0
        else if (failures == 1) then
           stop 1
        else
           stop 2
        end if
     end program vamp_test
```

6.1.2 Parallel Test

202a ⟨vampi_test.f90 202a⟩≡   202b ▷
```
      ! vampi_test.f90 --
```
      ⟨Copyleft notice 1⟩
      ⟨Module vamp_test_functions 192b⟩

The following is identical to vamp_tests, except for use vampi:

202b ⟨vampi_test.f90 202a⟩+≡   ◁ 202a 202c ▷
```
     module vampi_tests
       use kinds
       use exceptions
       use histograms
       use tao_random_numbers
       use coordinates
       use vampi
       use vamp_test_functions !NODEP!
       implicit none
       private
```
       ⟨Declaration of procedures in vamp_tests 196c⟩
```
     contains
```
       ⟨Implementation of procedures in vamp_tests 197a⟩
```
     end module vampi_tests
```

202c ⟨vampi_test.f90 202a⟩+≡   ◁ 202b
```
     program vampi_test
```

202

```
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

204a   ⟨`vamp_test.out` 204a⟩≡

6.2   Mapped Mode

In this chapter we perfom 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 reselt and error estimate.

6.2.1 Serial Test

204b   ⟨`vamp_test0.f90` 204b⟩≡   211a ▷
```
   ! vamp_test0.f90 --
```
⟨*Copyleft notice* 1⟩
⟨*Module* `vamp_test0_functions` 205⟩

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

205   ⟨*Module* `vamp_test0_functions` 205⟩≡   (204b 220b)

```
module vamp_test0_functions
  use kinds
  use vamp, only: vamp_grid, vamp_multi_channel0
  use vamp, only: vamp_data_t
  implicit none
  private
  public :: f, g, phi, w
  public :: create_sample, delete_sample
  private :: f0, psi, g0, f_norm
  real(kind=default), dimension(:), allocatable, private :: c, x_min, x_max
  real(kind=default), dimension(:,:,:), allocatable, public :: x0, gamma
contains
  ⟨Implementation of vamp_test0_functions procedures 206a⟩
end module vamp_test0_functions
```

We start from a model of n_p interfering resonances in one variable (cf. section **??**)

$$f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{N(x_{\min}, x_{\max}, x_0, \gamma)} \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \qquad (6.3)$$

where

$$N(x_{\min}, x_{\max}, x_0, \gamma) = \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \qquad (6.4)$$

such that

$$\int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \, f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = 1 \qquad (6.5)$$

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.

$$N(x_{\min}, x_{\max}, x_0, \gamma) = \sum_{p=1}^{n_p} \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \left| \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2$$

$$+ 2\operatorname{Re} \sum_{p=1}^{n_p} \sum_{q=1}^{n_p} \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \, \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} \qquad (6.6)$$

```
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
```

$$
\int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \, \frac{1}{x - x_{0,p} + i\gamma_p} \frac{1}{x - x_{0,q} - i\gamma_q} =
$$
$$
\frac{1}{x_{0,p} - x_{0,q} - i\gamma_p - i\gamma_q} \left(\ln \left(\frac{x_{\max} - x_{0,p} + i\gamma_p}{x_{\min} - x_{0,p} + i\gamma_p} \right) - \ln \left(\frac{x_{\max} - x_{0,q} - i\gamma_q}{x_{\min} - x_{0,q} - i\gamma_q} \right) \right)
$$
$$
(6.7)
$$

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

```
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:

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

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

207a   ⟨*Implementation of* vamp_test0_functions *procedures* 206a⟩+≡   (205) ◁206b 207b▷
```
pure function f (x, data, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  class(vamp_data_t), intent(in) :: data
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: f_x
  real(kind=default) :: fi_x
  integer :: i, j
  f_x = 0.0
  do i = 1, size (c)
     fi_x = 1.0
     do j = 1, size (x)
        if (all (gamma(:,i,j) > 0)) then
           fi_x = fi_x * f0 (x(j), x_min(j), x_max(j), &
                             x0(:,i,j), gamma(:,i,j))
        else
           fi_x = fi_x / (x_max(j) - x_min(j))
        end if
     end do
     f_x = f_x + c(i) * fi_x
  end do
  f_x = f_x / sum (c)
end function f
```

207b   ⟨*Implementation of* vamp_test0_functions *procedures* 206a⟩+≡   (205) ◁207a 207c▷
```
subroutine delete_sample ()
  deallocate (c, x_min, x_max, x0, gamma)
end subroutine delete_sample
```

207c   ⟨*Implementation of* vamp_test0_functions *procedures* 206a⟩+≡   (205) ◁207b 208▷
```
subroutine create_sample (num_poles, weights, region)
  integer, intent(in) :: num_poles
  real(kind=default), dimension(:), intent(in) :: weights
```

```fortran
    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

$$\psi(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] \to [x_{\min}, x_{\max}]$$
$$\xi \mapsto x = \psi(\xi | x_{\min}, x_{\max}, x_0, \gamma) \tag{6.9}$$

where

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

208   ⟨*Implementation of* `vamp_test0_functions` *procedures* 206a⟩+≡   (205) ◁207c 209a▷

```fortran
  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

$$\psi^{-1}(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] \to [x_{\min}, x_{\max}]$$
$$x \mapsto \xi = \psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) \tag{6.11}$$

with

$$\psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) =$$
$$\frac{x_{\max}(\operatorname{atan}\frac{x_0 - x_{\min}}{\gamma} + \operatorname{atan}\frac{x - x_0}{\gamma}) + x_{\min}(\operatorname{atan}\frac{x_{\max} - x_0}{\gamma} + \operatorname{atan}\frac{x_0 - x}{\gamma})}{\operatorname{atan}\frac{x_{\max} - x_0}{\gamma} + \operatorname{atan}\frac{x_0 - x_{\min}}{\gamma}} \tag{6.12}$$

with Jacobian

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

209a ⟨*Implementation of* `vamp_test0_functions` *procedures* 206a⟩+≡   (205) ◁208 209c▷

```
pure function g0 (x, x_min, x_max, x0, gamma) result (g_x)
  real(kind=default), intent(in) :: x, x_min, x_max, x0, gamma
  real(kind=default) :: g_x
  g_x = gamma / (atan ((x_max - x0) / gamma) - atan ((x_min - x0) / gamma)) &
        * (x_max - x_min) / ((x - x0)**2 + gamma**2)
end function g0
```

The function f has $n_c n_p^{n_d}$ peaks and we need a channel for each one, plus a constant function for the background. We encode the position on the grid linearly:

209b ⟨*Decode* `channel` *into* `ch` *and* `p(:)` 209b⟩≡   (209c 210a)

```
ch = channel - 1
do j = 1, size (x)
   p(j) = 1 + modulo (ch, np)
   ch = ch / np
end do
ch = ch + 1
```

The map ϕ is the direct product of ψs:

209c ⟨*Implementation of* `vamp_test0_functions` *procedures* 206a⟩+≡   (205) ◁209a 210a▷

```
pure function phi (xi, channel) result (x)
  real(kind=default), dimension(:), intent(in) :: xi
  integer, intent(in) :: channel
  real(kind=default), dimension(size(xi)) :: x
  integer, dimension(size(xi)) :: p
  integer :: j, ch, np, nch, nd, channels
  np = size (x0, dim = 1)
  nch = size (x0, dim = 2)
  nd = size (x0, dim = 3)
  channels = nch * np**nd
  if (channel >= 1 .and. channel <= channels) then
     ⟨Decode channel into ch and p(:) 209b⟩
     do j = 1, size (xi)
        if (all (gamma(:,ch,j) > 0)) then
           x(j) = psi (xi(j), x_min(j), x_max(j), &
                      x0(p(j),ch,j), gamma(p(j),ch,j))
        else
           x = xi
```

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

similarly for the Jacobians:

210a   ⟨*Implementation of* `vamp_test0_functions` *procedures* 206a⟩+≡   (205) ◁209c 210b▷

```
      pure recursive function g (x, data, channel) result (g_x)
        real(kind=default), dimension(:), intent(in) :: x
        class(vamp_data_t), intent(in) :: data
        integer, intent(in) :: channel
        real(kind=default) :: g_x
        integer, dimension(size(x)) :: p
        integer :: j, ch, np, nch, nd, channels
        np = size (x0, dim = 1)
        nch = size (x0, dim = 2)
        nd = size (x0, dim = 3)
        channels = nch * np**nd
        if (channel >= 1 .and. channel <= channels) then
          ⟨Decode channel into ch and p(:) 209b⟩
          g_x = 1.0
          do j = 1, size (x)
            if (all (gamma(:,ch,j) > 0)) then
              g_x = g_x * g0 (x(j), x_min(j), x_max(j), &
                              x0(p(j),ch,j), gamma(p(j),ch,j))
            end if
          end do
        else if (channel == channels + 1) then
          g_x = 1.0
        else
          g_x = 0
        end if
      end function g
```

210b   ⟨*Implementation of* `vamp_test0_functions` *procedures* 206a⟩+≡   (205) ◁210a

```
      function w (x, data, weights, channel, grids) result (w_x)
        real(kind=default), dimension(:), intent(in) :: x
        class(vamp_data_t), intent(in) :: data
        real(kind=default), dimension(:), intent(in), optional :: weights
        integer, intent(in), optional :: channel
```

```
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: w_x
      w_x = vamp_multi_channel0 (f, data, phi, g, x, weights, channel)
    end function w
```

<center>Driver Routines</center>

211a ⟨vamp_test0.f90 204b⟩+≡   ◁204b 217▷
```
      module vamp_tests0
        ⟨Modules used by vamp_tests0 211b⟩
        use vamp
        implicit none
        private
        ⟨Declaration of procedures in vamp_tests0 212a⟩
      contains
        ⟨Implementation of procedures in vamp_tests0 212b⟩
      end module vamp_tests0
```

211b ⟨Modules used by vamp_tests0 211b⟩≡   (211a 220b)
```
      use kinds
      use exceptions
      use histograms
      use tao_random_numbers
      use vamp_test0_functions !NODEP!
```

Verification

211c ⟨Declaration of procedures in vamp_tests0 (broken?) 211c⟩≡
```
      public :: check_jacobians
```

211d ⟨Implementation of procedures in vamp_tests0 (broken?) 211d⟩≡
```
      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
```

<center>211</center>

```
          end do
        end subroutine check_jacobians
```

Integration

212a ⟨*Declaration of procedures in* `vamp_tests0` 212a⟩≡   (211a 220b) 214a ▷
```
      public :: single_channel, multi_channel
```

212b ⟨*Implementation of procedures in* `vamp_tests0` 212b⟩≡   (211a 220b) 213a ▷
```
      subroutine single_channel (do_print, region, iterations, samples, rng, &
          acceptable, failures)
        logical, intent(in) :: do_print
        real(kind=default), dimension(:,:), intent(in) :: region
        integer, dimension(:), intent(in) :: iterations, samples
        type(tao_random_state), intent(inout) :: rng
        real(kind=default), intent(in) :: acceptable
        integer, intent(inout) :: failures
        type(vamp_grid) :: gr
        type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
        real(kind=default) :: integral, standard_dev, chi_squared, pull
        call vamp_create_history (history)
        call vamp_create_grid (gr, region, samples(1))
        call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
        call vamp_discard_integral (gr, samples(2))
        call vamp_sample_grid &
            (rng, gr, f, NO_DATA, iterations(2), &
             integral, standard_dev, chi_squared, &
             history = history(iterations(1)+1:))
        call vamp_write_grid (gr, "vamp_test0.grid")
        call vamp_delete_grid (gr)
        call vamp_print_history (history, "single")
        call vamp_delete_history (history)
        pull = (integral - 1) / standard_dev
        if (do_print) then
           print *, "    int, err, chi2:", integral, standard_dev, chi_squared
        end if
        if (abs (pull) > acceptable) then
           failures = failures + 1
           print *, " unacceptable pull:", pull
        else
           print *, "   acceptable pull:", pull
        end if
      end subroutine single_channel
```

213a   ⟨*Implementation of procedures in* `vamp_tests0` 212b⟩+≡   (211a 220b) ◁212b 214b▷

```
subroutine multi_channel (do_print, region, iterations, samples, rng, &
    acceptable, failures)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:,:), intent(in) :: region
  integer, dimension(:), intent(in) :: iterations, samples
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), intent(in) :: acceptable
  type(vamp_grids) :: grs
  integer, intent(inout) :: failures
  ⟨Body of multi_channel 199b⟩
end subroutine multi_channel
```

213b   ⟨*Body of* `multi_channel` 199b⟩+≡   (199a 213a) ◁199b

```
real(kind=default), &
    dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
    weight_vector
type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
real(kind=default) :: integral, standard_dev, chi_squared, pull
integer :: it
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
   call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
                           history = history(iterations(1)+it-1:), &
                           histories = histories(iterations(1)+it-1:,:))
   call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
    (rng, grs, w, NO_DATA, iterations(2), &
     integral, standard_dev, chi_squared, &
     history = history(iterations(1)+5:), &
     histories = histories(iterations(1)+5:,:))
call vamp_write_grids (grs, "vamp_test0.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
```

```fortran
call vamp_delete_history (histories)
if (do_print) then
   print *, integral, standard_dev, chi_squared
end if
pull = (integral - 1) / standard_dev
if (abs (pull) > acceptable) then
   failures = failures + 1
   print *, " unacceptable pull:", pull
else
   print *, "   acceptable pull:", pull
end if
```

Event Generation

214a ⟨*Declaration of procedures in* vamp␣tests0 212a⟩+≡   (211a 220b) ◁212a
```fortran
public :: single_channel_generator, multi_channel_generator
```

214b ⟨*Implementation of procedures in* vamp␣tests0 212b⟩+≡   (211a 220b) ◁213a 215▷
```fortran
subroutine single_channel_generator (do_print, region, iterations, samples, rng)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:,:), intent(in) :: region
  integer, dimension(:), intent(in) :: iterations, samples
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid) :: gr
  type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
  type(histogram) :: unweighted, reweighted, weighted, weights
  type(exception) :: exc
  real(kind=default) :: weight, integral, standard_dev
  integer :: i
  real(kind=default), dimension(size(region,dim=2)) :: x
  call vamp_create_grid (gr, region, samples(1))
  call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
  call vamp_discard_integral (gr, samples(2))
  call vamp_warmup_grid &
       (rng, gr, f, NO_DATA, iterations(2), history = history(iterations(1)+1:))
  call vamp_print_history (history, "single")
  call vamp_delete_history (history)
  call create_histogram (unweighted, region(1,1), region(2,1), 100)
  call create_histogram (reweighted, region(1,1), region(2,1), 100)
  call create_histogram (weighted, region(1,1), region(2,1), 100)
  call create_histogram (weights, 0.0_default, 10.0_default, 100)
  ! do i = 1, 1000000
  do i = 1, 100
     call clear_exception (exc)
```

```
            call vamp_next_event (x, rng, gr, f, NO_DATA, exc = exc)
            call handle_exception (exc)
            call fill_histogram (unweighted, x(1))
            call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
         end do
         integral = 0.0
         standard_dev = 0.0
         do i = 1, 10000
            call clear_exception (exc)
            call vamp_next_event (x, rng, gr, f, NO_DATA, weight, exc = exc)
            call handle_exception (exc)
            call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
            call fill_histogram (weights, x(1), weight)
            integral = integral + weight
            standard_dev = standard_dev + weight**2
         end do
         if (do_print) then
            print *, integral / (i-1), sqrt (standard_dev) / (i-1)
            call write_histogram (unweighted, "u_s.d")
            call write_histogram (reweighted, "r_s.d")
            call write_histogram (weighted, "w_s.d")
            call write_histogram (weights, "ws_s.d")
         end if
         call delete_histogram (unweighted)
         call delete_histogram (reweighted)
         call delete_histogram (weighted)
         call delete_histogram (weights)
         call vamp_delete_grid (gr)
      end subroutine single_channel_generator
```

215   ⟨*Implementation of procedures in* vamp_tests0 212b⟩+≡   (211a 220b) ◁214b
```
      subroutine multi_channel_generator (do_print, region, iterations, samples, rng)
         logical, intent(in) :: do_print
         real(kind=default), dimension(:,:), intent(in) :: region
         integer, dimension(:), intent(in) :: iterations, samples
         type(tao_random_state), intent(inout) :: rng
         type(vamp_grids) :: grs
         real(kind=default), &
               dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
               weight_vector
         type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
         type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
         type(histogram) :: unweighted, reweighted, weighted, weights
         type(exception) :: exc
```

```fortran
real(kind=default) :: weight, integral, standard_dev
real(kind=default), dimension(size(region,dim=2)) :: x
character(len=5) :: pfx
integer :: it, i, j
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
   call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
                           history = history(iterations(1)+it-1:), &
                           histories = histories(iterations(1)+it-1:,:))
   call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_warmup_grids &
     (rng, grs, w, NO_DATA, iterations(2), &
      history = history(iterations(1)+5:), &
      histories = histories(iterations(1)+5:,:))
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
!!! do i = 1, size (grs%grids)
!!!    do j = 1, size (grs%grids(i)%div)
!!!       write (pfx, "(I2.2,'/',I2.2)") i, j
!!!       call dump_division (grs%grids(i)%div(j), pfx)
!!!    end do
!!! end do
call create_histogram (unweighted, region(1,1), region(2,1), 100)
call create_histogram (reweighted, region(1,1), region(2,1), 100)
call create_histogram (weighted, region(1,1), region(2,1), 100)
call create_histogram (weights, 0.0_default, 10.0_default, 100)
! do i = 1, 1000000
do i = 1, 100
   call clear_exception (exc)
   call vamp_next_event (x, rng, grs, f, NO_DATA, phi, exc = exc)
   call handle_exception (exc)
   call fill_histogram (unweighted, x(1))
   call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
end do
```

```
      integral = 0.0
      standard_dev = 0.0
      do i = 1, 10000
         call clear_exception (exc)
         call vamp_next_event (x, rng, grs, f, NO_DATA, phi, weight, exc = exc)
         call handle_exception (exc)
         call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
         call fill_histogram (weights, x(1), weight)
         integral = integral + weight
         standard_dev = standard_dev + weight**2
      end do
      if (do_print) then
         print *, integral / (i-1), sqrt (standard_dev) / (i-1)
         call write_histogram (unweighted, "u_m.d")
         call write_histogram (reweighted, "r_m.d")
         call write_histogram (weighted, "w_m.d")
         call write_histogram (weights, "ws_m.d")
      end if
      call delete_histogram (unweighted)
      call delete_histogram (reweighted)
      call delete_histogram (weighted)
      call delete_histogram (weights)
      call vamp_delete_grids (grs)
   end subroutine multi_channel_generator
```

Main Program

217   ⟨vamp_test0.f90 204b⟩+≡   ◁211a

```
   program vamp_test0
      ⟨Modules used by vamp_test0 219d⟩
      implicit none
      ⟨Variables in vamp_test0 219b⟩
      do_print = .true.
      print *, "Starting VAMP 1.0 self test..."
      print *, "serial code"
      print *, VAMP_RCS_ID
      print *, DIVISIONS_RCS_ID
      call tao_random_create (rng, 0)
      call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
      if (status == 0) then
         call system_clock (ticks0)
      else
         ticks0 = 42
```

217

```
        end if
        call tao_random_seed (rng, ticks0)
        ⟨Set up integrand and region in vamp_test0 219f⟩
        ⟨Execute tests in vamp_test0 218a⟩
        ⟨Cleanup in vamp_test0 220a⟩
        if (failures == 0) then
           stop 0
        else if (failures == 1) then
           stop 1
        else
           stop 2
        end if
     end program vamp_test0
```

218a ⟨Execute tests in vamp_test0 218a⟩≡   (217) 218b ▷
```
     failures = 0
     call system_clock (ticks0)
     call single_channel (do_print, region, iterations, samples, rng, 10*ACCEPTABLE, failu
     call system_clock (ticks, ticks_per_second)
     print "(1X,A,F6.2,A)", &
          "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

218b ⟨Execute tests in vamp_test0 218a⟩+≡   (217) ◁218a 218c ▷
```
     call system_clock (ticks0)
     call single_channel_generator &
          (do_print, region, iterations, samples, rng)
     call system_clock (ticks, ticks_per_second)
     print "(1X,A,F6.2,A)", &
          "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

218c ⟨Execute tests in vamp_test0 218a⟩+≡   (217) ◁218b 218d ▷
```
     call system_clock (ticks0)
     call multi_channel (do_print, region, iterations, samples, rng, ACCEPTABLE, failures]
     call system_clock (ticks, ticks_per_second)
     print "(1X,A,F6.2,A)", &
          "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

218d ⟨Execute tests in vamp_test0 218a⟩+≡   (217) ◁218c 219a ▷
```
     call system_clock (ticks0)
     call multi_channel_generator &
          (do_print, region, iterations, samples, rng)
     call system_clock (ticks, ticks_per_second)
     print "(1X,A,F6.2,A)", &
          "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

219a ⟨*Execute tests in* `vamp_test0` 218a⟩+≡   (217) ◁218d
```
   call system_clock (ticks0)
   ! call check_jacobians (do_print, region, samples, rng)
   call system_clock (ticks, ticks_per_second)
   print "(1X,A,F6.2,A)", &
         "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

219b ⟨*Variables in* `vamp_test0` 219b⟩≡   (217 220c) 219e ▷
```
   logical :: do_print
```

219c ⟨*Execute* `command` 219c⟩≡   (220c)

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

219e ⟨*Variables in* `vamp_test0` 219b⟩+≡   (217 220c) ◁219b
```
   integer :: i, j, ticks, ticks_per_second, ticks0, status
   integer, dimension(2) :: iterations, samples
   real(kind=default), dimension(:,:), allocatable :: region
   type(tao_random_state) :: rng
   real(kind=default), parameter :: ACCEPTABLE = 4
   integer :: failures
```

219f ⟨*Set up integrand and region in* `vamp_test0` 219f⟩≡   (217 220c)
```
   iterations = (/ 4, 3 /)
   samples = (/ 10000, 50000 /)
   allocate (region(2,2))
   region(1,:)  = -1.0
   region(2,:)  =  2.0
   call create_sample &
        (num_poles = 2, weights = (/ 1.0_default, 2.0_default /), region = region)
   do i = 1, size (x0, dim=2)
      do j = 1, size (x0, dim=3)
         call tao_random_number (rng, x0(:,i,j))
      end do
   end do
   gamma = 0.001
   x0(1,:,:) = 0.2
   x0(2:,:,:) = 0.8
```

220a   ⟨*Cleanup in* `vamp_test0` 220a⟩≡   (217 220c)

```
  call delete_sample ()
  deallocate (region)
```

6.2.2   Parallel Test

220b   ⟨`vampi_test0.f90` 220b⟩≡   220c ▷

```
  ! vampi_test0.f90 --
```
⟨*Copyleft notice* 1⟩
⟨*Module* `vamp_test0_functions` 205⟩
```
  module vamp_tests0
```
  ⟨*Modules used by* `vamp_tests0` 211b⟩
```
    use vampi
    use mpi90
    implicit none
    private
```
  ⟨*Declaration of procedures in* `vamp_tests0` 212a⟩
```
  contains
```
  ⟨*Implementation of procedures in* `vamp_tests0` 212b⟩
```
  end module vamp_tests0
```

220c   ⟨`vampi_test0.f90` 220b⟩+≡   ◁ 220b

```
  program vampi_test0
```
  ⟨*Modules used by* `vamp_test0` 219d⟩
```
    use mpi90
    use vampi, only: VAMPI_RCS_ID
    implicit none
```
  ⟨*Variables in* `vamp_test0` 219b⟩
```
    integer :: num_proc, proc_id
    call mpi90_init ()
    call mpi90_size (num_proc)
    call mpi90_rank (proc_id)
    if (proc_id == 0) then
       do_print = .true.
       print *, "Starting VAMP 1.0 self test..."
       if (num_proc > 1) then
          print *, "parallel code running on ", num_proc, " processors"
       else
          print *, "parallel code running serially"
       end if
       print *, VAMP_RCS_ID
       print *, VAMPI_RCS_ID
       print *, DIVISIONS_RCS_ID
```

220

```
      else
         do_print = .false.
      end if
      call tao_random_create (rng, 0)
      call system_clock (ticks0)
      call tao_random_seed (rng, ticks0 + proc_id)
      ⟨Set up integrand and region in vamp_test0 219f⟩
      call mpi90_broadcast (x0, 0)
      call mpi90_broadcast (gamma, 0)
      command_loop: do
         if (proc_id == 0) then
            ⟨Read command line and decode it as command (never defined)⟩
         end if
         call mpi90_broadcast (command, 0)
         call system_clock (ticks0)
         ⟨Execute command 219c⟩
         call system_clock (ticks, ticks_per_second)
         if (proc_id == 0) then
            print "(1X,A,F6.2,A)", &
                  "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
         end if
      end do command_loop
      ⟨Cleanup in vamp_test0 220a⟩
      call mpi90_finalize ()
      if (proc_id == 0) then
         print *, "bye."
      end if
   end program vampi_test0
```

6.2.3   Output

221   ⟨vamp_test0.out 221⟩≡

—7—
APPLICATION

7.1 Cross section

222a ⟨application.f90 222a⟩≡

```
! application.f90 --
```
⟨*Copyleft notice* 1⟩
```
module cross_section
  use kinds
  use constants
  use utils
  use kinematics
  use tao_random_numbers
  use products, only: dot
  use helicity
  use vamp, only: vamp_grid, vamp_probability
  implicit none
  private
```
⟨*Declaration of* cross_section *procedures* 223d⟩
⟨*Types in* cross_section 228c⟩
⟨*Variables in* cross_section 222b⟩
```
contains
```
⟨*Implementation of* cross_section *procedures* 224a⟩
```
end module cross_section
```

222b ⟨*Variables in* cross_section 222b⟩≡   (222a) 223c ▷

```
real(kind=default), private, parameter :: &
     MA_0 = 0.0, &
     MB_0 = 0.0, &
     M1_0 = 0.0, &
     M2_0 = 0.0, &
     M3_0 = 0.0, &
```

```
          S_0 = 200.0 ** 2
```

223a   ⟨*XXX Variables in* cross_section 223a⟩≡   223b ▷

```
      real(kind=default), private, parameter :: &
          MA_0 = 0.01, &
          MB_0 = 0.01, &
          M1_0 = 0.01, &
          M2_0 = 0.01, &
          M3_0 = 0.01, &
          S_0 = 200.0 ** 2
```

223b   ⟨*XXX Variables in* cross_section 223a⟩+≡   ◁223a

```
      real(kind=default), private, parameter :: &
          S1_MIN_0 = 0.0 ** 2, &
          S2_MIN_0 = 0.0 ** 2, &
          S3_MIN_0 = 0.0 ** 2, &
          T1_MIN_0 = 0.0 ** 2, &
          T2_MIN_0 = 0.0 ** 2
```

223c   ⟨*Variables in* cross_section 222b⟩+≡   (222a) ◁222b   223f ▷

```
      real(kind=default), private, parameter :: &
          S1_MIN_0 = 1.0 ** 2, &
          S2_MIN_0 = 1.0 ** 2, &
          S3_MIN_0 = 1.0 ** 2, &
          T1_MIN_0 = 10.0 ** 2, &
          T2_MIN_0 = 10.0 ** 2
```


223d   ⟨*Declaration of* cross_section *procedures* 223d⟩≡   (222a)   225a ▷

```
      private :: cuts
```


223e   ⟨*XXX Implementation of* cross_section *procedures* 223e⟩≡

```
      pure function cuts (k1, k2, p1, p2, q) result (inside)
        real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
        logical :: inside
        inside =   (abs (dot (k1 - q, k1 - q)) >= T1_MIN_0) &
             .and. (abs (dot (k2 - q, k2 - q)) >= T2_MIN_0) &
             .and. (abs (dot (p1 + q, p1 + q)) >= S1_MIN_0) &
             .and. (abs (dot (p2 + q, p2 + q)) >= S2_MIN_0) &
             .and. (abs (dot (p1 + p2, p1 + p2)) >= S3_MIN_0)
      end function cuts
```


223f   ⟨*Variables in* cross_section 222b⟩+≡   (222a) ◁223c

```
      real(kind=default), private, parameter :: &
```

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

224a ⟨*Implementation of* cross_section *procedures* 224a⟩≡   (222a) 224b ▷
```
        pure function cuts (k1, k2, p1, p2, q) result (inside)
          real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
          logical :: inside
          real(kind=default), dimension(3) :: p1n, p2n, qn
          inside = .false.
          if ((p1(0) < E_MIN) .or. (p2(0) < E_MIN) .or. (q(0) < E_MIN)) then
             return
          end if
          p1n = p1(1:3) / sqrt (dot_product (p1(1:3), p1(1:3)))
          p2n = p2(1:3) / sqrt (dot_product (p2(1:3), p2(1:3)))
          qn = q(1:3) / sqrt (dot_product (q(1:3), q(1:3)))
          if ((abs (qn(3)) > COSTH_BEAM_MAX) &
               .or. (abs (p1n(3)) > COSTH_BEAM_MAX)&
               .or. (abs (p2n(3)) > COSTH_BEAM_MAX)) then
             return
          end if
          if (dot_product (p1n, qn) > COSTH_SEP_MAX) then
             return
          end if
          if (dot_product (p2n, qn) > COSTH_SEP_MAX) then
             return
          end if
          if (dot_product (p1n, p2n) > COSTH_SEP_MAX) then
             return
          end if
          inside = .true.
        end function cuts
```

224b ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁224a 226b ▷
```
        function xsect (k1, k2, p1, p2, q) result (xs)
          real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
          real(kind=default) :: xs
          complex(kind=default), dimension(-1:1,-1:1,-1:1,-1:1,-1:1) :: amp
          !!! xs = 1.0_double / phase_space_volume (3, k1(0) + k2(0))
          !!! xs = 1.0_double / dot (p1 + q, p1 + q) &
          !!!      + 1.0_double / dot (p2 + q, p2 + q)
          !!! return
          amp = nneeg (k1, k2, p1, p2, q)
```

```
        xs = sum (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2) &
                    * conjg (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2)))
      end function xsect
```

225a ⟨*Declaration of* `cross_section` *procedures* 223d⟩+≡   (222a) ◁223d 227b▷
```
      private :: xsect
```

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

where

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

225b ⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ 225b⟩≡   (226b)
```
      ! s2_min = S1_MIN_0
      s2_min = (m2 + m3)**2
      s2_max = (sqrt (s) - m1)**2
      s2 = s2_max * x(1) + s2_min * (1 - x(1))
      t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
          + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
      t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
          - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
      t1 = t1_max * x(2) + t1_min * (1 - x(2))
      phi = 2*PI * x(3)
      cos_theta3 = 2 * x(4) - 1
      phi3 = 2*PI * x(5)
```

225c ⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ *(massless case)* 225c⟩≡   (228b)
```
      ! s2_min = S1_MIN_0
      s2_min = 0
      s2_max = s
      s2 = s2_max * x(1) + s2_min * (1 - x(1))
      t1_min = - (s - s2)
      t1_max = 0
      t1 = t1_max * x(2) + t1_min * (1 - x(2))
      phi = 2*PI * x(3)
      cos_theta3 = 2 * x(4) - 1
      phi3 = 2*PI * x(5)
```

225

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

i.e.

$$J_\phi(x_1, \ldots, x_5) = 8\pi^2 \cdot \left| \frac{\mathrm{d}s_2}{\mathrm{d}x_1} \right| \cdot \left(t_1^{\max}(s_2) - t_1^{\min}(s_2) \right) \qquad (7.4)$$

226a   ⟨*Adjust Jacobian* 226a⟩≡   (226b 228b)

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

226b   ⟨*Implementation of* **cross_section** *procedures* 224a⟩+≡   (222a) ◁224b 227c▷

```
pure function phase_space (x, channel) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: channel
  type(LIPS3) :: p
  real(kind=default) :: &
       ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s = S_0
```
⟨$m_a \leftrightarrow m_b$, $m_1 \leftrightarrow m_2$ *for channel #1* 226c⟩
⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ 225b⟩
```
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
```
⟨*Adjust Jacobian* 226a⟩
⟨$p_1 \leftrightarrow p_2$ *for channel #2* 227a⟩
```
end function phase_space
```

226c   ⟨$m_a \leftrightarrow m_b$, $m_1 \leftrightarrow m_2$ *for channel #1* 226c⟩≡   (226b)

```
select case (channel)
case (1)
   ma = MA_0
   mb = MB_0
   m1 = M1_0
   m2 = M2_0
   m3 = M3_0
case (2)
   ma = MB_0
   mb = MA_0
   m1 = M2_0
   m2 = M1_0
   m3 = M3_0
case (3)
   ma = MA_0
   mb = MB_0
   m1 = M3_0
```

```
             m2 = M2_0
             m3 = M1_0
          case default
             ma = MA_0
             mb = MB_0
             m1 = M1_0
             m2 = M2_0
             m3 = M3_0
          end select
```

227a ⟨$p_1 \leftrightarrow p_2$ for channel #2 227a⟩≡   (226b 228b)
```
          select case (channel)
          case (1)
             ! OK
          case (2)
             call swap (p%p(1,:), p%p(2,:))
          case (3)
             call swap (p%p(1,:), p%p(3,:))
          case default
             ! OK
          end select
```

227b ⟨Declaration of cross_section procedures 223d⟩+≡   (222a) ◁225a 228a▷
```
          private :: jacobian
```

227c ⟨Implementation of cross_section procedures 224a⟩+≡   (222a) ◁226b 228b▷
```
          pure function jacobian (k1, k2, p1, p2, q) result (jac)
            real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
            real(kind=default) :: jac
            real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
            real(kind=default) :: s, s2, s2_min, s2_max, t1_min, t1_max
            ma_2 = max (dot (k1, k1), 0.0_double)
            mb_2 = max (dot (k2, k2), 0.0_double)
            m1_2 = max (dot (p1, p1), 0.0_double)
            m2_2 = max (dot (p2, p2), 0.0_double)
            m3_2 = max (dot (q, q), 0.0_double)
            s = dot (k1 + k2, k1 + k2)
            s2 = dot (p2 + q, p2 + q)
            ! s2_min = S1_MIN_0
            s2_min = (sqrt (m2_2) + sqrt (m3_2))**2
            s2_max = (sqrt (s) - sqrt (m1_2))**2
            t1_min = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
                  + sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
            t1_max = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
                  - sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
```

```
          jac = 1.0 / ((2*PI)**5 * 32 * s2) &
                * sqrt (lambda (s2, m2_2, m3_2) / lambda (s, ma_2, mb_2)) &
                * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
       end function jacobian
```

228a ⟨*Declaration of* cross_section *procedures* 223d⟩+≡   (222a) ◁227b 228e▷
```
       private :: phase_space, phase_space_massless
```

228b ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁227c 228f▷
```
       pure function phase_space_massless (x, channel) result (p)
         real(kind=default), dimension(:), intent(in) :: x
         integer, intent(in) :: channel
         type(LIPS3) :: p
         real(kind=default) :: s, t1, s2, phi, cos_theta3, phi3
         real(kind=default) :: s2_min, s2_max, t1_min, t1_max
         s = S_0
```
         ⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ *(massless case)* 225c⟩
```
         p = two_to_three (s, t1, s2, phi, cos_theta3, phi3)
```
         ⟨*Adjust Jacobian* 226a⟩
         ⟨$p_1 \leftrightarrow p_2$ *for channel #2* 227a⟩
```
       end function phase_space_massless
```

228c ⟨*Types in* cross_section 228c⟩≡   (222a) 228d▷
```
       type, public :: LIPS3_m5i2a3
          ! private
          real(kind=default) :: ma, mb, m1, m2, m3
          real(kind=default) :: s, s2, t1
          real(kind=default) :: phi, cos_theta3, phi3
          real(kind=default) :: jacobian
       end type LIPS3_m5i2a3
```

228d ⟨*Types in* cross_section 228c⟩+≡   (222a) ◁228c
```
       type, public :: x5
          ! private
          real(kind=default), dimension(5) :: x
          real(kind=default) :: jacobian
       end type x5
```

228e ⟨*Declaration of* cross_section *procedures* 223d⟩+≡   (222a) ◁228a 231a▷
```
       private :: invariants_from_p, invariants_to_p
       private :: invariants_from_x, invariants_to_x
```

228f ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁228b 229a▷
```
       pure function invariants_from_p (p, k1, k2) result (q)
         type(LIPS3), intent(in) :: p
```

```
        real(kind=default), dimension(0:), intent(in) :: k1, k2
        type(LIPS3_m5i2a3) :: q
        real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
        real(kind=default), dimension(0:3) :: k1k2, p2p3, k1p1, p3_23
        k1k2 = k1 + k2
        k1p1 = - k1 + p%p(1,:)
        p2p3 = p%p(2,:) + p%p(3,:)
        ma_2 = max (dot (k1, k1), 0.0_double)
        mb_2 = max (dot (k2, k2), 0.0_double)
        m1_2 = max (dot (p%p(1,:), p%p(1,:)), 0.0_double)
        m2_2 = max (dot (p%p(2,:), p%p(2,:)), 0.0_double)
        m3_2 = max (dot (p%p(3,:), p%p(3,:)), 0.0_double)
        q%ma = sqrt (ma_2)
        q%mb = sqrt (mb_2)
        q%m1 = sqrt (m1_2)
        q%m2 = sqrt (m2_2)
        q%m3 = sqrt (m3_2)
        q%s = dot (k1k2, k1k2)
        q%s2 = dot (p2p3, p2p3)
        q%t1 = dot (k1p1, k1p1)
        q%phi = atan2 (p%p(1,2), p%p(1,1))
        if (q%phi < 0) then
           q%phi = q%phi + 2*PI
        end if
        p3_23 = boost_momentum (p%p(3,:), p2p3)
        q%cos_theta3 = p3_23(3) / sqrt (dot_product (p3_23(1:3), p3_23(1:3)))
        q%phi3 = atan2 (p3_23(2), p3_23(1))
        if (q%phi3 < 0) then
           q%phi3 = q%phi3 + 2*PI
        end if
        q%jacobian = 1.0 / ((2*PI)**5 * 32 * q%s2) &
             * sqrt (lambda (q%s2, m2_2, m3_2) / lambda (q%s, ma_2, mb_2))
      end function invariants_from_p
```

229a ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁228f 229b▷
```
      pure function invariants_to_p (p) result (q)
        type(LIPS3_m5i2a3), intent(in) :: p
        type(LIPS3) :: q
        q = two_to_three (p%s, p%t1, p%s2, p%phi, p%cos_theta3, p%phi3)
        q%jacobian = q%jacobian * p%jacobian
      end function invariants_to_p
```

229b ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁229a 230▷

```
pure function invariants_from_x (x, s, ma, mb, m1, m2, m3) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(in) :: s, ma, mb, m1, m2, m3
  type(LIPS3_m5i2a3) :: p
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  p%ma = ma
  p%mb = mb
  p%m1 = m1
  p%m2 = m2
  p%m3 = m3
  p%s = s
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  p%s2 = s2_max * x(1) + s2_min * (1 - x(1))
  t1_min = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
           + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
             * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
           - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
             * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  p%t1 = t1_max * x(2) + t1_min * (1 - x(2))
  p%phi = 2*PI * x(3)
  p%cos_theta3 = 2 * x(4) - 1
  p%phi3 = 2*PI * x(5)
  p%jacobian = 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_from_x
```

230   ⟨*Implementation of* **cross_section** *procedures* 224a⟩+≡   (222a) ◁229b 231b▷
```
pure function invariants_to_x (p) result (x)
  type(LIPS3_m5i2a3), intent(in) :: p
  type(x5) :: x
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  t1_min = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
           + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
             * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
           - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
```

```
                    * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
         x%x(1) = (p%s2 - s2_min) / (s2_max - s2_min)
         x%x(2) = (p%t1 - t1_min) / (t1_max - t1_min)
         x%x(3) = p%phi / (2*PI)
         x%x(4) = (p%cos_theta3 + 1) / 2
         x%x(5) = p%phi3 / (2*PI)
         x%jacobian = p%jacobian * 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
       end function invariants_to_x
```

231a ⟨*Declaration of* `cross_section` *procedures* 223d⟩+≡   (222a) ◁228e 232b▷
```
         public :: sigma, sigma_raw, sigma_massless
```

231b ⟨*Implementation of* `cross_section` *procedures* 224a⟩+≡   (222a) ◁230 231c▷
```
       function sigma (x, weights, channel, grids) result (xs)
         real(kind=default), dimension(:), intent(in) :: x
         real(kind=default), dimension(:), intent(in), optional :: weights
         integer, intent(in), optional :: channel
         type(vamp_grid), dimension(:), intent(in), optional :: grids
         real(kind=default) :: xs
         real(kind=default), dimension(2,0:3) :: k
         type(LIPS3) :: p
         k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
         k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
         if (present (channel)) then
            p = phase_space (x, channel)
         else
            p = phase_space (x, 0)
         end if
         if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
            xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
                 * jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
                 !!! * p%jacobian
         else
            xs = 0.0
         end if
       end function sigma
```

231c ⟨*Implementation of* `cross_section` *procedures* 224a⟩+≡   (222a) ◁231b 232a▷
```
       function sigma_raw (k1, k2, p1, p2, q) result (xs)
         real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
         real(kind=default) :: xs
         if (cuts (k1, k2, p1, p2, q)) then
            xs = xsect (k1, k2, p1, p2, q)
```

```
        else
            xs = 0.0
        end if
    end function sigma_raw
```

232a ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁231c 232c▷
```
    function sigma_massless (x, weights, channel, grids) result (xs)
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default), dimension(:), intent(in), optional :: weights
      integer, intent(in), optional :: channel
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: xs
      real(kind=default), dimension(2,0:3) :: k
      type(LIPS3) :: p
      k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
      k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
      p = phase_space_massless (x, 0)
      if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
        xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
              * p%jacobian
      else
        xs = 0.0
      end if
    end function sigma_massless
```
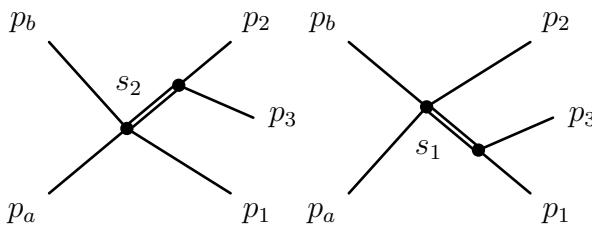
232b ⟨*Declaration of* cross_section *procedures* 223d⟩+≡   (222a) ◁231a 234a▷
```
    public :: w
```


232c ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁232a 233▷
```
    function w (x, weights, channel, grids) result (w_x)
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default), dimension(:), intent(in), optional :: weights
      integer, intent(in), optional :: channel
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: w_x
      real(kind=default), dimension(size(weights)) :: g_x
```

```
      real(kind=default), dimension(2,0:3) :: k
      type(LIPS3) :: p
      integer :: ch
      if (present (channel)) then
         ch = channel
      else
         ch = 0
      end if
      k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
      k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
      p = phase_space (x, abs (ch))
      g_x(1) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
      g_x(2) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(2,:), p%p(1,:), p%p(3,:))
      g_x(3) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(3,:), p%p(2,:), p%p(1,:))
      if (ch > 0) then
         w_x = sigma_raw (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
               / sum (weights * g_x)
      else if (ch < 0) then
         w_x = g_x(-ch) / sum (weights * g_x)
      else
         w_x = -1
      end if
   end function w
```

233 ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁232c 234c▷
```
   function sigma_rambo (x, weights, channel, grids) result (xs)
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default), dimension(:), intent(in), optional :: weights
      integer, intent(in), optional :: channel
      type(vamp_grid), dimension(:), intent(in), optional :: grids
      real(kind=default) :: xs
      real(kind=default), dimension(2,0:3) :: k
      real(kind=default), dimension(3,0:3) :: p
      k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
      k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
      p = massless_isotropic_decay (sum (k(:,0)), reshape (x, (/ 3, 4 /)))
      if (cuts (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:))) then
         xs = xsect (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:)) &
               * phase_space_volume (size (p, dim = 1), sum (k(:,0)))
      else
         xs = 0.0
      end if
   end function sigma_rambo
```

234a   ⟨*Declaration of* cross‑section *procedures* 223d⟩+≡   (222a) ◁232b 234b▷

```
public :: sigma_rambo
```

234b   ⟨*Declaration of* cross‑section *procedures* 223d⟩+≡   (222a) ◁234a 235a▷

```
public :: check_kinematics
private :: print_LIPS3_m5i2a3
```

234c   ⟨*Implementation of* cross‑section *procedures* 224a⟩+≡   (222a) ◁233 234d▷

```
subroutine check_kinematics (rng)
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), dimension(5) :: x
  real(kind=default), dimension(0:3) :: k1, k2
  type(x5) :: x1, x2
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q, q1, q2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  call tao_random_number (rng, x)
  q = invariants_from_x (x, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
  p1 = invariants_to_p (q)
  q1 = invariants_from_p (p1, k1, k2)
  p2 = phase_space (x, 1)
  q2 = invariants_from_p (p2, k1, k2)
  x1 = invariants_to_x (q1)
  x2 = invariants_to_x (q2)
  print *, p1%jacobian, p2%jacobian, x1%jacobian, x2%jacobian
  call print_lips3_m5i2a3 (q)
  call print_lips3_m5i2a3 (q1)
  call print_lips3_m5i2a3 (q2)
end subroutine check_kinematics
```

234d   ⟨*Implementation of* cross‑section *procedures* 224a⟩+≡   (222a) ◁234c 235b▷

```
subroutine print_LIPS3_m5i2a3 (p)
  type(LIPS3_m5i2a3), intent(in) :: p
  print "(1x,5('m',a1,'=',e9.2,' '))", &
        'a', p%ma, 'b', p%mb, '1', p%m1, '2', p%m2, '3', p%m3
  print "(1x,'s=',e9.2,' s2=',e9.2,' t1=',e9.2)", &
        p%s, p%s2, p%t1
  print "(1x,'phi=',e9.2,' cos(th3)=',e9.2,' phi2=',e9.2)", &
        p%phi, p%cos_theta3, p%phi3
  print "(1x,'j=',e9.2)", &
        p%jacobian
end subroutine print_LIPS3_m5i2a3
```

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

```
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
```

```
pure function phi21 (x2, dummy) result (x1)
  real(kind=default), dimension(:), intent(in) :: x2
  integer, intent(in) :: dummy
  real(kind=default), dimension(size(x2)) :: x1
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x51
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
  p2 = invariants_to_p (q2)
  p1%p(1,:) = p2%p(2,:)
  p1%p(2,:) = p2%p(1,:)
```

```
      p1%p(3,:) = p2%p(3,:)
      if (dummy < 0) then
          q1 = invariants_from_p (p1, k2, k1)
      else
          q1 = invariants_from_p (p1, k1, k2)
      end if
      x51 = invariants_to_x (q1)
      x1 = x51%x
    end function phi21
```

236a ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁235c 236b▷
```
    pure function phi1 (x1) result (p1)
      real(kind=default), dimension(:), intent(in) :: x1
      type(LIPS3) :: p1
      type(LIPS3_m5i2a3) :: q1
      q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
      p1 = invariants_to_p (q1)
    end function phi1
```

236b ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁236a 236c▷
```
    pure function phi2 (x2) result (p2)
      real(kind=default), dimension(:), intent(in) :: x2
      type(LIPS3) :: p2
      type(LIPS3_m5i2a3) :: q2
      q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
      p2 = invariants_to_p (q2)
    end function phi2
```

236c ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁236b 237a▷
```
    pure function g12 (x1) result (g)
      real(kind=default), dimension(:), intent(in) :: x1
      real(kind=default) :: g
      type(LIPS3) :: p1, p2
      type(LIPS3_m5i2a3) :: q1, q2
      type(x5) :: x52
      real(kind=default), dimension(0:3) :: k1, k2
      k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
      k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
      q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
      p1 = invariants_to_p (q1)
      p2%p(1,:) = p1%p(2,:)
      p2%p(2,:) = p1%p(1,:)
```

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```
      p2%p(3,:) = p1%p(3,:)
      q2 = invariants_from_p (p2, k2, k1)
      x52 = invariants_to_x (q2)
      g = x52%jacobian / p1%jacobian
    end function g12
```

237a ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁236c 237b▷
```
    pure function g21 (x2) result (g)
      real(kind=default), dimension(:), intent(in) :: x2
      real(kind=default) :: g
      type(LIPS3) :: p1, p2
      type(LIPS3_m5i2a3) :: q1, q2
      type(x5) :: x51
      real(kind=default), dimension(0:3) :: k1, k2
      k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
      k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
      q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
      p2 = invariants_to_p (q2)
      p1%p(1,:) = p2%p(2,:)
      p1%p(2,:) = p2%p(1,:)
      p1%p(3,:) = p2%p(3,:)
      q1 = invariants_from_p (p1, k2, k1)
      x51 = invariants_to_x (q1)
      g = x51%jacobian / p2%jacobian
    end function g21
```

237b ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁237a 237c▷
```
    pure function g1 (x1) result (g)
      real(kind=default), dimension(:), intent(in) :: x1
      real(kind=default) :: g
      type(LIPS3) :: p1
      type(LIPS3_m5i2a3) :: q1
      q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
      p1 = invariants_to_p (q1)
      g = 1 / p1%jacobian
    end function g1
```

237c ⟨*Implementation of* cross_section *procedures* 224a⟩+≡   (222a) ◁237b 238b▷
```
    pure function g2 (x2) result (g)
      real(kind=default), dimension(:), intent(in) :: x2
      real(kind=default) :: g
      type(LIPS3) :: p2
```

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```
            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
```

⟨*Declaration of* `cross_section` *procedures* 223d⟩+≡   (222a) ◁235a
```
          public :: wx
```

⟨*Implementation of* `cross_section` *procedures* 224a⟩+≡   (222a) ◁237c
```
          function wx (x, weights, channel, grids) result (w_x)
            real(kind=default), dimension(:), intent(in) :: x
            real(kind=default), dimension(:), intent(in) :: weights
            integer, intent(in) :: channel
            type(vamp_grid), dimension(:), intent(in) :: grids
            real(kind=default) :: w_x
            real(kind=default), dimension(size(weights)) :: g_x, p_q
            real(kind=default), dimension(size(x)) :: x1, x2
            real(kind=default), dimension(2,0:3) :: k
            type(LIPS3) :: q
            k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
            k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
            select case (abs (channel))
            case (1)
               x1 = x
               x2 = phi12 (x, 0)
               q = phi1 (x1)
            case (2)
               x1 = phi21 (x, 0)
               x2 = x
               q = phi2 (x2)
            end select
            p_q(1) = vamp_probability (grids(1), x1)
            p_q(2) = vamp_probability (grids(2), x2)
            g_x(1) = p_q(1) * g1 (x1)
            g_x(2) = p_q(2) * g2 (x2)
            g_x = g_x / p_q(abs(channel))
            if (channel > 0) then
               w_x = sigma_raw (k(1,:), k(2,:), q%p(1,:), q%p(2,:), q%p(3,:)) &
                     / dot_product (weights, g_x)
            else if (channel < 0) then
               w_x = vamp_probability (grids(-channel), x) / dot_product (weights, g_x)
            else
               w_x = 0
```

```
      end if
    end function wx
```

239 ⟨application.f90 222a⟩+≡   ◁222a
```
  program application
    use kinds
    use utils
    use vampi
    use mpi90
    use linalg
    use exceptions
    use kinematics, only: phase_space_volume
    use cross_section !NODEP!
    use tao_random_numbers
    implicit none
    type(vamp_grid) :: gr
    type(vamp_grids) :: grs
    real(kind=default), dimension(:,:), allocatable :: region
    real(kind=default) :: integral, standard_dev, chi_squared
    real(kind=default) :: &
         single_integral, single_standard_dev, &
         rambo_integral, rambo_standard_dev
    real(kind=default), dimension(2) :: weight_vector
    integer, dimension(2) :: calls, iterations
    type(vamp_history), dimension(100) :: history
    type(vamp_history), dimension(100,size(weight_vector)) :: histories
    type(exception) :: exc
    type(tao_random_state) :: rng
    real(kind=default), dimension(5) :: x
    real(kind=default) :: jac
    integer :: i
    integer :: num_proc, proc_id, ticks, ticks0, ticks_per_second, command
    character(len=72) :: command_line
    integer, parameter :: &
         CMD_SINGLE = 1, &
         CMD_MULTI = 2, &
         CMD_ROTATING = 3, &
         CMD_RAMBO = 4, &
         CMD_COMPARE = 5, &
         CMD_MASSLESS = 6, &
         CMD_ERROR = 0
    call mpi90_init ()
    call mpi90_size (num_proc)
```

```
call mpi90_rank (proc_id)
call system_clock (ticks0)
call tao_random_create (rng, 0)
call tao_random_seed (rng, ticks0 + proc_id)
!!! call tao_random_seed (rng, proc_id)
call vamp_create_history (history, verbose = .true.)
call vamp_create_history (histories, verbose = .true.)
iterations = (/ 3, 4 /)
calls =  (/  10000, 100000 /)
if (proc_id == 0) then
   read *, command_line
   if (command_line == "single") then
      command = CMD_SINGLE
   else if (command_line == "multi") then
      command = CMD_MULTI
   else if (command_line == "rotating") then
      command = CMD_ROTATING
   else if (command_line == "rambo") then
      command = CMD_RAMBO
   else if (command_line == "compare") then
      command = CMD_COMPARE
   else if (command_line == "massless") then
      command = CMD_MASSLESS
   else
      command = CMD_ERROR
   end if
end if
call mpi90_broadcast (command, 0)
call system_clock (ticks0)
select case (command)
case (CMD_SINGLE)
   ⟨Application in single channel mode 242a⟩
case (CMD_MASSLESS)
   ⟨Application in massless single channel mode 242b⟩
case (CMD_MULTI)
   ⟨Application in multi channel mode 243⟩
case (CMD_ROTATING)
   allocate (region(2,5))
   region(1,:) =  0.0
   region(2,:) =  1.0
   if (proc_id == 0) then
      print *, "rotating N/A yet ..."
   end if
```

```fortran
case (CMD_RAMBO)
   ⟨Application in Rambo mode 244⟩
case (CMD_COMPARE)
   ⟨Application in single channel mode 242a⟩
   single_integral = integral
   single_standard_dev = standard_dev
   ⟨Application in Rambo mode 244⟩
   if (proc_id == 0) then
      rambo_integral = integral
      rambo_standard_dev = standard_dev
      integral = &
           (single_integral / single_standard_dev**2 &
             + rambo_integral / rambo_standard_dev**2) &
         / (1.0_double / single_standard_dev**2 &
             + 1.0_double / rambo_standard_dev**2)
      standard_dev = 1.0_double &
           / sqrt (1.0_double / single_standard_dev**2 &
                   + 1.0_double / rambo_standard_dev**2)
      chi_squared = &
           ((single_integral - integral)**2 / single_standard_dev**2) &
               + ((rambo_integral - integral)**2 / rambo_standard_dev**2)
      print *, "S&R:    ", integral, standard_dev, chi_squared
   end if
case default
   if (proc_id == 0) then
      print *, "???: ", command
      !!! TO BE REMOVED !!!
      call check_kinematics (rng)
      allocate (region(2,5))
      region(1,:) = 0
      region(2,:) = 1
      do i = 1, 10
         call tao_random_number (rng, x)
         call vamp_jacobian (phi12, 0, x, region, jac)
         print *, "12: ", jac, 1 / g12 (x), jac * g12 (x) - 1
         call vamp_jacobian (phi21, 0, x, region, jac)
         print *, "21: ", jac, 1 / g21 (x), jac * g21 (x) - 1
         print *, "1:   ", real(x)
         print *, "2:   ", real(phi12(phi21(x,0),0))
         print *, "2’:  ", real(phi12(phi21(x,-1),-1))
         print *, "3:   ", real(phi21(phi12(x,0),0))
         print *, "3’:  ", real(phi21(phi12(x,-1),-1))
         print *, "2-1: ", real(phi12(phi21(x,0),0) - x)
```

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

242a ⟨*Application in single channel mode* 242a⟩≡   (239)
```
         allocate (region(2,5))
         region(1,:) =  0.0
         region(2,:) =  1.0
         call vamp_create_grid (gr, region, calls(1))
         call clear_exception (exc)
         call vamp_sample_grid &
              (rng, gr, sigma, iterations(1), history = history, exc = exc)
         call handle_exception (exc)
         call vamp_discard_integral (gr, calls(2))
         call vamp_sample_grid &
              (rng, gr, sigma, iterations(2), &
               integral, standard_dev, chi_squared, &
               history = history(iterations(1)+1:), exc = exc)
         call handle_exception (exc)
         call vamp_print_history (history, "single")
         if (proc_id == 0) then
            print *, "SINGLE: ", integral, standard_dev, chi_squared
         end if
         call vamp_write_grid (gr, "application.grid")
         call vamp_delete_grid (gr)
         deallocate (region)
```

242b ⟨*Application in massless single channel mode* 242b⟩≡   (239)
```
         allocate (region(2,5))
```

242

```
      region(1,:) =  0.0
      region(2,:) =  1.0
      call vamp_create_grid (gr, region, calls(1))
      call clear_exception (exc)
      call vamp_sample_grid &
           (rng, gr, sigma_massless, iterations(1), history = history, exc = exc)
      call handle_exception (exc)
      call vamp_discard_integral (gr, calls(2))
      call vamp_sample_grid &
           (rng, gr, sigma_massless, iterations(2), &
            integral, standard_dev, chi_squared, &
            history = history(iterations(1)+1:), exc = exc)
      call handle_exception (exc)
      call vamp_print_history (history, "single")
      if (proc_id == 0) then
         print *, "M=0:    ", integral, standard_dev, chi_squared
      end if
      call vamp_write_grid (gr, "application.grid")
      call vamp_delete_grid (gr)
      deallocate (region)
```

243   ⟨*Application in multi channel mode* 243⟩≡   (239)
```
      allocate (region(2,5))
      region(1,:) =  0.0
      region(2,:) =  1.0
      weight_vector = 1.0
      if (proc_id == 0) then
         read *, weight_vector
      end if
      call mpi90_broadcast (weight_vector, 0)
      weight_vector = weight_vector / sum (weight_vector)
      call vamp_create_grids (grs, region, calls(1), weight_vector)
      do i = 1, 3
         call clear_exception (exc)
         call vamp_sample_grids &
              (rng, grs, wx, iterations(1), &
               history = history(1+(i-1)*iterations(1):), &
               histories = histories(1+(i-1)*iterations(1):,:), exc = exc)
         call handle_exception (exc)
         call vamp_refine_weights (grs)
      end do
      call vamp_discard_integrals (grs, calls(2))
      call vamp_sample_grids &
           (rng, grs, wx, iterations(2), &
```

```
                integral, standard_dev, chi_squared, &
                history = history(3*iterations(1)+1:), &
                histories = histories(3*iterations(1)+1:,:), exc = exc)
        call handle_exception (exc)
        call vamp_print_history (history, "multi")
        call vamp_print_history (histories, "multi")
        if (proc_id == 0) then
           print *, "MULTI:  ", integral, standard_dev, chi_squared
        end if
        call vamp_write_grids (grs, "application.grids")
        call vamp_delete_grids (grs)
        deallocate (region)
```

244   ⟨*Application in Rambo mode* 244⟩≡   (239)

```
        allocate (region(2,12))
        region(1,:) =  0.0
        region(2,:) =  1.0
        call vamp_create_grid (gr, region, calls(1))
        call clear_exception (exc)
        call vamp_sample_grid &
             (rng, gr, sigma_rambo, iterations(1), history = history, exc = exc)
        call handle_exception (exc)
        call vamp_discard_integral (gr, calls(2))
        call vamp_sample_grid &
             (rng, gr, sigma_rambo, iterations(2), &
              integral, standard_dev, chi_squared, &
              history = history(iterations(1)+1:), exc = exc)
        call handle_exception (exc)
        call vamp_print_history (history, "rambo")
        if (proc_id == 0) then
           print *, "RAMBO:  ", integral, standard_dev, chi_squared
        end if
        call vamp_delete_grid (gr)
        deallocate (region)
```

—A—
Constants

A.1 Kinds

This borders on overkill, but it is the most portable way to get double precision in standard Fortran without relying on `kind (1.0D0)` Currently, it is possible to change `double` to any other supported real kind. The MPI interface is a potential trouble source for such things, however.

245a ⟨vamp_kinds.f90 245a⟩≡

```
! vamp_kinds.f90 --
⟨Copyleft notice 1⟩
module kinds
  implicit none
  integer, parameter, private :: single = &
      & selected_real_kind (precision(1.0), range(1.0))
  integer, parameter, private :: double = &
      & selected_real_kind (precision(1.0_single) + 1, range(1.0_single) + 1)
  integer, parameter, private :: extended = &
      & selected_real_kind (precision (1.0_double) + 1, range (1.0_double))
  integer, parameter, public :: default = double
  character(len=*), public, parameter :: KINDS_RCS_ID = &
      "$Id: kinds.nw 314 2010-04-17 20:32:33Z ohl $"
end module kinds
```

A.2 Mathematical and Physical Constants

245b ⟨constants.f90 245b⟩≡

```
! constants.f90 --
⟨Copyleft notice 1⟩
```

```fortran
module constants
  use kinds
  implicit none
  private
  real(kind=default), public, parameter :: &
       PI = 3.1415926535897932384626433832795028841972_default
  character(len=*), public, parameter :: CONSTANTS_RCS_ID = &
       "$Id: constants.nw 314 2010-04-17 20:32:33Z ohl $"
end module constants
```

—B—
ERRORS AND EXCEPTIONS

Fortran95 does not allow *any* I/O in `pure` and `elemental` procedures, not even output to the unit `*`. A `stop` statement is verboten as well. Therefore we have to use condition codes

247a ⟨exceptions.f90 247a⟩≡
```
  ! exceptions.f90 --
  ⟨Copyleft notice 1⟩
module exceptions
  use kinds
  implicit none
  private
  ⟨Declaration of exceptions procedures 248b⟩
  ⟨Interfaces of exceptions procedures (never defined)⟩
  ⟨Variables in exceptions 247c⟩
  ⟨Declaration of exceptions types 247b⟩
  character(len=*), public, parameter :: EXCEPTIONS_RCS_ID = &
       "$Id: exceptions.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of exceptions procedures 248c⟩
end module exceptions
```

247b ⟨Declaration of exceptions types 247b⟩≡   (247a)
```
type, public :: exception
   integer :: level = EXC_NONE
   character(len=NAME_LENGTH) :: message = ""
   character(len=NAME_LENGTH) :: origin = ""
end type exception
```

247c ⟨Variables in exceptions 247c⟩≡   (247a) 248a ▷
```
integer, public, parameter :: &
     EXC_NONE = 0, &
     EXC_INFO = 1, &
     EXC_WARN = 2, &
```

247

```
        EXC_ERROR = 3, &
        EXC_FATAL = 4
```

248a ⟨*Variables in* exceptions 247c⟩+≡   (247a) ◁247c
```
   integer, private, parameter :: EXC_DEFAULT = EXC_ERROR
   integer, private, parameter :: NAME_LENGTH = 64
```

248b ⟨*Declaration of* exceptions *procedures* 248b⟩≡   (247a) 248d ▷
```
   public :: handle_exception
```

248c ⟨*Implementation of* exceptions *procedures* 248c⟩≡   (247a) 248e ▷
```
   subroutine handle_exception (exc)
     type(exception), intent(inout) :: exc
     character(len=10) :: name
     if (exc%level > 0) then
        select case (exc%level)
           case (EXC_NONE)
              name = "(none)"
           case (EXC_INFO)
              name = "info"
           case (EXC_WARN)
              name = "warning"
           case (EXC_ERROR)
              name = "error"
           case (EXC_FATAL)
              name = "fatal"
           case default
              name = "invalid"
        end select
        print *, trim (exc%origin), ": ", trim(name), ": ", trim (exc%message)
        if (exc%level >= EXC_FATAL) then
           print *, "terminated."
           stop
        end if
     end if
   end subroutine handle_exception
```

248d ⟨*Declaration of* exceptions *procedures* 248b⟩+≡   (247a) ◁248b
```
   public :: raise_exception, clear_exception, gather_exceptions
```

Raise an exception, but don't overwrite the messages in exc if it holds a more
severe exception. This way we can accumulate error codes across procedure
calls. We have exc optional to simplify life for the cslling procedures, which
might have it optional themselves.

248e ⟨*Implementation of* exceptions *procedures* 248c⟩+≡   (247a) ◁248c 249a ▷
```
   elemental subroutine raise_exception (exc, level, origin, message)
```

```fortran
      type(exception), intent(inout), optional :: exc
      integer, intent(in), optional :: level
      character(len=*), intent(in), optional :: origin, message
      integer :: local_level
      if (present (exc)) then
         if (present (level)) then
            local_level = level
         else
            local_level = EXC_DEFAULT
         end if
         if (exc%level < local_level) then
            exc%level = local_level
            if (present (origin)) then
               exc%origin = origin
            else
               exc%origin = "[vamp]"
            end if
            if (present (message)) then
               exc%message = message
            else
               exc%message = "[vamp]"
            end if
         end if
      end if
   end subroutine raise_exception
```

249a   ⟨*Implementation of* exceptions *procedures* 248c⟩+≡   (247a) ◁248e 249b▷

```fortran
   elemental subroutine clear_exception (exc)
     type(exception), intent(inout) :: exc
     exc%level = 0
     exc%message = ""
     exc%origin = ""
   end subroutine clear_exception
```

249b   ⟨*Implementation of* exceptions *procedures* 248c⟩+≡   (247a) ◁249a

```fortran
   pure subroutine gather_exceptions (exc, excs)
     type(exception), intent(inout) :: exc
     type(exception), dimension(:), intent(in) :: excs
     integer :: i
     i = sum (maxloc (excs%level))
     if (exc%level < excs(i)%level) then
        call raise_exception (exc, excs(i)%level, excs(i)%origin, &
                              excs(i)%message)
     end if
   end subroutine gather_exceptions
```

Here's how to use gather_exceptions. elemental_procedure

250 ⟨Idioms 101c⟩+≡   ◁101c

```
call clear_exception (excs)
call elemental_procedure_1 (y, x, excs)
call elemental_procedure_2 (b, a, excs)
if (any (excs%level > 0)) then
   call gather_exceptions (exc, excs)
   return
end if
```

—C—
THE ART OF RANDOM NUMBERS

Volume two of Donald E. Knuth' *The Art of Computer Programming* [16] has always been celebrated as a prime reference for random number generation. Recently, the third edition has been published and it contains a gem of a *portable* random number generator. It generates 30-bit integers with the following desirable properties

- they pass all the tests from George Marsaglia's "diehard" suite of tests for random number generators [24] (but see [16] for a caveat regarding the "birthday-spacing" test)

- they can be generated with portable signed 32-bit arithmetic (Fortran can't do unsigned arithmetic)

- it is faster than other lagged Fibonacci generators

- it can create at least $2^{30} - 2$ independent sequences

We implement the improved versions available as FORTRAN77 code from

    http://www-cs-faculty.stanford.edu/~uno/programs.html#rng

that contain a streamlined seeding alorithm with better independence of substreams.

C.1   Application Program Interface

A function returning single reals and integers. Note that the static version without the `tao_random_state` argument does not require initialization. It will behave as if `call` `tao_random_seed`(0) had been executed. On the other hand, the parallelizable version with the explicit `tao_random_state` will fail

if none of the `tao_random_create` have been called for the state. (This is a deficiency of Fortran90 that can be fixed in Fortran95).

252a   ⟨*API documentation* 252a⟩≡   252b ▷
```
call tao_random_number (r)
call tao_random_number (s, r)
```

The state of the random number generator comes in two variaties: 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.

252b   ⟨*API documentation* 252a⟩+≡   ◁ 252a   252c ▷
```
type(tao_random_state) :: s
type(tao_random_raw_state) :: rs
```

Subroutines filling arrays of reals and integers:

252c   ⟨*API documentation* 252a⟩+≡   ◁ 252b   252d ▷
```
call tao_random_number (a, num = n)
call tao_random_number (s, a, num = n)
```

Subroutine for changing the seed:

252d   ⟨*API documentation* 252a⟩+≡   ◁ 252c   252e ▷
```
call tao_random_seed (seed = seed)
call tao_random_seed (s, seed = seed)
```

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

252e   ⟨*API documentation* 252a⟩+≡   ◁ 252d   252f ▷
```
call tao_random_luxury ()
call tao_random_luxury (s)
```

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

252f   ⟨*API documentation* 252a⟩+≡   ◁ 252e   252g ▷
```
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:

252g   ⟨*API documentation* 252a⟩+≡   ◁ 252f   252h ▷
```
call tao_random_luxury (x)
call tao_random_luxury (s, x)
```

Create a `tao_random_state`

252h   ⟨*API documentation* 252a⟩+≡   ◁ 252g   253a ▷
```
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`

253a ⟨*API documentation* 252a⟩+≡   ◁252h 253b▷
```
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`

253b ⟨*API documentation* 252a⟩+≡   ◁253a 253c▷
```
call tao_random_destroy (s)
```

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

253c ⟨*API documentation* 252a⟩+≡   ◁253b 253d▷
```
call tao_random_copy (lhs, rhs)
lhs = rhs
```

253d ⟨*API documentation* 252a⟩+≡   ◁253c 253e▷
```
call tao_random_flush (s)
```

253e ⟨*API documentation* 252a⟩+≡   ◁253d 253f▷
```
call tao_random_read (s, unit)
call tao_random_write (s, unit)
```

253f ⟨*API documentation* 252a⟩+≡   ◁253e 253g▷
```
call tao_random_test (name = name)
```

Here is a sample application of random number states:

253g ⟨*API documentation* 252a⟩+≡   ◁253f 253h▷
```
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.

253h ⟨*API documentation* 252a⟩+≡   ◁253g
```
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

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

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

254a ⟨*Parameters in* `tao_random_numbers` 254a⟩≡   (273d 274a) 255a ▷
```
   integer, parameter, private :: K = 100, L = 37
```

Other good choices for K and L are (cf. [16], table 1 in section 3.2.2, p. 29)

254b ⟨*Parameters in* `tao_random_numbers` *(alternatives)* 254b⟩≡
```
   integer, parameter, private :: K =  55, L =  24
   integer, parameter, private :: K =  89, L =  38
   integer, parameter, private :: K = 100, L =  37
   integer, parameter, private :: K = 127, L =  30
   integer, parameter, private :: K = 258, L =  83
   integer, parameter, private :: K = 378, L = 107
   integer, parameter, private :: K = 607, L = 273
```

A modulus of 2^{30} is the largest we can handle in *portable* (i.e. *signed*) 32-bit arithmetic

254c ⟨*Variables in 30-bit* `tao_random_numbers` 254c⟩≡   (273d) 256b ▷
```
   integer(kind=tao_i32), parameter, private :: M = 2**30
```

254

generate fills the array $a_1, \ldots, a_n$ with random integers $0 \le a_i < 2^{30}$. We *must* have at least $n \ge K$. Higher values don't change the results, but make generate more efficient (about a factor of two, asymptotically). For $K = 100$, DEK recommends $n \ge 1000$. 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:

255a ⟨*Parameters in* tao_random_numbers 254a⟩+≡   (273d 274a) ◁254a
```
integer, parameter, private :: DEFAULT_BUFFER_SIZE = 1009
```

Since users are not expected to call generate directly, we do *not* check for $n \ge K$ and assume that the caller knows what (s)he's doing . . .

255b ⟨*Implementation of 30-bit* tao_random_numbers 255b⟩≡   (273d) 256e▷
```
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 255d⟩
end subroutine generate
```

255c ⟨*Declaration of* tao_random_numbers 255c⟩≡   (273d 274a) 259b▷
```
private :: generate
```

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

255d ⟨*Load* a *and refresh* state 255d⟩≡   (255b) 255e▷
```
a(1:K) = state(1:K)
```

The remaining $n - K$ random numbers can be gotten directly from the recursion (C.1). Note that Fortran90's modulo intrinsic does the right thing, since it guarantees (unlike Fortran77's mod) that $0 \le \texttt{modulo}(a, m) < a$ if $m > 0$).

255e ⟨*Load* a *and refresh* state 255d⟩+≡   (255b) ◁255d 255f▷
```
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 invokation of generate.

255f ⟨*Load* a *and refresh* state 255d⟩+≡   (255b) ◁255e
```
state(1:L) = modulo (a(n+1-K:n+L-K) - a(n+1-L:n), M)
do j = L+1, K
    state(j) = modulo (a(n+j-K) - state(j-L), M)
end do
```

C.2.2 Initialization of 30-bit Random Numbers

The non-trivial and most beautiful part is the algorithm to initialize the random number generator state `state` with the first K numbers. I haven't studied algebra over finite fields in sufficient depth to consider the mathematics behind it straightforward. The commentary below is rather verbose and reflects my understanding of DEK's rather terse remarks (solution to exercise 3.6-9 [16]).

256a ⟨*Implementation of* `tao_random_numbers` 256a⟩≡   (273d 274a) 256c ▷
```
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`:

256b ⟨*Variables in 30-bit* `tao_random_numbers` 254c⟩+≡   (273d) ◁254c 275c ▷
```
integer(kind=tao_i32), dimension(K), save, private :: s_state
logical, save, private :: s_virginal = .true.
```

256c ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁256a 256d ▷
```
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
```

256d ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁256c 262d ▷
```
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`.

256e ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁255b 267c ▷
```
pure subroutine seed_stateless (state, seed)
  integer(kind=tao_i32), dimension(:), intent(out) :: state
  integer, optional, intent(in) :: seed
  ⟨Parameters local to tao_random_seed 257a⟩
  integer :: seed_value, j, s, t
  integer(kind=tao_i32), dimension(2*K-1) :: x
  ⟨Set up seed_value from seed or DEFAULT_SEED 257c⟩
```

$\langle$*Bootstrap the* x *buffer* 257d$\rangle$
$\langle$*Set up* s *and* t 257f$\rangle$
```
do
```
    $\langle p(z) \to p(z)^2 \ (modulo \ z^K + z^L + 1)$ 258a$\rangle$
    $\langle p(z) \to zp(z) \ (modulo \ z^K + z^L + 1)$ 258c$\rangle$
    $\langle$*Shift* s *or* t *and exit if* t ≤ 0 258d$\rangle$
```
end do
```
$\langle$*Fill* state *from* x 258e$\rangle$
$\langle$*Warm up* state 258f$\rangle$
```
  end subroutine seed_stateless
```

Any default will do

257a $\langle$*Parameters local to* tao_random_seed 257a$\rangle\equiv$ (256e 260a)   257b $\triangleright$
```
   integer, parameter :: DEFAULT_SEED = 0
```

These must not be changed:

257b $\langle$*Parameters local to* tao_random_seed 257a$\rangle+\equiv$ (256e 260a) $\triangleleft$257a
```
   integer, parameter :: MAX_SEED = 2**30 - 3
   integer, parameter :: TT = 70
```

257c $\langle$*Set up* seed_value *from* seed *or* DEFAULT_SEED 257c$\rangle\equiv$ (256e 260a)
```
   if (present (seed)) then
      seed_value = modulo (seed, MAX_SEED + 1)
   else
      seed_value = DEFAULT_SEED
   end if
```

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

257d $\langle$*Bootstrap the* x *buffer* 257d$\rangle\equiv$ (256e)   257e $\triangleright$
```
   s = seed_value - modulo (seed_value, 2) + 2
   do j = 1, K
      x(j) = s
      s = 2*s
      if (s >= M) then
         s = s - M + 2
      end if
   end do
   x(K+1:2*K-1) = 0
```

Make x_2 (and only x_2) odd:

257e $\langle$*Bootstrap the* x *buffer* 257d$\rangle+\equiv$ (256e) $\triangleleft$257d
```
   x(2) = x(2) + 1
```

257f $\langle$*Set up* s *and* t 257f$\rangle\equiv$ (256e 260a)
```
   s = seed_value
   t = TT - 1
```

Consider the polynomial

$$p(z) = \sum_{n=1}^{K} x_n z^{n-1} = x_K z^{K-1} + \ldots + x_2 z + x_1 \qquad (C.2)$$

We have $p(z)^2 = p(z^2) \mod 2$ because cross terms have an even coefficient and $x_n^2 = x_n \mod 2$. Therefore we can square the polynomial by shifting the coefficients. The coefficients for $n > K$ will be reduced.

258a $\langle p(z) \to p(z)^2 \ (modulo \ z^K + z^L + 1) \ 258a\rangle\equiv$ (256e) 258b$\triangleright$
```
  x(3:2*K-1:2) = x(2:K)
  x(2:2*K-2:2) = 0
```

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

258b $\langle p(z) \to p(z)^2 \ (modulo \ z^K + z^L + 1) \ 258a\rangle+\equiv$ (256e) $\triangleleft$258a
```
  do j = 2*K-1, K+1, -1
    x(j-(K-L)) = modulo (x(j-(K-L))-x(j), M)
    x(j-K)=modulo (x(j-K)-x(j), M)
  end do
```

258c $\langle p(z) \to zp(z) \ (modulo \ z^K + z^L + 1) \ 258c\rangle\equiv$ (256e)
```
  if (modulo (s, 2) == 1) then
    x(2:K+1) = x(1:K)
    x(1) = x(K+1)
    x(L+1) = modulo (x(L+1) - x(K+1), M)
  end if
```

258d $\langle$*Shift* s *or* t *and exit if* t ≤ 0 258d$\rangle\equiv$ (256e 260a)
```
  if (s /= 0) then
    s = s / 2
  else
    t = t - 1
  end if
  if (t <= 0) then
    exit
  end if
```

258e $\langle$*Fill* state *from* x 258e$\rangle\equiv$ (256e 260a)
```
  state(1:K-L) = x(L+1:K)
  state(K-L+1:K) = x(1:L)
```

258f $\langle$*Warm up* state 258f$\rangle\equiv$ (256e 260a)
```
  do j = 1, 10
    call generate (x, state)
  end do
```

259a   ⟨*Interfaces of* `tao_random_numbers` *259a*⟩≡   (273d 274a) 262a▷

```
interface tao_random_seed
   module procedure ⟨Specific procedures for tao_random_seed 259c⟩
end interface
```

259b   ⟨*Declaration of* `tao_random_numbers` *255c*⟩+≡   (273d 274a) ◁255c 260b▷

```
private :: ⟨Specific procedures for tao_random_seed 259c⟩
```

259c   ⟨*Specific procedures for* `tao_random_seed` *259c*⟩≡   (259)

```
seed_static, seed_state, seed_raw_state
```

C.2.3   Generation of 52-bit Random Numbers

$$X_j = (X_{j-K} + X_{j-L}) \mod 1 \qquad\qquad (C.3)$$

259d   ⟨*Variables in 52-bit* `tao_random_numbers` *259d*⟩≡   (274a) 259e▷

```
real(kind=tao_r64), parameter, private :: M = 1.0_tao_r64
```

The state of the internal routines

259e   ⟨*Variables in 52-bit* `tao_random_numbers` *259d*⟩+≡   (274a) ◁259d 276b▷

```
real(kind=tao_r64), dimension(K), save, private :: s_state
logical, save, private :: s_virginal = .true.
```

259f   ⟨*Implementation of 52-bit* `tao_random_numbers` *259f*⟩≡   (274a) 260a▷

```
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 259g⟩
end subroutine generate
```

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

259g   ⟨*Load 52-bit* `a` *and refresh* `state` *259g*⟩≡   (259f)

```
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`.

260a ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁259f 268a▷

```
pure subroutine seed_stateless (state, seed)
  real(kind=tao_r64), dimension(:), intent(out) :: state
  integer, optional, intent(in) :: seed
  ⟨Parameters local to tao_random_seed 257a⟩
  ⟨Variables local to 52-bit tao_random_seed 260c⟩
  ⟨Set up seed_value from seed or DEFAULT_SEED 257c⟩
  ⟨Bootstrap the 52-bit x buffer 260e⟩
  ⟨Set up s and t 257f⟩
  do
      ⟨52-bit p(z) → p(z)² (modulo zᴷ + zᴸ + 1) 261a⟩
      ⟨52-bit p(z) → zp(z) (modulo zᴷ + zᴸ + 1) 261c⟩
      ⟨Shift s or t and exit if t ≤ 0 258d⟩
  end do
  ⟨Fill state from x 258e⟩
  ⟨Warm up state 258f⟩
end subroutine seed_stateless
```

260b ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁259b 262b▷

```
private :: seed_stateless
```

260c ⟨*Variables local to 52-bit* `tao_random_seed` 260c⟩≡   (260a) 260d▷

```
real(kind=tao_r64), parameter :: ULP = 2.0_tao_r64**(-52)
```

260d ⟨*Variables local to 52-bit* `tao_random_seed` 260c⟩+≡   (260a) ◁260c

```
real(kind=tao_r64), dimension(2*K-1) :: x
real(kind=tao_r64) :: ss
integer :: seed_value, t, s, j
```

260e ⟨*Bootstrap the 52-bit* `x` *buffer* 260e⟩≡   (260a) 260f▷

```
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
```

260f ⟨*Bootstrap the 52-bit* `x` *buffer* 260e⟩+≡   (260a) ◁260e

```
x(2) = x(2) + ULP
```

261a $\langle$*52-bit $p(z) \to p(z)^2$ (modulo $z^K + z^L + 1$) 261a*$\rangle\equiv$ (260a) 261b $\triangleright$

```
  x(3:2*K-1:2) = x(2:K)
  x(2:2*K-2:2) = 0
```

This works because 2*K-1 is odd

261b $\langle$*52-bit $p(z) \to p(z)^2$ (modulo $z^K + z^L + 1$) 261a*$\rangle+\equiv$ (260a) $\triangleleft$261a

```
  do j = 2*K-1, K+1, -1
     x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
     x(j-K) = modulo (x(j-K) + x(j), M)
  end do
```

261c $\langle$*52-bit $p(z) \to zp(z)$ (modulo $z^K + z^L + 1$) 261c*$\rangle\equiv$ (260a)

```
  if (modulo (s, 2) == 1) THEN
     x(2:K+1) = x(1:K)
     x(1) = x(K+1)
     x(L+1) = modulo (x(L+1) + x(K+1), M)
  end if
```

C.3   The State

261d $\langle$*Declaration of 30-bit* tao_random_numbers *types* 261d$\rangle\equiv$ (273d) 261e $\triangleright$

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

261e $\langle$*Declaration of 30-bit* tao_random_numbers *types* 261d$\rangle+\equiv$ (273d) $\triangleleft$261d

```
  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
```

261f $\langle$*Declaration of 52-bit* tao_random_numbers *types* 261f$\rangle\equiv$ (274a) 261g $\triangleright$

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

261g $\langle$*Declaration of 52-bit* tao_random_numbers *types* 261f$\rangle+\equiv$ (274a) $\triangleleft$261f

```
  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

⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁259a 263e▷
```
    interface tao_random_create
       module procedure ⟨Specific procedures for tao_random_create 262c⟩
    end interface
```

262b ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁260b 264a▷
```
    private :: ⟨Specific procedures for tao_random_create 262c⟩
```

262c ⟨*Specific procedures for* `tao_random_create` 262c⟩≡   (262)
```
    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.

262d ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁256d 262e▷
```
    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
```

262e ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁262d 263a▷
```
    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)
```

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```
        end subroutine create_state_from_state
```

263a ⟨*Implementation of* tao‿random‿numbers 256a⟩+≡   (273d 274a) ◁262e 263b▷
```
    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
```

263b ⟨*Implementation of* tao‿random‿numbers 256a⟩+≡   (273d 274a) ◁263a 263c▷
```
    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
```

263c ⟨*Implementation of* tao‿random‿numbers 256a⟩+≡   (273d 274a) ◁263b 263d▷
```
    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
```

263d ⟨*Implementation of* tao‿random‿numbers 256a⟩+≡   (273d 274a) ◁263c 264b▷
```
    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

263e ⟨*Interfaces of* tao‿random‿numbers 259a⟩+≡   (273d 274a) ◁262a 264d▷
```
    interface tao_random_destroy
       module procedure destroy_state, destroy_raw_state
    end interface
```

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264a   ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁262b 264f▷
```
private :: destroy_state, destroy_raw_state
```

264b   ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁263d 264c▷
```
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

264c   ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁264b 264h▷
```
elemental subroutine destroy_raw_state (s)
  type(tao_random_raw_state), intent(inout) :: s
end subroutine destroy_raw_state
```

C.3.3   Copying

264d   ⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁263e 264e▷
```
interface tao_random_copy
   module procedure ⟨Specific procedures for tao_random_copy 264g⟩
end interface
```

264e   ⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁264d 265e▷
```
interface assignment(=)
   module procedure ⟨Specific procedures for tao_random_copy 264g⟩
end interface
```

264f   ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁264a 266a▷
```
public :: assignment(=)
private :: ⟨Specific procedures for tao_random_copy 264g⟩
```

264g   ⟨*Specific procedures for* `tao_random_copy` 264g⟩≡   (264)
```
copy_state, copy_raw_state, &
copy_raw_state_to_state, copy_state_to_raw_state
```

264h   ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁264c 265a▷
```
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
```

265a ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁264h 265b▷

```
    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
```

265b ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁265a 265c▷

```
    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
```

265c ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁265b 265d▷

```
    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

265d ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁265c 266d▷

```
    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

265e ⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁264e 266b▷

```
    interface tao_random_write
      module procedure &
           write_state_unit, write_state_name, &
           write_raw_state_unit, write_raw_state_name
    end interface
```

266a ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁264f 266c▷
```
  private :: write_state_unit, write_state_name
  private :: write_raw_state_unit, write_raw_state_name
```

266b ⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁265e 270b▷
```
  interface tao_random_read
     module procedure &
          read_state_unit, read_state_name, &
          read_raw_state_unit, read_raw_state_name
  end interface
```

266c ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁266a 269b▷
```
  private :: read_state_unit, read_state_name
  private :: read_raw_state_unit, read_raw_state_name
```

266d ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁265d 266e▷
```
  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
```

266e ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁266d 267a▷
```
  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)
```

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```
        read (unit = unit, fmt = *)
        read (unit = unit, fmt = *)
      end subroutine read_state_unit
```

267a ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁266e 267b▷
```
      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
```

267b ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁267a 268e▷
```
      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
```

267c ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁256e 267e▷
```
      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
```

267d ⟨*Declaration of 30-bit* `tao_random_numbers` 267d⟩≡   (273d) 267f▷
```
      private :: write_state_array
```

267e ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁267c 270d▷
```
      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
```

267f ⟨*Declaration of 30-bit* `tao_random_numbers` 267d⟩+≡   (273d) ◁267d 281c▷
```
      private :: read_state_array
```

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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 …

268a ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁260a 268c▷

```
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
```

268b ⟨*Declaration of 52-bit* `tao_random_numbers` 268b⟩≡   (274a) 268d▷

```
private :: write_state_array
```

268c ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁268a 272b▷

```
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
```

268d ⟨*Declaration of 52-bit* `tao_random_numbers` 268b⟩+≡   (274a) ◁268b 281g▷

```
private :: read_state_array
```

268e ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁267b 269c▷

```
subroutine find_free_unit (u, iostat)
  integer, intent(out) :: u
  integer, intent(out), optional :: iostat
  logical :: exists, is_open
  integer :: i, status
  do i = MIN_UNIT, MAX_UNIT
     inquire (unit = i, exist = exists, opened = is_open, &
              iostat = status)
     if (status == 0) then
        if (exists .and. .not. is_open) then
           u = i
           if (present (iostat)) then
```

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```
                iostat = 0
            end if
            return
        end if
      end if
    end do
    if (present (iostat)) then
        iostat = -1
    end if
    u = -1
  end subroutine find_free_unit
```

269a ⟨*Variables in* tao_random_numbers 269a⟩≡   (273d 274a)
      `integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99`

269b ⟨*Declaration of* tao_random_numbers 255c⟩+≡   (273d 274a) ◁266c 270c▷
      `private :: find_free_unit`

269c ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁268e 269d▷
```
    subroutine write_state_name (s, name)
      type(tao_random_state), intent(in) :: s
      character(len=*), intent(in) :: name
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "write", status = "replace", file = name)
      call write_state_unit (s, unit)
      close (unit = unit)
    end subroutine write_state_name
```

269d ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁269c 269e▷
```
    subroutine write_raw_state_name (s, name)
      type(tao_random_raw_state), intent(in) :: s
      character(len=*), intent(in) :: name
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "write", status = "replace", file = name)
      call write_raw_state_unit (s, unit)
      close (unit = unit)
    end subroutine write_raw_state_name
```

269e ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁269d 270a▷
```
    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
```

270a ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁269e 281i▷
```
      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!

270b ⟨*Interfaces of* `tao_random_numbers` 259a⟩+≡   (273d 274a) ◁266b
```
      interface tao_random_marshal_size
        module procedure marshal_state_size, marshal_raw_state_size
      end interface
      interface tao_random_marshal
        module procedure marshal_state, marshal_raw_state
      end interface
      interface tao_random_unmarshal
        module procedure unmarshal_state, unmarshal_raw_state
      end interface
```

270c ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁269b 274b▷
```
      public :: tao_random_marshal
      private :: marshal_state, marshal_raw_state
      public :: tao_random_marshal_size
      private :: marshal_state_size, marshal_raw_state_size
      public :: tao_random_unmarshal
      private :: unmarshal_state, unmarshal_raw_state
```

270d ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁267e 271a▷
```
      pure subroutine marshal_state (s, ibuf, dbuf)
        type(tao_random_state), intent(in) :: s
```

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```
        integer, dimension(:), intent(inout) :: ibuf
        real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
        integer :: buf_size
        buf_size = size (s%buffer)
        ibuf(1) = s%buffer_end
        ibuf(2) = s%last
        ibuf(3) = buf_size
        ibuf(4:3+buf_size) = s%buffer
        call marshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
      end subroutine marshal_state
```

271a ⟨*Implementation of 30-bit* tao‗random‗numbers 255b⟩+≡   (273d) ◁270d 271b▷
```
      pure subroutine marshal_state_size (s, iwords, dwords)
        type(tao_random_state), intent(in) :: s
        integer, intent(out) :: iwords, dwords
        call marshal_raw_state_size (s%state, iwords, dwords)
        iwords = iwords + 3 + size (s%buffer)
      end subroutine marshal_state_size
```

271b ⟨*Implementation of 30-bit* tao‗random‗numbers 255b⟩+≡   (273d) ◁271a 271c▷
```
      pure subroutine unmarshal_state (s, ibuf, dbuf)
        type(tao_random_state), intent(inout) :: s
        integer, dimension(:), intent(in) :: ibuf
        real(kind=tao_r64), dimension(:), intent(in) :: dbuf
        integer :: buf_size
        s%buffer_end = ibuf(1)
        s%last = ibuf(2)
        buf_size = ibuf(3)
        s%buffer = ibuf(4:3+buf_size)
        call unmarshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
      end subroutine unmarshal_state
```

271c ⟨*Implementation of 30-bit* tao‗random‗numbers 255b⟩+≡   (273d) ◁271b 271d▷
```
      pure subroutine marshal_raw_state (s, ibuf, dbuf)
        type(tao_random_raw_state), intent(in) :: s
        integer, dimension(:), intent(inout) :: ibuf
        real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
        ibuf(1) = size (s%x)
        ibuf(2:1+size(s%x)) = s%x
      end subroutine marshal_raw_state
```

271d ⟨*Implementation of 30-bit* tao‗random‗numbers 255b⟩+≡   (273d) ◁271c 272a▷
```
      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)
```

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```
        dwords = 0
      end subroutine marshal_raw_state_size
```

272a ⟨*Implementation of 30-bit* tao_random_numbers 255b⟩+≡   (273d) ◁271d 275a▷
```
  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
```

272b ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁268c 272c▷
```
  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
```

272c ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁272b 272d▷
```
  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
```

272d ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁272c 273a▷
```
  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
```

273a ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁272d 273b▷
```
        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
```

273b ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁273a 273c▷
```
        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
```

273c ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁273b 276a▷
```
        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

273d ⟨tao_random_numbers.f90 273d⟩≡
```
        ! 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 255c⟩
⟨*Declaration of 30-bit* tao_random_numbers 267d⟩
⟨*Interfaces of* tao_random_numbers 259a⟩
⟨*Interfaces of 30-bit* tao_random_numbers 281a⟩

⟨*Parameters in* `tao_random_numbers` 254a⟩
⟨*Variables in* `tao_random_numbers` 269a⟩
⟨*Variables in 30-bit* `tao_random_numbers` 254c⟩
⟨*Declaration of 30-bit* `tao_random_numbers` *types* 261d⟩
```
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` 256a⟩
⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩
```
end module tao_random_numbers
```

274a   ⟨`tao52_random_numbers.f90` 274a⟩≡
```
! tao52_random_numbers.f90 --
```
⟨*Copyleft notice* 1⟩
```
module tao52_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
```
⟨*Declaration of* `tao_random_numbers` 255c⟩
⟨*Declaration of 52-bit* `tao_random_numbers` 268b⟩
⟨*Interfaces of* `tao_random_numbers` 259a⟩
⟨*Interfaces of 52-bit* `tao_random_numbers` 281e⟩
⟨*Parameters in* `tao_random_numbers` 254a⟩
⟨*Variables in* `tao_random_numbers` 269a⟩
⟨*Variables in 52-bit* `tao_random_numbers` 259d⟩
⟨*Declaration of 52-bit* `tao_random_numbers` *types* 261f⟩
```
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` 256a⟩
⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩
```
end module tao52_random_numbers
```

Ten functions are exported

274b   ⟨*Declaration of* `tao_random_numbers` 255c⟩+≡   (273d 274a) ◁270c
```
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
```

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```
    ! public :: tao_random_luxury
    public :: tao_random_test
```

C.4.1 Single Random Numbers

A random integer r with $0 \le r < 2^{30} = 1073741824$:

275a ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁272a 275e▷
```
    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_* 275b⟩
    end subroutine integer_stateless
```

275b ⟨*Body of* `tao_random_*` 275b⟩≡   (275 276a)
```
    ⟨Step last and reload buffer iff necessary 275d⟩
    r = NORM * buffer(last)
```

The low level routine `generate` will fill an array $a_1, \ldots, a_n$, which will be consumed and refilled like an input buffer. We need at least $n \ge K$ for the call to `generate`.

275c ⟨*Variables in 30-bit* `tao_random_numbers` 254c⟩+≡   (273d) ◁256b
```
    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.

275d ⟨*Step* `last` *and reload* `buffer` *iff necessary* 275d⟩≡   (275b)
```
    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.

275e ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁275a 276c▷
```
    pure subroutine real_stateless (state, buffer, buffer_end, last, r)
```

```fortran
      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_*` 275b⟩
```fortran
   end subroutine real_stateless
```

A random real $r \in [0, 1)$.

276a ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁273c 278b▷
```fortran
   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_*` 275b⟩
```fortran
   end subroutine real_stateless
```

The low level routine `generate` will fill an array $a_1, \ldots, a_N$, which will be consumed and refilled like an input buffer.

276b ⟨*Variables in 52-bit* `tao_random_numbers` 259d⟩+≡   (274a) ◁259e
```fortran
   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 $j_1, \ldots, j_\nu$ with random integers $0 \le j_i < 2^{30} = 1073741824$. This has to be done such that the underlying array length in `generate` is transparent to the user. At the same time we want to avoid the overhead of calling `tao_random_real` ν times.

276c ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁275e 278a▷
```fortran
   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` 277a⟩
```fortran
   end subroutine integer_array_stateless
```

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277a   ⟨*Body of* `tao_random_*_array` 277a⟩≡   (276c 278)

```
integer :: nu, done, todo, chunk
```
⟨*Set* `nu` *to* `num` *or* `size(v)` 277b⟩
⟨*Prepare array* `buffer` *and* `done`, `todo`, `chunk` 277c⟩
```
v(1:chunk) = NORM * buffer(last+1:last+chunk)
do
```
     ⟨*Update* `last`, `done` *and* `todo` *and set new* `chunk` 277d⟩
     ⟨*Reload* `buffer` *or exit* 277e⟩
```
    v(done+1:done+chunk) = NORM * buffer(1:chunk)
end do
```

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

```
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.

277c   ⟨*Prepare array* `buffer` *and* `done`, `todo`, `chunk` 277c⟩≡   (277a)

```
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.

277d   ⟨*Update* `last`, `done` *and* `todo` *and set new* `chunk` 277d⟩≡   (277a)

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

277e   ⟨*Reload* `buffer` *or exit* 277e⟩≡   (277a)

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

278a   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁276c 278c▷

```
  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 277a⟩
  end subroutine real_array_stateless
```

Fill the array $v_1, \ldots, v_\nu$ with uniform deviates $v_i \in [0, 1)$.

278b   ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁276a 279a▷

```
  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 277a⟩
  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:

278c   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁278a 278d▷

```
  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
```

278d   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁278c 279b▷

```
  elemental subroutine real_state (s, r)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(out) :: r
    call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
  end subroutine real_state
```

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279a   ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁278b 279d▷

```fortran
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
```

279b   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁278d 279c▷

```fortran
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
```

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

```fortran
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
```

279d   ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁279a 280c▷

```fortran
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:

279e   ⟨*Initialize a virginal random number generator* 279e⟩≡   (280 282)

```fortran
if (s_virginal) then
   call tao_random_seed ()
end if
```

279

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

```
subroutine integer_static (r)
   integer, intent(out) :: r
   ⟨Initialize a virginal random number generator 279e⟩
   call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine integer_static
```

280b   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁280a 280d▷

```
subroutine real_static (r)
   real(kind=default), intent(out) :: r
   ⟨Initialize a virginal random number generator 279e⟩
   call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static
```

280c   ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁279d 280f▷

```
subroutine real_static (r)
   real(kind=default), intent(out) :: r
   ⟨Initialize a virginal random number generator 279e⟩
   call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static
```

280d   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁280b 280e▷

```
subroutine integer_array_static (v, num)
   integer, dimension(:), intent(out) :: v
   integer, optional, intent(in) :: num
   ⟨Initialize a virginal random number generator 279e⟩
   call integer_array_stateless &
       (s_state, s_buffer, s_buffer_end, s_last, v, num)
end subroutine integer_array_static
```

280e   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁280d 283e▷

```
subroutine real_array_static (v, num)
   real(kind=default), dimension(:), intent(out) :: v
   integer, optional, intent(in) :: num
   ⟨Initialize a virginal random number generator 279e⟩
   call real_array_stateless &
       (s_state, s_buffer, s_buffer_end, s_last, v, num)
end subroutine real_array_static
```

280f   ⟨*Implementation of 52-bit* `tao_random_numbers` 259f⟩+≡   (274a) ◁280c 286a▷

```
subroutine real_array_static (v, num)
   real(kind=default), dimension(:), intent(out) :: v
   integer, optional, intent(in) :: num
   ⟨Initialize a virginal random number generator 279e⟩
   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

281a   ⟨*Interfaces of 30-bit* `tao_random_numbers` 281a⟩≡   (273d)
```
interface tao_random_number
   module procedure ⟨Specific procedures for 30-bit tao_random_number 281b⟩
end interface
```

281b   ⟨*Specific procedures for 30-bit* `tao_random_number` 281b⟩≡   (281)
```
integer_static, integer_state, &
integer_array_static, integer_array_state, &
real_static, real_state, real_array_static, real_array_state
```
These are not exported

281c   ⟨*Declaration of 30-bit* `tao_random_numbers` 267d⟩+≡   (273d) ◁267f 281d ▷
```
private :: &
      integer_stateless, integer_array_stateless, &
      real_stateless, real_array_stateless
```

281d   ⟨*Declaration of 30-bit* `tao_random_numbers` 267d⟩+≡   (273d) ◁281c
```
private :: ⟨Specific procedures for 30-bit tao_random_number 281b⟩
```

281e   ⟨*Interfaces of 52-bit* `tao_random_numbers` 281e⟩≡   (274a)
```
interface tao_random_number
   module procedure ⟨Specific procedures for 52-bit tao_random_number 281f⟩
end interface
```

281f   ⟨*Specific procedures for 52-bit* `tao_random_number` 281f⟩≡   (281)
```
real_static, real_state, real_array_static, real_array_state
```
Thes are not exported

281g   ⟨*Declaration of 52-bit* `tao_random_numbers` 268b⟩+≡   (274a) ◁268d 281h ▷
```
private :: real_stateless, real_array_stateless
```

281h   ⟨*Declaration of 52-bit* `tao_random_numbers` 268b⟩+≡   (274a) ◁281g
```
private :: ⟨Specific procedures for 52-bit tao_random_number 281f⟩
```

C.4.6   Luxury

281i   ⟨*Implementation of* `tao_random_numbers` 256a⟩+≡   (273d 274a) ◁270a 282a ▷
```
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
```

282a ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁281i 282b▷
```
   elemental subroutine luxury_state (s)
      type(tao_random_state), intent(inout) :: s
      call luxury_state_integer (s, size (s%buffer))
   end subroutine luxury_state
```

282b ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁282a 282c▷
```
   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
```

282c ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁282b 282d▷
```
   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
```

282d ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁282c 282e▷
```
   subroutine luxury_static ()
      ⟨Initialize a virginal random number generator 279e⟩
      call luxury_static_integer (size (s_buffer))
   end subroutine luxury_static
```

282e ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁282d 282f▷
```
   subroutine luxury_static_integer (consumption)
      integer, intent(in) :: consumption
      ⟨Initialize a virginal random number generator 279e⟩
      call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
   end subroutine luxury_static_integer
```

282f ⟨*Implementation of* tao_random_numbers 256a⟩+≡   (273d 274a) ◁282e
```
   subroutine luxury_static_real (consumption)
      real(kind=default), intent(in) :: consumption
      ⟨Initialize a virginal random number generator 279e⟩
      call luxury_static_integer (int (consumption * size (s_buffer)))
   end subroutine luxury_static_real
```

283a   ⟨*Interfaces of* `tao_random_numbers` *(unused luxury)* 283a⟩≡

```
interface tao_random_luxury
   module procedure ⟨Specific procedures for tao_random_luxury 283d⟩
end interface
```

283b   ⟨*Declaration of* `tao_random_numbers` *(unused luxury)* 283b⟩≡   283c ▷

```
private :: luxury_stateless
```

283c   ⟨*Declaration of* `tao_random_numbers` *(unused luxury)* 283b⟩+≡   ◁ 283b

```
private :: ⟨Specific procedures for tao_random_luxury 283d⟩
```

283d   ⟨*Specific procedures for* `tao_random_luxury` 283d⟩≡   (283)

```
luxury_static, luxury_state, &
luxury_static_integer, luxury_state_integer, &
luxury_static_real, luxury_state_real
```

C.5   Testing

C.5.1   30-bit

283e   ⟨*Implementation of 30-bit* `tao_random_numbers` 255b⟩+≡   (273d) ◁ 280e

```
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 283f⟩
   integer, parameter :: &
       A_2027082 = 995235265
   integer, dimension(N) :: a
   type(tao_random_state) :: s, t
   integer, dimension(:), allocatable :: ibuf
   real(kind=tao_r64), dimension(:), allocatable :: dbuf
   integer :: i, ibuf_size, dbuf_size
   print *, TAO_RANDOM_NUMBERS_RCS_ID
   print *, "testing the 30-bit tao_random_numbers ..."
   ⟨Perform simple tests of tao_random_numbers 284a⟩
   ⟨Perform more tests of tao_random_numbers 284d⟩
end subroutine tao_random_test
```

283f   ⟨*Parameters in* `tao_random_test` 283f⟩≡   (283e 286a)

```
integer, parameter :: &
    SEED = 310952, &
```

```
        N = 2009, M = 1009, &
        N_SHORT = 1984
```

DEK's "official" test expects $a_{1009\cdot2009+1} = a_{2027082} = 995235265$:

284a ⟨*Perform simple tests of* `tao_random_numbers` 284a⟩≡   (283e 286a) 284c ▷
```
! 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` 284b⟩

284b ⟨*Test* `a(1)` = `A_2027082` 284b⟩≡   (284 285)
```
if (a(1) == A_2027082) then
   print OK, a(1)
else
   print NOT_OK, a(1), A_2027082
   stop 1
end if
```

Deja vu all over again, but 2027081 is factored the other way around this time

284c ⟨*Perform simple tests of* `tao_random_numbers` 284a⟩+≡   (283e 286a) ◁284a
```
call tao_random_seed (SEED)
do i = 1, M+1
   call tao_random_number (a)
end do
```
⟨*Test* `a(1)` = `A_2027082` 284b⟩

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

284d ⟨*Perform more tests of* `tao_random_numbers` 284d⟩≡   (283e 286a) 284e ▷
```
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` 284b⟩

and restart the saved generator

284e ⟨*Perform more tests of* `tao_random_numbers` 284d⟩+≡   (283e 286a) ◁284d 285a ▷
```
do i = 1, N+1 - N_SHORT
   call tao_random_number (t, a, M)
```

```
      end do
      ⟨Test a(1) = A_2027082 284b⟩
```

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

285a ⟨*Perform more tests of* tao_random_numbers 284d⟩+≡   (283e 286a) ◁284e 285b▷
```
   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 284b⟩
      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 284b⟩
   end if
```

And finally using marshaling/unmarshaling:

285b ⟨*Perform more tests of* tao_random_numbers 284d⟩+≡   (283e 286a) ◁285a
```
   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_marshal_size (s, ibuf_size, dbuf_size)
   allocate (ibuf(ibuf_size), dbuf(dbuf_size))
   call tao_random_marshal (s, ibuf, dbuf)
   do i = 1, N+1 - N_SHORT
      call tao_random_number (s, a, M)
   end do
   ⟨Test a(1) = A_2027082 284b⟩
   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 284b⟩
```

285

C.5.2 52-bit

DEK's "official" test expects $x_{1009 \cdot 2009+1} = x_{2027082} = 0.36410514377569680455$:

286a ⟨*Implementation of 52-bit* tao_random_numbers 259f⟩+≡   (274a) ◁280f
```
  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 283f⟩
    real(kind=default), parameter :: &
         A_2027082 = 0.36410514377569680455_tao_r64
    real(kind=default), dimension(N) :: a
    type(tao_random_state) :: s, t
    integer, dimension(:), allocatable :: ibuf
    real(kind=tao_r64), dimension(:), allocatable :: dbuf
    integer :: i, ibuf_size, dbuf_size
    print *, TAO52_RANDOM_NUMBERS_RCS_ID
    print *, "testing the 52-bit tao_random_numbers ..."
    ⟨Perform simple tests of tao_random_numbers 284a⟩
    ⟨Perform more tests of tao_random_numbers 284d⟩
  end subroutine tao_random_test
```

C.5.3 Test Program

286b ⟨tao_test.f90 286b⟩≡
```
  program tao_test
    use tao_random_numbers, only: test30 => tao_random_test
    use tao52_random_numbers, only: test52 => tao_random_test
    implicit none
    call test30 ("tmp.tao")
    call test52 ("tmp.tao")
    stop 0
  end program tao_test
```

—D—
Special Functions

287a   ⟨specfun.f90 287a⟩≡

```
! specfun.f90 --
⟨Copyleft notice 1⟩
module specfun
  use kinds
! use constants
  implicit none
  private
  ⟨Declaration of specfun procedures 287b⟩
  character(len=*), public, parameter :: SPECFUN_RCS_ID = &
       "$Id: specfun.nw 314 2010-04-17 20:32:33Z ohl $"
  !WK:
  real(kind=default), public, parameter :: &
       PI = 3.1415926535897932384626433832795028841972_default
contains
  ⟨Implementation of specfun procedures 288c⟩
end module specfun
```

The algorithm is stolen from the FORTRAN version in routine C303 of the CERN library [25]. It has an accuracy which is approximately one digit less than machine precision.

287b   ⟨Declaration of specfun procedures 287b⟩≡   (287a)

```
public :: gamma
```

The so-called reflection formula is used for negative arguments:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \qquad (D.1)$$

Here's the identity transformation that pulls the argument of Γ into $[3, 4]$:

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

287

288a   ⟨*Pull u into the intervall* $[3, 4]$ *288a*⟩≡   (288c)

```
f = 1
if (u < 3) then
   do i = 1, int (4 - u)
      f = f / u
      u = u + 1
   end do
else
   do i = 1, int (u - 3)
      u = u - 1
      f = f * u
   end do
end if
```

A Chebyshev approximation for $\Gamma(x)$ is used after mapping $x \in [3, 4]$ linearly to $h \in [-1, 1]$. The series is evaluted by Clenshaw's recurrence formula:

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

288b   ⟨*Clenshaw's recurrence formula 288b*⟩≡   (288c)

```
alpha = 2*g
b1 = 0
b2 = 0
do i = 15, 0, -1
   b0 = c(i) + alpha * b1 - b2
   b2 = b1
   b1 = b0
end do
g = f * (b0 - g * b2)
```

Note that we're assuming that `c(0)` is in fact $c_0/2$. This is for compatibility with the CERN library routines.

288c   ⟨*Implementation of* `specfun` *procedures 288c*⟩≡   (287a)

```
pure function gamma (x) result (g)
  real(kind=default), intent(in) :: x
  real(kind=default) :: g
  integer :: i
  real(kind=default) :: u, f, alpha, b0, b1, b2
  real(kind=default), dimension(0:15), parameter :: &
       c = ⟨c_0/2, c_1, c_2, ..., c_15 for Γ(x) 289a⟩
  u = x
  if (u <= 0.0) then
```

288

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

289a ⟨$c_0/2, c_1, c_2, \ldots, c_{15}$ for $\Gamma(x)$ 289a⟩≡   (288c)
```
    (/ 3.65738772508338244_default, &
       1.95754345666126827_default, &
       0.33829711382616039_default, &
       0.04208951276557549_default, &
       0.00428765048212909_default, &
       0.00036521216929462_default, &
       0.00002740064222642_default, &
       0.00000181240233365_default, &
       0.00000010965775866_default, &
       0.00000000598718405_default, &
       0.00000000030769081_default, &
       0.00000000001431793_default, &
       0.00000000000065109_default, &
       0.00000000000002596_default, &
       0.00000000000000111_default, &
       0.00000000000000004_default /)
```

D.1   Test

289b ⟨stest.f90 289b⟩≡   290c ▷
```
    ! stest.f90 --
    ⟨Copyleft notice 1⟩
    module stest_functions
        use kinds
        use constants
        use specfun
```

```
      private
      ⟨Declaration of stest_functions procedures 290a⟩
    contains
      ⟨Implementation of stest_functions procedures 290b⟩
    end module stest_functions
```

290a ⟨Declaration of stest_functions procedures 290a⟩≡   (289b)
```
      public :: gauss_multiplication
```

Gauss' multiplication fomula can serve as a non-trivial test

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \qquad \text{(D.4)}$$

290b ⟨Implementation of stest_functions procedures 290b⟩≡   (289b)
```
    pure function gauss_multiplication (x, n) result (delta)
      real(kind=default), intent(in) :: x
      integer, intent(in) :: n
      real(kind=default) :: delta
      real(kind=default) :: gxn
      integer :: k
      gxn = (2*PI)**(0.5_double*(1-n)) * n**(n*x-0.5_double)
      do k = 0, n - 1
         gxn = gxn * gamma (x + real (k, kind=default) / n)
      end do
      delta = abs ((gamma (n*x) - gxn) / gamma (n*x))
    end function gauss_multiplication
```

290c ⟨stest.f90 289b⟩+≡   ◁289b
```
    program stest
      use kinds
      use specfun
      use stest_functions !NODEP!
      implicit none
      integer :: i, steps
      real(kind=default) :: x, g, xmin, xmax
      xmin = -4.5
      xmax =  4.5
      steps = 100 ! 9
      do i = 0, steps
         x = xmin + ((xmax - xmin) / real (steps)) * i
         print "(f6.3,4(1x,e9.2))", x, &
              gauss_multiplication (x, 2), &
              gauss_multiplication (x, 3), &
              gauss_multiplication (x, 4), &
```

```fortran
            gauss_multiplication (x, 5)
  end do
end program stest
```

—E—
STATISTICS

292a ⟨vamp_stat.f90 292a⟩≡

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

292b ⟨*Declaration of* vamp_stat *procedures* 292b⟩≡   (292a) 293c ▷
```
  public :: average, standard_deviation, value_spread
```

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

292c ⟨*Implementation of* vamp_stat *procedures* 292c⟩≡   (292a) 293a ▷
```
  pure function average (x) result (a)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default) :: a
    integer :: n
    n = size (x)
    if (n == 0) then
       a = 0.0
    else
       a = sum (x) / n
    end if
  end function average
```

292

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

293a ⟨*Implementation of* `vamp_stat` *procedures* 292c⟩+≡   (292a) ◁292c 293b▷

```
pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
     s = huge (s)
  else
     s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
               0.0_default))
  end if
end function standard_deviation
```

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

293b ⟨*Implementation of* `vamp_stat` *procedures* 292c⟩+≡   (292a) ◁293a 293d▷

```
pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread
```

293c ⟨*Declaration of* `vamp_stat` *procedures* 292b⟩+≡   (292a) ◁292b

```
public :: standard_deviation_percent, value_spread_percent
```

293d ⟨*Implementation of* `vamp_stat` *procedures* 292c⟩+≡   (292a) ◁293b 293e▷

```
pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
     s = huge (s)
  else
     s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent
```

293e ⟨*Implementation of* `vamp_stat` *procedures* 292c⟩+≡   (292a) ◁293d

```
pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
```

```fortran
  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.*

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

295b ⟨Declaration of histograms types 295b⟩≡   (295a) 296a ▷
```
type, public :: histogram
   private
   integer :: n_bins
   real(kind=default) :: x_min, x_max
```

```
           real(kind=default), dimension(:), pointer :: bins => null ()
           real(kind=default), dimension(:), pointer :: bins2 => null ()
           real(kind=default), dimension(:), pointer :: bins3 => null ()
         end type histogram
```

296a ⟨*Declaration of* histograms *types* 295b⟩+≡   (295a) ◁295b
```
       type, public :: histogram2
          private
          integer, dimension(2) :: n_bins
          real(kind=default), dimension(2) :: x_min, x_max
          real(kind=default), dimension(:,:), pointer :: bins => null ()
          real(kind=default), dimension(:,:), pointer :: bins2 => null ()
       end type histogram2
```

296b ⟨*Declaration of* histograms *procedures* 296b⟩≡   (295a) 296d▷
```
       public :: create_histogram
       public :: fill_histogram
       public :: delete_histogram
       public :: write_histogram
```

296c ⟨*Interfaces of* histograms *procedures* 296c⟩≡   (295a) 301b▷
```
       interface create_histogram
          module procedure create_histogram1, create_histogram2
       end interface
       interface fill_histogram
          module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
       end interface
       interface delete_histogram
          module procedure delete_histogram1, delete_histogram2
       end interface
       interface write_histogram
          module procedure write_histogram1, write_histogram2
          module procedure write_histogram1_unit
       end interface
```

296d ⟨*Declaration of* histograms *procedures* 296b⟩+≡   (295a) ◁296b 300a▷
```
       private :: create_histogram1, create_histogram2
       private :: fill_histogram1, fill_histogram2s, fill_histogram2v
       private :: delete_histogram1, delete_histogram2
       private :: write_histogram1, write_histogram2
```

296e ⟨*Variables in* histograms 296e⟩≡   (295a)
```
       integer, parameter, private :: N_BINS_DEFAULT = 10
```

296f ⟨*Implementation of* histograms *procedures* 296f⟩≡   (295a) 297a▷
```
       elemental subroutine create_histogram1 (h, x_min, x_max, nb)
         type(histogram), intent(out) :: h
```

296

```
      real(kind=default), intent(in) :: x_min, x_max
      integer, intent(in), optional :: nb
      if (present (nb)) then
         h%n_bins = nb
      else
         h%n_bins = N_BINS_DEFAULT
      end if
      h%x_min = x_min
      h%x_max = x_max
      allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
      h%bins = 0
      h%bins2 = 0
      allocate (h%bins3(0:h%n_bins+1))
      h%bins3 = 0
    end subroutine create_histogram1
```

297a ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁296f 297b▷

```
    pure subroutine create_histogram2 (h, x_min, x_max, nb)
      type(histogram2), intent(out) :: h
      real(kind=default), dimension(:), intent(in) :: x_min, x_max
      integer, intent(in), dimension(:), optional :: nb
      if (present (nb)) then
         h%n_bins = nb
      else
         h%n_bins = N_BINS_DEFAULT
      end if
      h%x_min = x_min
      h%x_max = x_max
      allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
                h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
      h%bins = 0
      h%bins2 = 0
    end subroutine create_histogram2
```

297b ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁297a 298a▷

```
    elemental subroutine fill_histogram1 (h, x, weight, excess)
      type(histogram), intent(inout) :: h
      real(kind=default), intent(in) :: x
      real(kind=default), intent(in), optional :: weight
      real(kind=default), intent(in), optional :: excess
      integer :: i
      if (x < h%x_min) then
         i = 0
      else if (x > h%x_max) then
         i = h%n_bins + 1
```

```
        else
            i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
    !WK! i = min (max (i, 0), h%n_bins + 1)
        end if
        if (present (weight)) then
            h%bins(i) = h%bins(i) + weight
            h%bins2(i) = h%bins2(i) + weight*weight
        else
            h%bins(i) = h%bins(i) + 1
            h%bins2(i) = h%bins2(i) + 1
        end if
        if (present (excess)) h%bins3(i) = h%bins3(i) + excess
    end subroutine fill_histogram1
```

298a ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁297b 298b▷

```
    elemental subroutine fill_histogram2s (h, x1, x2, weight)
        type(histogram2), intent(inout) :: h
        real(kind=default), intent(in) :: x1, x2
        real(kind=default), intent(in), optional :: weight
        call fill_histogram2v (h, (/ x1, x2 /), weight)
    end subroutine fill_histogram2s
```

298b ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁298a 298c▷

```
    pure subroutine fill_histogram2v (h, x, weight)
        type(histogram2), intent(inout) :: h
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(in), optional :: weight
        integer, dimension(2) :: i
        i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
        i = min (max (i, 0), h%n_bins + 1)
        if (present (weight)) then
            h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight
            h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight*weight
        else
            h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1
            h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1
        end if
    end subroutine fill_histogram2v
```

298c ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁298b 299a▷

```
    elemental subroutine delete_histogram1 (h)
        type(histogram), intent(inout) :: h
        deallocate (h%bins, h%bins2)
        deallocate (h%bins3)
    end subroutine delete_histogram1
```

⟨*Implementation of* `histograms` *procedures* 296f⟩+≡   (295a) ◁298c 299b▷

```
elemental subroutine delete_histogram2 (h)
  type(histogram2), intent(inout) :: h
  deallocate (h%bins, h%bins2)
end subroutine delete_histogram2
```

⟨*Implementation of* `histograms` *procedures* 296f⟩+≡   (295a) ◁299a 300b▷

```
subroutine write_histogram1 (h, name, over)
  type(histogram), intent(in) :: h
  character(len=*), intent(in), optional :: name
  logical, intent(in), optional :: over
  integer :: i, iounit
  if (present (name)) then
     call find_free_unit (iounit)
     if (iounit > 0) then
        open (unit = iounit, action = "write", status = "replace", &
             file = name)
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                "underflow", h%bins(0), sqrt (h%bins2(0))
           end if
        end if
        do i = 1, h%n_bins
           write (unit = iounit, fmt = *) &
                midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
        end do
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                "overflow", h%bins(h%n_bins+1), &
                sqrt (h%bins2(h%n_bins+1))
           end if
        end if
        close (unit = iounit)
     else
        print *, "write_histogram: Can't find a free unit!"
     end if
  else
     if (present (over)) then
        if (over) then
           print *, "underflow", h%bins(0), sqrt (h%bins2(0))
        end if
     end if
```

```
            do i = 1, h%n_bins
               print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
            end do
            if (present (over)) then
               if (over) then
                  print *, "overflow", h%bins(h%n_bins+1), &
                            sqrt (h%bins2(h%n_bins+1))
               end if
            end if
         end if
      end subroutine write_histogram1
```

300a ⟨*Declaration of* histograms *procedures* 296b⟩+≡   (295a) ◁296d 301a▷
```
      !WK! public :: write_histogram1_unit
```

> ✎ I don't like the `format` statement with the line number. Use a character
> constant instead (after we have merged with WHIZARD's branch).

300b ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁299b 301d▷
```
      subroutine write_histogram1_unit (h, iounit, over, show_excess)
        type(histogram), intent(in) :: h
        integer, intent(in) :: iounit
        logical, intent(in), optional :: over, show_excess
        integer :: i
        logical :: show_exc
        show_exc = .false.; if (present(show_excess)) show_exc = show_excess
        if (present (over)) then
           if (over) then
              if (show_exc) then
                 write (unit = iounit, fmt = 1) &
                       "underflow", h%bins(0), sqrt (h%bins2(0)), h%bins3(0)
              else
                 write (unit = iounit, fmt = 1) &
                       "underflow", h%bins(0), sqrt (h%bins2(0))
              end if
           end if
        end if
        do i = 1, h%n_bins
           if (show_exc) then
              write (unit = iounit, fmt = 1) &
                    midpoint (h, i), h%bins(i), sqrt (h%bins2(i)), h%bins3(i)
           else
              write (unit = iounit, fmt = 1) &
                    midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
```

```
            end if
          end do
          if (present (over)) then
            if (over) then
              if (show_exc) then
                write (unit = iounit, fmt = 1) &
                      "overflow", h%bins(h%n_bins+1), &
                      sqrt (h%bins2(h%n_bins+1)), &
                      h%bins3(h%n_bins+1)
              else
                write (unit = iounit, fmt = 1) &
                      "overflow", h%bins(h%n_bins+1), &
                      sqrt (h%bins2(h%n_bins+1))
              end if
            end if
          end if
        1 format (1x,4(G16.9,2x))
        end subroutine write_histogram1_unit
```

301a ⟨*Declaration of* histograms *procedures* 296b⟩+≡   (295a) ◁300a 301c▷
```
      private :: midpoint
```

301b ⟨*Interfaces of* histograms *procedures* 296c⟩+≡   (295a) ◁296c
```
      interface midpoint
         module procedure midpoint1, midpoint2
      end interface
```

301c ⟨*Declaration of* histograms *procedures* 296b⟩+≡   (295a) ◁301a
```
      private :: midpoint1, midpoint2
```

301d ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁300b 301e▷
```
      elemental function midpoint1 (h, bin) result (x)
        type(histogram), intent(in) :: h
        integer, intent(in) :: bin
        real(kind=default) :: x
        x = h%x_min + (h%x_max - h%x_min) * (bin - 0.5) / h%n_bins
      end function midpoint1
```

301e ⟨*Implementation of* histograms *procedures* 296f⟩+≡   (295a) ◁301d 302▷
```
      elemental function midpoint2 (h, bin, d) result (x)
        type(histogram2), intent(in) :: h
        integer, intent(in) :: bin, d
        real(kind=default) :: x
        x = h%x_min(d) + (h%x_max(d) - h%x_min(d)) * (bin - 0.5) / h%n_bins(d)
      end function midpoint2
```

```
subroutine write_histogram2 (h, name, over)
  type(histogram2), intent(in) :: h
  character(len=*), intent(in), optional :: name
  logical, intent(in), optional :: over
  integer :: i1, i2, iounit
  if (present (name)) then
     call find_free_unit (iounit)
     if (iounit > 0) then
        open (unit = iounit, action = "write", status = "replace", &
              file = name)
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                   "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
              do i2 = 1, h%n_bins(2)
                 write (unit = iounit, fmt = *) &
                      "x1 underflow", midpoint (h, i2, 2), &
                      h%bins(0,i2), sqrt (h%bins2(0,i2))
              end do
              do i1 = 1, h%n_bins(1)
                 write (unit = iounit, fmt = *) &
                      "x2 underflow", midpoint (h, i1, 1), &
                      h%bins(i1,0), sqrt (h%bins2(i1,0))
              end do
           end if
        end if
        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)
```

```fortran
               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), &
```

```fortran
                h%bins(i1,h%n_bins(2)+1), &
                sqrt (h%bins2(i1,h%n_bins(2)+1))
         end do
         print *, "double overflow", &
               h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
               sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
       end if
     end if
   end if
end subroutine write_histogram2
```

—G—
MISCELLANEOUS UTILITIES

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

G.1   Memory Management

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

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

305

```
                     create_integer_array2_pointer, &
                     create_real_array2_pointer
         end interface
```

306a   ⟨*Body of* `create_*_array_pointer` 306a⟩≡   (306c 307a)
```
         if (associated (lhs)) then
            if (size (lhs) /= n) then
               deallocate (lhs)
               if (present (lb)) then
                  allocate (lhs(lb:n+lb-1))
               else
                  allocate (lhs(n))
               end if
            end if
         else
            if (present (lb)) then
               allocate (lhs(lb:n+lb-1))
            else
               allocate (lhs(n))
            end if
         end if
         lhs = 0
```

306b   ⟨*Body of* `create_*_array2_pointer` 306b⟩≡   (307)
```
         if (associated (lhs)) then
            if (any (ubound (lhs) /= n)) then
               deallocate (lhs)
               if (present (lb)) then
                  allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
               else
                  allocate (lhs(n(1),n(2)))
               end if
            end if
         else
            if (present (lb)) then
               allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
            else
               allocate (lhs(n(1),n(2)))
            end if
         end if
         lhs = 0
```

306c   ⟨*Implementation of* `utils` *procedures* 306c⟩≡   (305a) 307a ▷
```
         pure subroutine create_integer_array_pointer (lhs, n, lb)
            integer, dimension(:), pointer :: lhs
```

```
      integer, intent(in) :: n
      integer, intent(in), optional :: lb
      ⟨Body of create_*_array_pointer 306a⟩
    end subroutine create_integer_array_pointer
```

307a   ⟨Implementation of utils procedures 306c⟩+≡   (305a) ◁306c 307b▷
```
    pure subroutine create_real_array_pointer (lhs, n, lb)
      real(kind=default), dimension(:), pointer :: lhs
      integer, intent(in) :: n
      integer, intent(in), optional :: lb
      ⟨Body of create_*_array_pointer 306a⟩
    end subroutine create_real_array_pointer
```

307b   ⟨Implementation of utils procedures 306c⟩+≡   (305a) ◁307a 307c▷
```
    pure subroutine create_integer_array2_pointer (lhs, n, lb)
      integer, dimension(:,:), pointer :: lhs
      integer, dimension(:), intent(in) :: n
      integer, dimension(:), intent(in), optional :: lb
      ⟨Body of create_*_array2_pointer 306b⟩
    end subroutine create_integer_array2_pointer
```

307c   ⟨Implementation of utils procedures 306c⟩+≡   (305a) ◁307b 308a▷
```
    pure subroutine create_real_array2_pointer (lhs, n, lb)
      real(kind=default), dimension(:,:), pointer :: lhs
      integer, dimension(:), intent(in) :: n
      integer, dimension(:), intent(in), optional :: lb
      ⟨Body of create_*_array2_pointer 306b⟩
    end subroutine create_real_array2_pointer
```

Copy an allocatable array component of a derived type, reshaping the target
if necessary. The target can be disassociated, but its association *must not*
be undefined.

307d   ⟨Declaration of utils procedures 305b⟩+≡   (305a) ◁305b 308e▷
```
    public :: copy_array_pointer
    private :: copy_integer_array_pointer
    private :: copy_real_array_pointer
    private :: copy_integer_array2_pointer
    private :: copy_real_array2_pointer
```

307e   ⟨Interfaces of utils procedures 305c⟩+≡   (305a) ◁305c 309a▷
```
    interface copy_array_pointer
       module procedure &
            copy_integer_array_pointer, &
            copy_real_array_pointer, &
            copy_integer_array2_pointer, &
            copy_real_array2_pointer
```

```
                  end interface
```

308a ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁307c 308b▷
```
      pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
        integer, dimension(:), pointer :: lhs
        integer, dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_integer_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
      end subroutine copy_integer_array_pointer
```

308b ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁308a 308c▷
```
      pure subroutine copy_real_array_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:), pointer :: lhs
        real(kind=default), dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_real_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
      end subroutine copy_real_array_pointer
```

308c ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁308b 308d▷
```
      pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
        integer, dimension(:,:), pointer :: lhs
        integer, dimension(:,:), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_integer_array2_pointer &
             (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
      end subroutine copy_integer_array2_pointer
```

308d ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁308c 309b▷
```
      pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:,:), pointer :: lhs
        real(kind=default), dimension(:,:), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_real_array2_pointer &
             (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
      end subroutine copy_real_array2_pointer
```

G.2   Sorting

308e ⟨*Declaration of* `utils` *procedures* 305b⟩+≡   (305a) ◁307d 310d▷
```
      public :: swap
      private :: swap_integer, swap_real
```

309a   ⟨*Interfaces of* `utils` *procedures* 305c⟩+≡   (305a) ◁307e 311a▷

```
interface swap
   module procedure swap_integer, swap_real
end interface
```

309b   ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁308d 309c▷

```
elemental subroutine swap_integer (a, b)
  integer, intent(inout) :: a, b
  integer :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_integer
```

309c   ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁309b 309d▷

```
elemental subroutine swap_real (a, b)
  real(kind=default), intent(inout) :: a, b
  real(kind=default) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_real
```

Straight insertion:

309d   ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁309c 310b▷

```
pure subroutine sort_real (key, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  ⟨Set rev to reverse or .false. 309e⟩
  do i = 1, size (key) - 1
     ⟨Set j to minloc(key) 310a⟩
     if (j /= i) then
        call swap (key(i), key(j))
     end if
  end do
end subroutine sort_real
```

309e   ⟨*Set* `rev` *to* `reverse` *or* `.false.` 309e⟩≡   (309 310)

```
if (present (reverse)) then
   rev = reverse
else
   rev = .false.
end if
```

310a   ⟨*Set* `j` *to* `minloc(key)` 310a⟩≡   (309 310)

```
if (rev) then
   j = sum (maxloc (key(i:))) + i - 1
else
   j = sum (minloc (key(i:))) + i - 1
end if
```

310b   ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁309d 310c▷

```
pure subroutine sort_real_and_real_array (key, table, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  real(kind=default), dimension(:,:), intent(inout) :: table
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
```
      ⟨*Set* `rev` *to* `reverse` *or* `.false.` 309e⟩
```
  do i = 1, size (key) - 1
```
         ⟨*Set* `j` *to* `minloc(key)` 310a⟩
```
     if (j /= i) then
        call swap (key(i), key(j))
        call swap (table(:,i), table(:,j))
     end if
  end do
end subroutine sort_real_and_real_array
```

310c   ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁310b 311c▷

```
pure subroutine sort_real_and_integer (key, table, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  integer, dimension(:), intent(inout) :: table
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
```
      ⟨*Set* `rev` *to* `reverse` *or* `.false.` 309e⟩
```
  do i = 1, size (key) - 1
```
         ⟨*Set* `j` *to* `minloc(key)` 310a⟩
```
     if (j /= i) then
        call swap (key(i), key(j))
        call swap (table(i), table(j))
     end if
  end do
end subroutine sort_real_and_integer
```

310d   ⟨*Declaration of* `utils` *procedures* 305b⟩+≡   (305a) ◁308e 311b▷

```
public :: sort
private :: sort_real, sort_real_and_real_array, sort_real_and_integer
```

311a ⟨*Interfaces of* `utils` *procedures* 305c⟩+≡   (305a) ◁309a
```
   interface sort
     module procedure &
           sort_real, sort_real_and_real_array, &
           sort_real_and_integer
   end interface
```

G.3   Mathematics

311b ⟨*Declaration of* `utils` *procedures* 305b⟩+≡   (305a) ◁310d 311d▷
```
   public :: outer_product
```

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

311c ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁310c 311e▷
```
   pure function outer_product (x, y) result (xy)
     real(kind=default), dimension(:), intent(in) :: x, y
     real(kind=default), dimension(size(x),size(y)) :: xy
     xy = spread (x, dim=2, ncopies=size(y)) &
           * spread (y, dim=1, ncopies=size(x))
   end function outer_product
```

Greatest common divisor and least common multiple

311d ⟨*Declaration of* `utils` *procedures* 305b⟩+≡   (305a) ◁311b 313a▷
```
   public :: factorize, gcd, lcm
   private :: gcd_internal
```

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

311e ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁311c 311f▷
```
   pure recursive function gcd_internal (m, n) result (gcd_m_n)
     integer, intent(in) :: m, n
     integer :: gcd_m_n
     if (n <= 0) then
        gcd_m_n = m
     else
        gcd_m_n = gcd_internal (n, modulo (m, n))
     end if
   end function gcd_internal
```

Wrap an elemental procedure around the recursive procedure:

311f ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁311e 312a▷
```
   elemental function gcd (m, n) result (gcd_m_n)
     integer, intent(in) :: m, n
     integer :: gcd_m_n
```

```
      gcd_m_n = gcd_internal (m, n)
    end function gcd
```

As long as `m*n` does not overflow, we can use $\gcd(m, n)\operatorname{lcm}(m, n) = mn$:

312a ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁311f 312b▷
```
    elemental function lcm (m, n) result (lcm_m_n)
      integer, intent(in) :: m, n
      integer :: lcm_m_n
      lcm_m_n = (m * n) / gcd (m, n)
    end function lcm
```

A very simple minded factorization procedure, that is not fool proof at all.
It maintains `n == product (factors(1:i))`, however, and will work in all
cases of practical relevance.

312b ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁312a 313c▷
```
    pure subroutine factorize (n, factors, i)
      integer, intent(in) :: n
      integer, dimension(:), intent(out) :: factors
      integer, intent(out) :: i
      integer :: nn, p
      nn = n
      i = 0
      do p = 1, size (PRIMES)
        try: do
          if (modulo (nn, PRIMES(p)) == 0) then
            i = i + 1
            factors(i) = PRIMES(p)
            nn = nn / PRIMES(p)
            if (i >= size (factors)) then
              factors(i) = nn
              return
            end if
          else
            exit try
          end if
        end do try
        if (nn == 1) then
          return
        end if
      end do
    end subroutine factorize
```

312c ⟨*Parameters in* `utils` 312c⟩≡   (305a)
```
    integer, dimension(13), parameter, private :: &
        PRIMES = (/ 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41 /)
```

G.4 I/O

313a ⟨*Declaration of* `utils` *procedures* 305b⟩+≡   (305a) ◁311d
```
public :: find_free_unit
```

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

313c ⟨*Implementation of* `utils` *procedures* 306c⟩+≡   (305a) ◁312b
```
subroutine find_free_unit (u, iostat)
   integer, intent(out) :: u
   integer, intent(out), optional :: iostat
   logical :: exists, is_open
   integer :: i, status
   do i = MIN_UNIT, MAX_UNIT
      inquire (unit = i, exist = exists, opened = is_open, &
               iostat = status)
      if (status == 0) then
         if (exists .and. .not. is_open) then
            u = i
            if (present (iostat)) then
               iostat = 0
            end if
            return
         end if
      end if
   end do
   if (present (iostat)) then
      iostat = -1
   end if
   u = -1
end subroutine find_free_unit
```

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

H.1   LU Decomposition

314b ⟨Declaration of linalg procedures 314b⟩≡   (314a) 317a ▷
```
   public :: lu_decompose
```

$$A = LU \tag{H.1a}$$

In more detail

$$\begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ l_{21} & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \ldots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \ldots & u_{1n} \\ 0 & u_{22} & \ldots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & u_{nn} \end{pmatrix} \tag{H.1b}$$

Rewriting (H.1) in block matrix notation

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

we can solve it easily

$$u_{11} = a_{11} \tag{H.3a}$$

$$u_{1.} = a_{1.} \tag{H.3b}$$

$$l_{.1} = \frac{a_{.1}}{a_{11}} \tag{H.3c}$$

$$LU = A - \frac{a_{.1} \otimes a_{1.}}{a_{11}} \tag{H.3d}$$

and (H.3c) and (H.3d) define a simple iterative algorithm if we work from the outside in. It just remains to add pivoting.

315   ⟨*Implementation of* `linalg` *procedures* 315⟩≡   (314a) 317b ▷

```
pure subroutine lu_decompose (a, pivots, eps, l, u)
  real(kind=default), dimension(:,:), intent(inout) :: a
  integer, dimension(:), intent(out), optional :: pivots
  real(kind=default), intent(out), optional :: eps
  real(kind=default), dimension(:,:), intent(out), optional :: l, u
  real(kind=default), dimension(size(a,dim=1)) :: vv
  integer, dimension(size(a,dim=1)) :: p
  integer :: j, pivot
  ⟨eps = 1 316a⟩
  vv = maxval (abs (a), dim=2)
  if (any (vv == 0.0)) then
     a = 0.0
     ⟨pivots = 0 and eps = 0 316c⟩
     return
  end if
  vv = 1.0 / vv
  do j = 1, size (a, dim=1)
     pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
     if (j /= pivot) then
        call swap (a(pivot,:), a(j,:))
        ⟨eps = - eps 316b⟩
        vv(pivot) = vv(j)
     end if
     p(j) = pivot
     if (a(j,j) == 0.0) then
        a(j,j) = tiny (a(j,j))
```

315

```
            end if
            a(j+1:,j) = a(j+1:,j) / a(j,j)
            a(j+1:,j+1:) &
                  = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
         end do
       ⟨Return optional arguments in lu_decompose 316d⟩
     end subroutine lu_decompose
```

316a ⟨eps = 1 316a⟩≡ (315)
```
     if (present (eps)) then
        eps = 1.0
     end if
```

316b ⟨eps = - eps 316b⟩≡ (315)
```
     if (present (eps)) then
        eps = - eps
     end if
```

316c ⟨pivots = 0 *and* eps = 0 316c⟩≡ (315)
```
     if (present (pivots)) then
        pivots = 0
     end if
     if (present (eps)) then
        eps = 0
     end if
```

316d ⟨*Return optional arguments in* lu_decompose 316d⟩≡ (315)
```
     if (present (pivots)) then
        pivots = p
     end if
     if (present (l)) then
        do j = 1, size (a, dim=1)
           l(1:j-1,j) = 0.0
           l(j,j) = 1.0
           l(j+1:,j) = a(j+1:,j)
        end do
        do j = size (a, dim=1), 1, -1
           call swap (l(j,:), l(p(j),:))
        end do
     end if
     if (present (u)) then
        do j = 1, size (a, dim=1)
           u(1:j,j) = a(1:j,j)
           u(j+1:,j) = 0.0
        end do
     end if
```

316

H.2 Determinant

317a ⟨*Declaration of* `linalg` *procedures* 314b⟩+≡   (314a) ◁314b 318a▷
```
public :: determinant
```

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

317b ⟨*Implementation of* `linalg` *procedures* 315⟩+≡   (314a) ◁315 318b▷
```
pure subroutine determinant (a, det)
  real(kind=default), dimension(:,:), intent(in) :: a
  real(kind=default), intent(out) :: det
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu
  integer :: i
  lu = a
  call lu_decompose (lu, eps = det)
  do i = 1, size (a, dim = 1)
     det = det * lu(i,i)
  end do
end subroutine determinant
```

H.3 Diagonalization

The code is an implementation of the algorithm presented in [17, 18], but independent from the code presented in [19] to avoid legal problems.

A Jacobi rotation around the angle ϕ in row p and column q

$$P(\phi; p, q) = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos\phi & \cdots & \sin\phi & & \\ & & \vdots & 1 & \vdots & & \\ & & -\sin\phi & \cdots & \cos\phi & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \tag{H.4}$$

317

results in

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

318a ⟨*Declaration of* `linalg` *procedures* 314b⟩+≡   (314a) ◁317a 321c▷
    `public :: diagonalize_real_symmetric`

318b ⟨*Implementation of* `linalg` *procedures* 315⟩+≡   (314a) ◁317b 321b▷
```
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 321e⟩
  sweeps: do sweep = 1, MAX_SWEEPS
    off_diagonal_norm = sum (abs (aa), mask=upper_triangle)
    if (off_diagonal_norm == 0.0) then
       eval = diag (aa)
       return
    end if
    if (sweep < 4) then
       threshold = 0.2 * off_diagonal_norm / ndim**2
    else
```

```
            threshold = 0.0
         end if
         do p = 1, ndim - 1
            do q = p + 1, ndim
               〈Perform the Jacobi rotation resulting in A'_pq = 0 319〉
            end do
         end do
      end do sweeps
      if (present (num_rot)) then
         num_rot = -1
      end if
    !!! print *, "linalg::diagonalize_real_symmetric: exceeded sweep count"
    end subroutine diagonalize_real_symmetric
```

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

```
   g = 100 * abs (aa (p,q))
   if ((sweep > 4) &
       .and. (g <= min (spacing (aa(p,p)), spacing (aa(q,q))))) then
      aa(p,q) = 0.0
   else if (abs (aa(p,q)) > threshold) then
      〈Determine φ for the Jacobi rotation P(φ; p, q) with A'_pq = 0 320a〉
      〈A' = P^T(φ; p, q) · A · P(φ; p, q) 320c〉
      〈V' = V · P(φ; p, q) 321d〉
      〈Update num_rot 321f〉
   end if
```

We want

$$A'_{pq} = (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) = 0 \tag{H.6}$$

and therefore

$$\cot 2\phi = \frac{1 - \tan^2 \phi}{2\tan\phi} = \frac{\cos^2 \phi - \sin^2 \phi}{2\sin\phi\cos\phi} = \frac{A_{pp} - A_{qq}}{2A_{pq}} \tag{H.7}$$

i.e. with $t = \tan\phi = s/c$

$$t^2 + 2t\cot 2\phi - 1 = 0 \tag{H.8}$$

This quadratic equation has the roots

$$t = -\cot 2\phi \pm \sqrt{1 + \cot^2 2\phi} = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| \pm \epsilon(\cot 2\phi)\sqrt{1 + \cot^2 2\phi}} \tag{H.9}$$

and the smaller in magnitude of these is

$$t = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| + \sqrt{1 + \cot^2 2\phi}} \tag{H.10}$$

and since $|t| \leq 1$, it corresponds to $|\phi| \leq \pi/4$. For very large $\cot 2\phi$ we will use

$$t = \frac{1}{2\cot 2\phi} = \frac{A_{pq}}{A_{pp} - A_{qq}} \tag{H.11}$$

$$h = A_{qq} - A_{pp} \tag{H.12}$$

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

```
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

$$\cos^2 \phi = \frac{\cos^2 \phi}{\cos^2 \phi + \sin^2 \phi} = \frac{1}{1 + \tan^2 \phi} \tag{H.13a}$$

$$\sin \phi = \tan \phi \cos \phi \tag{H.13b}$$

$$\tau \sin \phi = \frac{\sin^2}{1 + \cos \phi} = \frac{1 - \cos^2}{1 + \cos \phi} = 1 - \cos \phi \tag{H.13c}$$

320b ⟨*Determine ϕ for the Jacobi rotation $P(\phi; p, q)$ with $A'_{pq} = 0$* 320a⟩+≡   (319) ◁ 320a

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

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

320c ⟨$A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$ 320c⟩≡   (319) 321a ▷

```
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
```

$$\begin{aligned}
r \neq p < q \neq r : A'_{rp} &= cA_{rp} - sA_{rq} \\
A'_{rq} &= sA_{rp} + cA_{rq}
\end{aligned} \tag{H.15}$$

Here's how we cover the upper triangular region using array notation:

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

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

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

321b $\langle \textit{Implementation of } \texttt{linalg} \textit{ procedures } 315\rangle+\equiv$ (314a) ◁318b 322a▷
```
pure subroutine jacobi_rotation (s, tau, vp, vq)
  real(kind=default), intent(in) :: s, tau
  real(kind=default), dimension(:), intent(inout) :: vp, vq
  real(kind=default), dimension(size(vp)) :: vp_tmp
  vp_tmp = vp
  vp = vp - s * (vq      + tau * vp)
  vq = vq + s * (vp_tmp - tau * vq)
end subroutine jacobi_rotation
```

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

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

321e $\langle \textit{Initialize } \texttt{num\_rot}\ 321e\rangle\equiv$ (318b)
```
if (present (num_rot)) then
   num_rot = 0
end if
```

321f $\langle \textit{Update } \texttt{num\_rot}\ 321f\rangle\equiv$ (319)
```
if (present (num_rot)) then
   num_rot = num_rot + 1
end if
```

322a ⟨*Implementation of* `linalg` *procedures* 315⟩+≡   (314a) ◁321b 322b▷
```
pure subroutine unit (u)
  real(kind=default), dimension(:,:), intent(out) :: u
  integer :: i
  u = 0.0
  do i = 1, min (size (u, dim = 1), size (u, dim = 2))
     u(i,i) = 1.0
  end do
end subroutine unit
```

322b ⟨*Implementation of* `linalg` *procedures* 315⟩+≡   (314a) ◁322a
```
pure function diag (a) result (d)
  real(kind=default), dimension(:,:), intent(in) :: a
  real(kind=default), dimension(min(size(a,dim=1),size(a,dim=2))) :: d
  integer :: i
  do i = 1, min (size (a, dim = 1), size (a, dim = 2))
     d(i) = a(i,i)
  end do
end function diag
```

322c ⟨*Declaration of* `linalg` *procedures* 314b⟩+≡   (314a) ◁321c
```
public :: unit, diag
```

H.4   Test

322d ⟨`la_sample.f90` 322d⟩≡
```
! la_sample.f90 --
```
⟨*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
```

```fortran
       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

⟨products.f90 324⟩≡

```
! 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), kind=default) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
         - cmplx (q(2), q(3), kind=default) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
  end function sp
  pure function spc (p, q) result (spcpq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: spcpq
    spcpq = conjg (sp (p, q))
  end function spc
end module products
```

—J—
KINEMATICS

325a   ⟨kinematics.f90 325a⟩≡   330d ▷

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

J.1 Lorentz Transformations

325b   ⟨Declaration of kinematics procedures 325b⟩≡   (325a) 327d ▷

```
  public :: boost_velocity
  private :: boost_one_velocity, boost_many_velocity
  public :: boost_momentum
  private :: boost_one_momentum, boost_many_momentum
```

325c   ⟨Interfaces of kinematics procedures 325c⟩≡   (325a) 327f ▷

```
  interface boost_velocity
     module procedure boost_one_velocity, boost_many_velocity
  end interface
```

```
interface boost_momentum
   module procedure boost_one_momentum, boost_many_momentum
end interface
```

Boost a four vector p to the inertial frame moving with the velocity β:

$$p_0' = \gamma \left(p_0 - \vec{\beta}\vec{p} \right) \tag{J.1a}$$

$$\vec{p}' = \gamma \left(\vec{p}_\parallel - \vec{\beta}p_0 \right) + \vec{p}_\perp \tag{J.1b}$$

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

$$p_0' = \gamma p_0 - \vec{b}\vec{p} \tag{J.2a}$$

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

326a   ⟨*Implementation of* `kinematics` *procedures* 326a⟩≡   (325a)   326b ▷

```
pure function boost_one_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(0:3) :: p_prime
  real(kind=default), dimension(1:3) :: b
  real(kind=default) :: gamma, b_dot_p
  gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
  b = gamma * beta
  b_dot_p = dot_product (b, p(1:3))
  p_prime(0) = gamma * p(0) - b_dot_p
  p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
end function boost_one_velocity
```

326b   ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a)   ◁326a 327a ▷

```
pure function boost_many_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  integer :: i
  do i = 1, size (p, dim=1)
     p_prime(i,:) = boost_one_velocity (p(i,:), beta)
  end do
end function boost_many_velocity
```

Boost a four vector p to the rest frame of the four vector q. The velocity is $\vec{\beta} = \vec{q}/|q_0|$:

327a $\quad\langle$*Implementation of* `kinematics` *procedures* 326a$\rangle+\equiv$ $\qquad$ (325a) ◁326b 327b▷

```
pure function boost_one_momentum (p, q) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p, q
  real(kind=default), dimension(0:3) :: p_prime
  p_prime = boost_velocity (p, q(1:3) / abs (q(0)))
end function boost_one_momentum
```

327b $\quad\langle$*Implementation of* `kinematics` *procedures* 326a$\rangle+\equiv$ $\qquad$ (325a) ◁327a 327c▷

```
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

$$\lambda(a, b, c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca = (a - b - c)^2 - 4bc \qquad \text{(J.3)}$$

and permutations

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

```
pure function lambda (a, b, c) result (lam)
  real(kind=default), intent(in) :: a, b, c
  real(kind=default) :: lam
  lam = a**2 + b**2 + c**2 - 2*(a*b + b*c + c*a)
end function lambda
```

327d $\quad\langle$*Declaration of* `kinematics` *procedures* 325b$\rangle+\equiv$ $\qquad$ (325a) ◁325b 327e▷

```
public :: lambda
```

327e $\quad\langle$*Declaration of* `kinematics` *procedures* 325b$\rangle+\equiv$ $\qquad$ (325a) ◁327d 329a▷

```
public :: two_to_three
private :: two_to_three_massive, two_to_three_massless
```

327f $\quad\langle$*Interfaces of* `kinematics` *procedures* 325c$\rangle+\equiv$ $\qquad$ (325a) ◁325c 329b▷

```
interface two_to_three
  module procedure two_to_three_massive, two_to_three_massless
end interface
```

327g $\quad\langle$*Declaration of* `kinematics` *types* 327g$\rangle\equiv$ $\qquad$ (325a)

```
type, public :: LIPS3
  real(kind=default), dimension(3,0:3) :: p
  real(kind=default) :: jacobian
end type LIPS3
```

$$\mathrm{dLIPS}_3 = \int \frac{\mathrm{d}^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{\mathrm{d}^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{\mathrm{d}^3\vec{p}_3}{(2\pi)^3 2E_3} \, (2\pi)^4 \delta^4(p_1+p_2+p_3-p_a-p_b) \quad \text{(J.4)}$$

The jacobian is given by

$$\mathrm{dLIPS}_3 = \frac{1}{(2\pi)^5} \int \mathrm{d}\phi \mathrm{d}t_1 \mathrm{d}s_2 \mathrm{d}\Omega_3^{[23]} \frac{1}{32\sqrt{ss_2}} \frac{|\vec{p}_3^{\,[23]}|}{|\vec{p}_a^{\,[ab]}|} \quad \text{(J.5)}$$

where $\vec{p}_i^{\,[jk]}$ denotes the momentum of particle i in the center of mass system of particles j and k.

328a ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁327c 328b▷

```
pure function two_to_three_massive &
     (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
       s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
       1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive
```

A specialized version for massless particles can be faster, because the kinematics is simpler:

328b ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁328a 329c▷

```
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
```
⟨*Declaration of* `kinematics` *procedures* 325b⟩+≡   (325a) ◁327e 330a▷
```
          public :: one_to_two
          private :: one_to_two_massive, one_to_two_massless
```

⟨*Interfaces of* `kinematics` *procedures* 325c⟩+≡   (325a) ◁327f
```
          interface one_to_two
             module procedure one_to_two_massive, one_to_two_massless
          end interface
```

⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁328b 329d▷
```
          pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
            real(kind=default), dimension(0:), intent(in) :: p12
            real(kind=default), intent(in) :: cos_theta, phi, m1, m2
            real(kind=default), dimension(2,0:3) :: p
            real(kind=default) :: s, p1_abs
            s = dot (p12, p12)
            p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
            p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
            p(2,1:3) = - p(1,1:3)
            p(1,0) = on_shell (p(1,:), m1)
            p(2,0) = on_shell (p(2,:), m2)
            p = boost_momentum (p, - p12)
          end function one_to_two_massive
```

⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁329c 330b▷
```
          pure function one_to_two_massless (p12, cos_theta, phi) result (p)
            real(kind=default), dimension(0:), intent(in) :: p12
            real(kind=default), intent(in) :: cos_theta, phi
            real(kind=default), dimension(2,0:3) :: p
            real(kind=default) :: p1_abs
            p1_abs = sqrt (dot (p12, p12)) / 2
            p(1,0) = p1_abs
            p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
            p(2,0) = p1_abs
            p(2,1:3) = - p(1,1:3)
            p = boost_momentum (p, - p12)
```

```
          end function one_to_two_massless
```

330a ⟨*Declaration of* `kinematics` *procedures* 325b⟩+≡   (325a) ◁329a 333c▷
```
    public :: polar_to_cartesian, on_shell
```

330b ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁329d 330c▷
```
    pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
      real(kind=default), intent(in) :: v_abs, cos_theta, phi
      real(kind=default), dimension(3) :: v
      real(kind=default) :: sin_phi, cos_phi, sin_theta
      sin_theta = sqrt (1.0 - cos_theta**2)
      cos_phi = cos (phi)
      sin_phi = sin (phi)
      v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
    end function polar_to_cartesian
```

330c ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁330b 333d▷
```
    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

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

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

330d ⟨`kinematics.f90` 325a⟩+≡   ◁325a
```
  module phase_space
    use kinds
    use constants
    use kinematics !NODEP!
    use tao_random_numbers
    implicit none
    private
```

330

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

$$\texttt{LIPS3\_unit} : [0, 1]^5 \qquad\qquad (\text{J.8})$$

331a ⟨*Declaration of* `phase_space` *types* 331a⟩≡   (330d) 331b▷
```
type, public :: LIPS3_unit
   real(kind=default), dimension(5) :: x
   real(kind=default) :: s
   real(kind=default), dimension(2) :: mass_in
   real(kind=default), dimension(3) :: mass_out
   real(kind=default) :: jacobian
end type LIPS3_unit
```

331b ⟨*Declaration of* `phase_space` *types* 331a⟩+≡   (330d) ◁331a 331c▷
```
type, public :: LIPS3_unit_massless
   real(kind=default), dimension(5) :: x
   real(kind=default) :: s
   real(kind=default) :: jacobian
end type LIPS3_unit_massless
```

$$\texttt{LIPS3\_s2\_t1\_angles} : (s_2, t_1, \phi, \cos\theta_3, \phi_3) \qquad\qquad (\text{J.9})$$

331c ⟨*Declaration of* `phase_space` *types* 331a⟩+≡   (330d) ◁331b 331d▷
```
type, public :: LIPS3_s2_t1_angles
   real(kind=default) :: s2, t1, phi, cos_theta3, phi3
   real(kind=default) :: s
   real(kind=default), dimension(2) :: mass_in
   real(kind=default), dimension(3) :: mass_out
   real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles
```

331d ⟨*Declaration of* `phase_space` *types* 331a⟩+≡   (330d) ◁331c 331e▷
```
type, public :: LIPS3_s2_t1_angles_massless
   real(kind=default) :: s2, t1, phi, cos_theta3, phi3
   real(kind=default) :: s
   real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles_massless
```

$$\texttt{LIPS3\_momenta} : (p_1, p_2, p_3) \qquad\qquad (\text{J.10})$$

331e ⟨*Declaration of* `phase_space` *types* 331a⟩+≡   (330d) ◁331d 332a▷

331

```
      type, public :: LIPS3_momenta
         real(kind=default), dimension(0:3,3) :: p
         real(kind=default) :: s
         real(kind=default), dimension(2) :: mass_in
         real(kind=default), dimension(3) :: mass_out
         real(kind=default) :: jacobian
      end type LIPS3_momenta
```

332a ⟨*Declaration of* phase_space *types* 331a⟩+≡   (330d) ◁331e
```
      type, public :: LIPS3_momenta_massless
         real(kind=default), dimension(0:3,3) :: p
         real(kind=default) :: s
         real(kind=default) :: jacobian
      end type LIPS3_momenta_massless
```

332b ⟨*Declaration of* phase_space *procedures* 332b⟩≡   (330d) 332f▷
```
      public :: random_LIPS3
      private :: random_LIPS3_unit, random_LIPS3_unit_massless
```

332c ⟨*Interfaces of* phase_space *procedures* 332c⟩≡   (330d)
```
      interface random_LIPS3
         module procedure random_LIPS3_unit, random_LIPS3_unit_massless
      end interface
```

332d ⟨*Implementation of* phase_space *procedures* 332d⟩≡   (330d) 332e▷
```
      pure subroutine random_LIPS3_unit (rng, lips)
        type(tao_random_state), intent(inout) :: rng
        type(LIPS3_unit), intent(inout) :: lips
        call tao_random_number (rng, lips%x)
        lips%jacobian = 1
      end subroutine random_LIPS3_unit
```

332e ⟨*Implementation of* phase_space *procedures* 332d⟩+≡   (330d) ◁332d 333a▷
```
      pure subroutine random_LIPS3_unit_massless (rng, lips)
        type(tao_random_state), intent(inout) :: rng
        type(LIPS3_unit_massless), intent(inout) :: lips
        call tao_random_number (rng, lips%x)
        lips%jacobian = 1
      end subroutine random_LIPS3_unit_massless
```

332f ⟨*Declaration of* phase_space *procedures* 332b⟩+≡   (330d) ◁332b
```
      private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
```

332g ⟨*(Unused) Interfaces of* phase_space *procedures* 332g⟩≡
```
      interface assignment(=)
         module procedure &
              LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
      end interface
```

⟨*Implementation of* **phase_space** *procedures* 332d⟩+≡   (330d) ◁332e 333b▷

```fortran
pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
  type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
  type(LIPS3_unit), intent(in) :: unit
end subroutine  LIPS3_unit_to_s2_t1_angles
```

333b ⟨*Implementation of* **phase_space** *procedures* 332d⟩+≡   (330d) ◁333a

```fortran
pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
  type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
  type(LIPS3_unit_massless), intent(in) :: unit
end subroutine  LIPS3_unit_to_s2_t1_angles_m0
```

J.4   Massless n-Particle Phase Space: `RAMBO`

333c ⟨*Declaration of* **kinematics** *procedures* 325b⟩+≡   (325a) ◁330a 334b▷

```fortran
public :: massless_isotropic_decay
```

The massless `RAMBO` algorithm [26]:

333d ⟨*Implementation of* **kinematics** *procedures* 326a⟩+≡   (325a) ◁330c 334c▷

```fortran
pure function massless_isotropic_decay (roots, ran) result (p)
  real (kind=default), intent(in) :: roots
  real (kind=default), dimension(:,:), intent(in) :: ran
  real (kind=default), dimension(size(ran,dim=1),0:3) :: p
  real (kind=default), dimension(size(ran,dim=1),0:3) :: q
  real (kind=default), dimension(0:3) :: qsum
  real (kind=default) :: cos_theta, sin_theta, phi, qabs, x, r, z
  integer :: k
  ⟨Generate isotropic null vectors 333e⟩
  ⟨Boost and rescale the vectors 334a⟩
end function massless_isotropic_decay
```

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

333e ⟨*Generate isotropic null vectors* 333e⟩≡   (333d)

```fortran
do k = 1, size (p, dim = 1)
   q(k,0) = - log (ran(k,1) * ran(k,2))
   cos_theta = 2 * ran(k,3) - 1
   sin_theta = sqrt (1 - cos_theta**2)
   phi = 2 * PI * ran(k,4)
   q(k,1) = q(k,0) * sin_theta * cos (phi)
   q(k,2) = q(k,0) * sin_theta * sin (phi)
   q(k,3) = q(k,0) * cos_theta
enddo
```

The proof that the Jacobian of the transformation vanishes can be found in [26]. The transformation is really a Lorentz boost (as can be seen easily).

334a   ⟨*Boost and rescale the vectors* 334a⟩≡   (333d)

```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
   r = dot (q(k,:), qsum) / qabs
   z = (q(k,0) + r) / (qsum(0) + qabs)
   p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
   p(k,0) = x * r
enddo
```

334b   ⟨*Declaration of* `kinematics` *procedures* 325b⟩+≡   (325a) ◁333c

```
public :: phase_space_volume
```

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

334c   ⟨*Implementation of* `kinematics` *procedures* 326a⟩+≡   (325a) ◁333d

```
pure function phase_space_volume (n, roots) result (volume)
   integer, intent(in) :: n
   real (kind=default), intent(in) :: roots
   real (kind=default) :: volume
   real (kind=default) :: nd
   nd = n
   volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

J.5   Tests

334d   ⟨ktest.f90 334d⟩≡

```
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
```

334

```
      integer :: i
      character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
      ma = 1.0
      mb = 1.0
      m1 = 10.0
      m2 = 20.0
      m3 = 30.0
      s = 100.0 ** 2
      do i = 1, 10
         call tao_random_number (r)
         s2 = (r(1) * (sqrt (s) - m1) + (1 - r(1)) * (m2 + m3)) ** 2
         t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
               + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
         t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
               - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
         t1 = r(2) * t1_max + (1 - r(2)) * t1_min
         phi = 2*PI * r(3)
         cos_theta3 = 2 * r(4) - 1
         phi3 = 2*PI * r(5)
         p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
         print fmt, "p1       = ", p%p(1,:)
         print fmt, "p2       = ", p%p(2,:)
         print fmt, "p3       = ", p%p(3,:)
         print fmt, "p1,2,3^2 = ", dot (p%p(1,:), p%p(1,:)), &
               dot (p%p(2,:), p%p(2,:)), dot (p%p(3,:), p%p(3,:))
         print fmt, "sum(p)   = ", p%p(1,:) + p%p(2,:) + p%p(3,:)
         print fmt, "|J|      = ", p%jacobian
      end do
   end program ktest
```

⚠ Trivial check for typos, should be removed from the finalized program!

335 ⟨*Trivial* `ktest.f90` 335⟩≡

```
   program ktest
      use kinds
      use constants
      use products
      use kinematics
      use tao_random_numbers
      implicit none
      real(kind=default), dimension(0:3) :: p, q, p_prime, p0
      real(kind=default) :: m
      character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
      integer :: i
```

```
   do i = 1, 5
      if (i == 1) then
         p = (/ 1.0_double, 0.0_double, 0.0_double, 0.0_double /)
         m = 1.0
      else
         call tao_random_number (p)
         m = sqrt (PI)
      end if
      call tao_random_number (q(1:3))
      q(0) = sqrt (m**2 + dot_product (q(1:3), q(1:3)))
      p_prime = boost_momentum (p, q)
      print fmt, "p    = ", p
      print fmt, "q    = ", q
      print fmt, "p'   = ", p_prime
      print fmt, "p^2  = ", dot (p, p)
      print fmt, "p'^2 = ", dot (p_prime, p_prime)
      if (dot (p, p) > 0.0) then
         p0 = boost_momentum (p, p)
         print fmt, "p0   = ", p0
         print fmt, "p0^2 = ", dot (p0, p0)
      end if
   end do
end program ktest
```

—K—
Coordinates

337   ⟨coordinates.f90 337⟩≡

```
! coordinates.f90 --
⟨Copyleft notice 1⟩
module coordinates
  use kinds
  use constants, only: PI
  use specfun, only: gamma
  implicit none
  private
  ⟨Declaration of coordinates procedures 338a⟩
contains
  ⟨Implementation of coordinates procedures 338b⟩
end module coordinates
```

K.1   Angular Spherical Coordinates

$$\begin{aligned}
x_n &= r \cos \theta_{n-2} \\
x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
&\cdots \\
x_3 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \cos \theta_1 \\
x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \cos \phi \\
x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \sin \phi
\end{aligned} \tag{K.1}$$

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

$$P_j = \prod_{i=j}^{n-2} \sin \theta_i \tag{K.3}$$

Then

$$
\begin{aligned}
x_n &= r \cos \theta_{n-2} \\
x_{n-1} &= r P_{n-2} \cos \theta_{n-3} \\
&\cdots \\
x_3 &= r P_2 \cos \theta_1 \\
x_2 &= r P_1 \cos \phi \\
x_1 &= r P_1 \sin \phi
\end{aligned}
\tag{K.4}
$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} P_i \tag{K.5}$$

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

$$\sin \theta_i = \sqrt{1 - \cos^2 \theta_i} \tag{K.6}$$

which is not true for ϕ. Since `sqrt` is typically much faster than `sin` and `cos`, we use (K.6) where ever possible.

338a ⟨*Declaration of* `coordinates` *procedures* 338a⟩≡   (337) 339c ▷
```
  public :: spherical_to_cartesian_2, &
        spherical_to_cartesian, spherical_to_cartesian_j
```

338b ⟨*Implementation of* `coordinates` *procedures* 338b⟩≡   (337) 339a ▷
```
  pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: theta
    real(kind=default), dimension(:), intent(out), optional :: x
    real(kind=default), intent(out), optional :: jacobian
    real(kind=default), dimension(size(theta)) :: cos_theta
    real(kind=default), dimension(size(theta)+1) :: product_sin_theta
    integer :: n, i
    n = size (theta) + 2
    cos_theta = cos (theta)
    product_sin_theta(n-1) = 1.0_default
    do i = n - 2, 1, -1
       product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
    end do
```

```
     if (present (x)) then
         x(1) = r * product_sin_theta(1) * sin (phi)
         x(2) = r * product_sin_theta(1) * cos (phi)
         x(3:) = r * product_sin_theta(2:n-1) * cos_theta
     end if
     if (present (jacobian)) then
         jacobian = r**(n-1) * product (product_sin_theta)
     end if
   end subroutine spherical_to_cartesian_2
```

⚠ Note that **call** inside of a function breaks F-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where **theta** could not be assumed shape . . .

339a   ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁338b 339b▷
```
   pure function spherical_to_cartesian (r, phi, theta) result (x)
     real(kind=default), intent(in) :: r, phi
     real(kind=default), dimension(:), intent(in) :: theta
     real(kind=default), dimension(size(theta)+2) :: x
     call spherical_to_cartesian_2 (r, phi, theta, x = x)
   end function spherical_to_cartesian
```

339b   ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁339a 339d▷
```
   pure function spherical_to_cartesian_j (r, phi, theta) &
         result (jacobian)
     real(kind=default), intent(in) :: r, phi
     real(kind=default), dimension(:), intent(in) :: theta
     real(kind=default) :: jacobian
     call spherical_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
   end function spherical_to_cartesian_j
```

339c   ⟨*Declaration of* `coordinates` *procedures* 338a⟩+≡   (337) ◁338a 341c▷
```
   public :: cartesian_to_spherical_2, &
         cartesian_to_spherical, cartesian_to_spherical_j
```

339d   ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁339b 341a▷
```
   pure subroutine cartesian_to_spherical_2 (x, r, phi, theta, jacobian)
     real(kind=default), dimension(:), intent(in) :: x
     real(kind=default), intent(out), optional :: r, phi
     real(kind=default), dimension(:), intent(out), optional :: theta
     real(kind=default), intent(out), optional :: jacobian
     real(kind=default) :: local_r
     real(kind=default), dimension(size(x)-2) :: cos_theta
     real(kind=default), dimension(size(x)-1) :: product_sin_theta
```

```fortran
integer :: n, i
n = size (x)
local_r = sqrt (dot_product (x, x))
if (local_r == 0) then
  if (present (r)) then
    r = 0
  end if
  if (present (phi)) then
    phi = 0
  end if
  if (present (theta)) then
    theta = 0
  end if
  if (present (jacobian)) then
    jacobian = 1
  end if
else
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
    if (product_sin_theta(i-1) == 0) then
      cos_theta(i-2) = 0
    else
      cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    end if
    product_sin_theta(i-2) = &
        product_sin_theta(i-1) * sqrt (1 - cos_theta(i-2)**2)
  end do
  if (present (r)) then
    r = local_r
  end if
  if (present (phi)) then
    !  Set phi = 0 for vanishing vector
    if (x(1) == 0 .and. x(2)==0) then
     phi = 0
    else
       phi = atan2 (x(1), x(2))
    end if
  end if
  if (present (theta)) then
    theta = acos (cos_theta)
  end if
  if (present (jacobian)) then
    jacobian = local_r**(1-n) / product (product_sin_theta)
```

```
          end if
        end if
      end subroutine cartesian_to_spherical_2
```

341a ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁339d 341b▷
```
      pure subroutine cartesian_to_spherical (x, r, phi, theta)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out) :: r, phi
        real(kind=default), dimension(:), intent(out) :: theta
        call cartesian_to_spherical_2 (x, r, phi, theta)
      end subroutine cartesian_to_spherical
```

341b ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁341a 341d▷
```
      pure function cartesian_to_spherical_j (x) result (jacobian)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default) :: jacobian
        call cartesian_to_spherical_2 (x, jacobian = jacobian)
      end function cartesian_to_spherical_j
```

K.2   Trigonometric Spherical Coordinates

341c ⟨*Declaration of* `coordinates` *procedures* 338a⟩+≡   (337) ◁339c 342c▷
```
      public :: spherical_cos_to_cartesian_2, &
          spherical_cos_to_cartesian, spherical_cos_to_cartesian_j
```

Using the cosine, we have to drop P_1 from the Jacobian

341d ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁341b 342a▷
```
      pure subroutine spherical_cos_to_cartesian_2 (r, phi, cos_theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: cos_theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(cos_theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (cos_theta) + 2
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
          product_sin_theta(i) = &
              product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do
        if (present (x)) then
          x(1) = r * product_sin_theta(1) * sin (phi)
          x(2) = r * product_sin_theta(1) * cos (phi)
          x(3:) = r * product_sin_theta(2:n-1) * cos_theta
```

```
      end if
      if (present (jacobian)) then
          jacobian = r**(n-1) * product (product_sin_theta(2:))
      end if
   end subroutine spherical_cos_to_cartesian_2
```

342a ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁341d 342b▷
```
   pure function spherical_cos_to_cartesian (r, phi, theta) result (x)
     real(kind=default), intent(in) :: r, phi
     real(kind=default), dimension(:), intent(in) :: theta
     real(kind=default), dimension(size(theta)+2) :: x
     call spherical_cos_to_cartesian_2 (r, phi, theta, x = x)
   end function spherical_cos_to_cartesian
```

342b ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁342a 342d▷
```
   pure function spherical_cos_to_cartesian_j (r, phi, theta) &
        result (jacobian)
     real(kind=default), intent(in) :: r, phi
     real(kind=default), dimension(:), intent(in) :: theta
     real(kind=default) :: jacobian
     call spherical_cos_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
   end function spherical_cos_to_cartesian_j
```

342c ⟨*Declaration of* `coordinates` *procedures* 338a⟩+≡   (337) ◁341c 344b▷
```
   public :: cartesian_to_spherical_cos_2, &
        cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
```

342d ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁342b 343▷
```
   pure subroutine cartesian_to_spherical_cos_2 (x, r, phi, cos_theta, jacobian)
     real(kind=default), dimension(:), intent(in) :: x
     real(kind=default), intent(out), optional :: r, phi
     real(kind=default), dimension(:), intent(out), optional :: cos_theta
     real(kind=default), intent(out), optional :: jacobian
     real(kind=default) :: local_r
     real(kind=default), dimension(size(x)-2) :: local_cos_theta
     real(kind=default), dimension(size(x)-1) :: product_sin_theta
     integer :: n, i
     n = size (x)
     local_r = sqrt (dot_product (x, x))
     if (local_r == 0) then
       if (present (r)) then
         r = 0
       end if
       if (present (phi)) then
         phi = 0
       end if
```

```fortran
        if (present (cos_theta)) then
          cos_theta = 0
        end if
        if (present (jacobian)) then
          jacobian = 1
        end if
      else
        product_sin_theta(n-1) = 1
        do i = n, 3, -1
          if (product_sin_theta(i-1) == 0) then
            local_cos_theta(i-2) = 0
          else
            local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
          end if
          product_sin_theta(i-2) = &
                product_sin_theta(i-1) * sqrt (1 - local_cos_theta(i-2)**2)
        end do
        if (present (r)) then
          r = local_r
        end if
        if (present (phi)) then
          !  Set phi = 0 for vanishing vector
          if (x(1) == 0 .and. x(2)==0) then
           phi = 0
          else
            phi = atan2 (x(1), x(2))
          end if
        end if
        if (present (cos_theta)) then
          cos_theta = local_cos_theta
        end if
        if (present (jacobian)) then
          jacobian = local_r**(1-n) / product (product_sin_theta(2:))
        end if
      end if
    end subroutine cartesian_to_spherical_cos_2
```

343 ⟨*Implementation of* coordinates *procedures* 338b⟩+≡   (337) ◁342d 344a▷

```fortran
    pure subroutine cartesian_to_spherical_cos (x, r, phi, cos_theta)
      real(kind=default), dimension(:), intent(in) :: x
      real(kind=default), intent(out) :: r, phi
      real(kind=default), dimension(:), intent(out), optional :: cos_theta
      call cartesian_to_spherical_cos_2 (x, r, phi, cos_theta)
    end subroutine cartesian_to_spherical_cos
```

344a   ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁343 344c▷

```
pure function cartesian_to_spherical_cos_j (x) result (jacobian)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: jacobian
  call cartesian_to_spherical_cos_2 (x, jacobian = jacobian)
end function cartesian_to_spherical_cos_j
```

K.3 Surface of a Sphere

344b   ⟨*Declaration of* `coordinates` *procedures* 338a⟩+≡   (337) ◁342c

```
public :: surface
```

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

344c   ⟨*Implementation of* `coordinates` *procedures* 338b⟩+≡   (337) ◁344a

```
pure function surface (n) result (vol)
  integer, intent(in) :: n
  real(kind=default) :: vol
  real(kind=default) :: n_by_2
  n_by_2 = 0.5_default * n
  vol = 2 * PI**n_by_2 / gamma (n_by_2)
end function surface
```

—L—
Idiomatic Fortran90 Interface for MPI

345a ⟨mpi90.f90 345a⟩≡

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

L.1   Basics

345b ⟨Declaration of mpi90 procedures 345b⟩≡   (345a) 348b ▷

```
      public :: mpi90_init
      public :: mpi90_finalize
      public :: mpi90_abort
      public :: mpi90_print_error
      public :: mpi90_size
      public :: mpi90_rank
```

346a　⟨*Implementation of* `mpi90` *procedures* 346a⟩≡　　　　　　　　(345a)　346d ▷

```
subroutine mpi90_init (error)
  integer, intent(out), optional :: error
  integer :: local_error
  character(len=*), parameter :: FN = "mpi90_init"
  external mpi_init
  call mpi_init (local_error)
```
⟨*Handle* `local_error` *(no* `mpi90_abort`*)* 346b⟩
```
end subroutine mpi90_init
```

346b　⟨*Handle* `local_error` *(no* `mpi90_abort`*)* 346b⟩≡　　　　　　　　(346)

```
if (present (error)) then
  error = local_error
else
  if (local_error /= MPI_SUCCESS) then
    call mpi90_print_error (local_error, FN)
    stop
  end if
end if
```

346c　⟨*Handle* `local_error` 346c⟩≡　　　　　　　　(346–49 351c 353d 354b 356a)

```
if (present (error)) then
  error = local_error
else
  if (local_error /= MPI_SUCCESS) then
    call mpi90_print_error (local_error, FN)
    call mpi90_abort (local_error)
    stop
  end if
end if
```

346d　⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡　　　　　(345a)　◁346a　346e ▷

```
subroutine mpi90_finalize (error)
  integer, intent(out), optional :: error
  integer :: local_error
  character(len=*), parameter :: FN = "mpi90_finalize"
  external mpi_finalize
  call mpi_finalize (local_error)
```
⟨*Handle* `local_error` 346c⟩
```
end subroutine mpi90_finalize
```

346e　⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡　　　　　(345a)　◁346d　347a ▷

```
subroutine mpi90_abort (code, domain, error)
  integer, intent(in), optional :: code, domain
  integer, intent(out), optional :: error
  character(len=*), parameter :: FN = "mpi90_abort"
```

```
      integer :: local_domain, local_code, local_error
      external mpi_abort
      if (present (code)) then
         local_code = code
      else
         local_code = MPI_ERR_UNKNOWN
      end if
      ⟨Set default for domain 347b⟩
      call mpi_abort (local_domain, local_code, local_error)
      ⟨Handle local_error (no mpi90_abort) 346b⟩
   end subroutine mpi90_abort
```

347a ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁346e 347c▷
```
   subroutine mpi90_print_error (error, msg)
      integer, intent(in) :: error
      character(len=*), optional :: msg
      character(len=*), parameter :: FN = "mpi90_print_error"
      integer :: msg_len, local_error
      external mpi_error_string
      call mpi_error_string (error, msg, msg_len, local_error)
      if (local_error /= MPI_SUCCESS) then
         print *, "PANIC: even MPI_ERROR_STRING() failed!!!"
         call mpi90_abort (local_error)
      else if (present (msg)) then
         print *, trim (msg), ": ", trim (msg(msg_len+1:))
      else
         print *, "mpi90: ", trim (msg(msg_len+1:))
      end if
   end subroutine mpi90_print_error
```

347b ⟨*Set default for* domain 347b⟩≡   (346–50 356a) 354f▷
```
   if (present (domain)) then
      local_domain = domain
   else
      local_domain = MPI_COMM_WORLD
   end if
```

347c ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁347a 348a▷
```
   subroutine mpi90_size (sz, domain, error)
      integer, intent(out) :: sz
      integer, intent(in), optional :: domain
      integer, intent(out), optional :: error
      character(len=*), parameter :: FN = "mpi90_size"
      integer :: local_domain, local_error
      external mpi_comm_size
```

```
        ⟨Set default for domain 347b⟩
        call mpi_comm_size (local_domain, sz, local_error)
        ⟨Handle local_error 346c⟩
      end subroutine mpi90_size
```

348a   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁347c 348d▷
```
      subroutine mpi90_rank (rank, domain, error)
        integer, intent(out) :: rank
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_rank"
        integer :: local_domain, local_error
        external mpi_comm_rank
        ⟨Set default for domain 347b⟩
        call mpi_comm_rank (local_domain, rank, local_error)
        ⟨Handle local_error 346c⟩
      end subroutine mpi90_rank
```

L.2   Point to Point

348b   ⟨*Declaration of* `mpi90` *procedures* 345b⟩+≡   (345a) ◁345b 351d▷
```
      public :: mpi90_send
      public :: mpi90_receive
      public :: mpi90_receive_pointer
```

348c   ⟨*Interfaces of* `mpi90` *procedures* 348c⟩≡   (345a) 350d▷
```
      interface mpi90_send
        module procedure &
            mpi90_send_integer, mpi90_send_double, &
            mpi90_send_integer_array, mpi90_send_double_array, &
            mpi90_send_integer_array2, mpi90_send_double_array2
      end interface
```

348d   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁348a 348e▷
```
      subroutine mpi90_send_integer (value, target, tag, domain, error)
        integer, intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        call mpi90_send_integer_array ((/ value /), target, tag, domain, error)
      end subroutine mpi90_send_integer
```

348e   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁348d 349a▷
```
      subroutine mpi90_send_double (value, target, tag, domain, error)
```

```
        real(kind=default), intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        call mpi90_send_double_array ((/ value /), target, tag, domain, error)
      end subroutine mpi90_send_double
```

349a ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁348e 349c▷
```
      subroutine mpi90_send_integer_array (buffer, target, tag, domain, error)
        integer, dimension(:), intent(in) :: buffer
        integer, intent(in) ::  target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
```
        ⟨*Body of* mpi90_send_*_array 349b⟩
```
      end subroutine mpi90_send_integer_array
```

349b ⟨*Body of* mpi90_send_*_array 349b⟩≡   (349)
```
        integer :: local_domain, local_error
        external mpi_send
```
        ⟨*Set default for* domain 347b⟩
```
        call mpi_send (buffer, size (buffer), datatype, target, tag, &
                       local_domain, local_error)
```
        ⟨*Handle* local_error 346c⟩

349c ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁349a 349d▷
```
      subroutine mpi90_send_double_array (buffer, target, tag, domain, error)
        real(kind=default), dimension(:), intent(in) :: buffer
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_double_array"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
```
        ⟨*Body of* mpi90_send_*_array 349b⟩
```
      end subroutine mpi90_send_double_array
```

349d ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁349c 350a▷
```
      subroutine mpi90_send_integer_array2 (value, target, tag, domain, error)
        integer, dimension(:,:), intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(size(value)) :: buffer
        buffer = reshape (value, shape(buffer))
        call mpi90_send_integer_array (buffer, target, tag, domain, error)
```

```
          end subroutine mpi90_send_integer_array2
```

350a   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁349d 350c▷

```
    subroutine mpi90_send_double_array2 (value, target, tag, domain, error)
      real(kind=default), dimension(:,:), intent(in) :: value
      integer, intent(in) :: target, tag
      integer, intent(in), optional :: domain
      integer, intent(out), optional :: error
      real(kind=default), dimension(size(value)) :: buffer
      buffer = reshape (value, shape(buffer))
      call mpi90_send_double_array (buffer, target, tag, domain, error)
    end subroutine mpi90_send_double_array2
```

350b   ⟨*Declaration of* `mpi90` *types* 350b⟩≡   (345a)

```
    type, public :: mpi90_status
       integer :: count, source, tag, error
    end type mpi90_status
```

350c   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁350a 351a▷

```
    subroutine mpi90_receive_integer (value, source, tag, domain, status, error)
      integer, intent(out) :: value
      integer, intent(in), optional :: source, tag, domain
      type(mpi90_status), intent(out), optional :: status
      integer, intent(out), optional :: error
      integer, dimension(1)  :: buffer
      call mpi90_receive_integer_array (buffer, source, tag, domain, status, error)
      value = buffer(1)
    end subroutine mpi90_receive_integer
```

350d   ⟨*Interfaces of* `mpi90` *procedures* 348c⟩+≡   (345a) ◁348c 353a▷

```
    interface mpi90_receive
       module procedure &
            mpi90_receive_integer, mpi90_receive_double, &
            mpi90_receive_integer_array, mpi90_receive_double_array, &
            mpi90_receive_integer_array2, mpi90_receive_double_array2
    end interface
```

350e   ⟨*Set defaults for* `source`, `tag` *and* `domain` 350e⟩≡   (351c 353c)

```
    if (present (source)) then
       local_source = source
    else
       local_source = MPI_ANY_SOURCE
    end if
    if (present (tag)) then
       local_tag = tag
    else
```

```
        local_tag = MPI_ANY_TAG
      end if
      ⟨Set default for domain 347b⟩
```

351a ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁350c 351b▷
```
      subroutine mpi90_receive_double (value, source, tag, domain, status, error)
        real(kind=default), intent(out) :: value
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        call mpi90_receive_double_array (buffer, source, tag, domain, status, error)
        value = buffer(1)
      end subroutine mpi90_receive_double
```

351b ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁351a 351e▷
```
      subroutine mpi90_receive_integer_array &
          (buffer, source, tag, domain, status, error)
        integer, dimension(:), intent(out) :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        ⟨Body of mpi90_receive_*_array 351c⟩
      end subroutine mpi90_receive_integer_array
```

351c ⟨Body of mpi90_receive_*_array 351c⟩≡   (351b 352a)
```
      integer :: local_source, local_tag, local_domain, local_error
      integer, dimension(MPI_STATUS_SIZE) :: local_status
      external mpi_receive, mpi_get_count
      ⟨Set defaults for source, tag and domain 350e⟩
      call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
                     local_domain, local_status, local_error)
      ⟨Handle local_error 346c⟩
      if (present (status)) then
         call decode_status (status, local_status, datatype)
      end if
```

351d ⟨Declaration of mpi90 procedures 345b⟩+≡   (345a) ◁348b 354d▷
```
      private :: decode_status
```

⟐ Can we ignore ierror???

351e ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁351b 352a▷
```
      subroutine decode_status (status, mpi_status, datatype)
```

```
      type(mpi90_status), intent(out) :: status
      integer, dimension(:), intent(in) :: mpi_status
      integer, intent(in), optional :: datatype
      integer :: ierror
      if (present (datatype)) then
         call mpi_get_count (mpi_status, datatype, status%count, ierror)
      else
         status%count = 0
      end if
      status%source = mpi_status(MPI_SOURCE)
      status%tag = mpi_status(MPI_TAG)
      status%error = mpi_status(MPI_ERROR)
   end subroutine decode_status
```

352a ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁351e 352b▷
```
   subroutine mpi90_receive_double_array &
        (buffer, source, tag, domain, status, error)
      real(kind=default), dimension(:), intent(out) :: buffer
      integer, intent(in), optional :: source, tag, domain
      type(mpi90_status), intent(out), optional :: status
      integer, intent(out), optional :: error
      character(len=*), parameter :: FN = "mpi90_receive_double_array"
      integer, parameter :: datatype = MPI_DOUBLE_PRECISION
```
      ⟨*Body of* mpi90_receive_*_array 351c⟩
```
   end subroutine mpi90_receive_double_array
```

352b ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁352a 352c▷
```
   subroutine mpi90_receive_integer_array2 &
        (value, source, tag, domain, status, error)
      integer, dimension(:,:), intent(out) :: value
      integer, intent(in), optional :: source, tag, domain
      type(mpi90_status), intent(out), optional :: status
      integer, intent(out), optional :: error
      integer, dimension(size(value)) :: buffer
      call mpi90_receive_integer_array &
           (buffer, source, tag, domain, status, error)
      value = reshape (buffer, shape(value))
   end subroutine mpi90_receive_integer_array2
```

352c ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁352b 353b▷
```
   subroutine mpi90_receive_double_array2 &
        (value, source, tag, domain, status, error)
      real(kind=default), dimension(:,:), intent(out) :: value
      integer, intent(in), optional :: source, tag, domain
      type(mpi90_status), intent(out), optional :: status
```

```
            integer, intent(out), optional :: error
            real(kind=default), dimension(size(value)) :: buffer
            call mpi90_receive_double_array &
                    (buffer, source, tag, domain, status, error)
            value = reshape (buffer, shape(value))
          end subroutine mpi90_receive_double_array2
```

353a ⟨*Interfaces of* mpi90 *procedures* 348c⟩+≡   (345a) ◁350d 354e▷
```
          interface mpi90_receive_pointer
            module procedure &
                    mpi90_receive_integer_pointer, mpi90_receive_double_pointer
          end interface
```

353b ⟨*Implementation of* mpi90 *procedures* 346a⟩+≡   (345a) ◁352c 354c▷
```
          subroutine mpi90_receive_integer_pointer &
                  (buffer, source, tag, domain, status, error)
            integer, dimension(:), pointer :: buffer
            integer, intent(in), optional :: source, tag, domain
            type(mpi90_status), intent(out), optional :: status
            integer, intent(out), optional :: error
            character(len=*), parameter :: FN = "mpi90_receive_integer_pointer"
            integer, parameter :: datatype = MPI_INTEGER
            ⟨Body of mpi90_receive_*_pointer 353c⟩
          end subroutine mpi90_receive_integer_pointer
```

353c ⟨*Body of* mpi90_receive_*_pointer 353c⟩≡   (353b 354c) 353d▷
```
          integer :: local_source, local_tag, local_domain, local_error, buffer_size
          integer, dimension(MPI_STATUS_SIZE) :: local_status
          integer :: ierror
          external mpi_receive, mpi_get_count
          ⟨Set defaults for source, tag and domain 350e⟩
```

353d ⟨*Body of* mpi90_receive_*_pointer 353c⟩+≡   (353b 354c) ◁353c 353e▷
```
          call mpi_probe (local_source, local_tag, local_domain, &
                          local_status, local_error)
          ⟨Handle local_error 346c⟩
```

⟨⚠⟩ Can we ignore ierror???

353e ⟨*Body of* mpi90_receive_*_pointer 353c⟩+≡   (353b 354c) ◁353d 354a▷
```
          call mpi_get_count (local_status, datatype, buffer_size, ierror)
          if (associated (buffer)) then
            if (size (buffer) /= buffer_size) then
              deallocate (buffer)
              allocate (buffer(buffer_size))
            end if
```

```
      else
         allocate (buffer(buffer_size))
      end if
```

354a   ⟨*Body of* `mpi90_receive_*_pointer` 353c⟩+≡   (353b 354c) ◁353e 354b▷
```
      call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
                     local_domain, local_status, local_error)
```

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

354c   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁353b 355a▷
```
      subroutine mpi90_receive_double_pointer &
            (buffer, source, tag, domain, status, error)
        real(kind=default), dimension(:), pointer :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_double_pointer"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        ⟨Body of mpi90_receive_*_pointer 353c⟩
      end subroutine mpi90_receive_double_pointer
```

L.3   Collective Communication

354d   ⟨*Declaration of* `mpi90` *procedures* 345b⟩+≡   (345a) ◁351d
```
      public :: mpi90_broadcast
```

354e   ⟨*Interfaces of* `mpi90` *procedures* 348c⟩+≡   (345a) ◁353a
```
      interface mpi90_broadcast
         module procedure &
              mpi90_broadcast_integer, mpi90_broadcast_integer_array, &
              mpi90_broadcast_integer_array2, mpi90_broadcast_integer_array3, &
              mpi90_broadcast_double, mpi90_broadcast_double_array, &
              mpi90_broadcast_double_array2, mpi90_broadcast_double_array3, &
              mpi90_broadcast_logical, mpi90_broadcast_logical_array, &
              mpi90_broadcast_logical_array2, mpi90_broadcast_logical_array3
      end interface
```

354f   ⟨*Set default for* `domain` 347b⟩+≡   (346–50 356a) ◁347b
```
      if (present (domain)) then
         local_domain = domain
```

```
        else
            local_domain = MPI_COMM_WORLD
        end if
```

355a ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁354c 355b▷
```
    subroutine mpi90_broadcast_integer (value, root, domain, error)
        integer, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_integer_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_integer
```

355b ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁355a 355c▷
```
    subroutine mpi90_broadcast_double (value, root, domain, error)
        real(kind=default), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_double_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_double
```

355c ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁355b 355d▷
```
    subroutine mpi90_broadcast_logical (value, root, domain, error)
        logical, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        logical, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_logical_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_logical
```

355d ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁355c 356b▷
```
    subroutine mpi90_broadcast_integer_array (buffer, root, domain, error)
        integer, dimension(:), intent(inout) :: buffer
        integer, intent(in) ::  root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
```

```
              character(len=*), parameter :: FN = "mpi90_broadcast_integer_array"
              integer, parameter :: datatype = MPI_INTEGER
              ⟨Body of mpi90_broadcast_*_array 356a⟩
            end subroutine mpi90_broadcast_integer_array
```

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

356b   ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁355d 356c▷
```
              subroutine mpi90_broadcast_double_array (buffer, root, domain, error)
                real(kind=default), dimension(:), intent(inout) :: buffer
                integer, intent(in) :: root
                integer, intent(in), optional :: domain
                integer, intent(out), optional :: error
                integer, parameter :: datatype = MPI_DOUBLE_PRECISION
                character(len=*), parameter :: FN = "mpi90_broadcast_double_array"
```
              ⟨Body of mpi90_broadcast_*_array 356a⟩
```
              end subroutine mpi90_broadcast_double_array
```

356c   ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁356b 356d▷
```
              subroutine mpi90_broadcast_logical_array (buffer, root, domain, error)
                logical, dimension(:), intent(inout) :: buffer
                integer, intent(in) :: root
                integer, intent(in), optional :: domain
                integer, intent(out), optional :: error
                integer, parameter :: datatype = MPI_LOGICAL
                character(len=*), parameter :: FN = "mpi90_broadcast_logical_array"
```
              ⟨Body of mpi90_broadcast_*_array 356a⟩
```
              end subroutine mpi90_broadcast_logical_array
```

356d   ⟨Implementation of mpi90 procedures 346a⟩+≡   (345a) ◁356c 357a▷
```
              subroutine mpi90_broadcast_integer_array2 (value, root, domain, error)
                integer, dimension(:,:), intent(inout) :: value
                integer, intent(in) :: root
                integer, intent(in), optional :: domain
                integer, intent(out), optional :: error
                integer, dimension(size(value)) :: buffer
                buffer = reshape (value, shape(buffer))
                call mpi90_broadcast_integer_array (buffer, root, domain, error)
                value = reshape (buffer, shape(value))
              end subroutine mpi90_broadcast_integer_array2
```

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357a   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁356d 357b▷

```
subroutine mpi90_broadcast_double_array2 (value, root, domain, error)
  real(kind=default), dimension(:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  real(kind=default), dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_double_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_double_array2
```

357b   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁357a 357c▷

```
subroutine mpi90_broadcast_logical_array2 (value, root, domain, error)
  logical, dimension(:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  logical, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_logical_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_logical_array2
```

357c   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁357b 357d▷

```
subroutine mpi90_broadcast_integer_array3 (value, root, domain, error)
  integer, dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_integer_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_integer_array3
```

357d   ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁357c 358▷

```
subroutine mpi90_broadcast_double_array3 (value, root, domain, error)
  real(kind=default), dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  real(kind=default), dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_double_array (buffer, root, domain, error)
```

```
      value = reshape (buffer, shape(value))
    end subroutine mpi90_broadcast_double_array3
```

358 ⟨*Implementation of* `mpi90` *procedures* 346a⟩+≡   (345a) ◁357d
```
    subroutine mpi90_broadcast_logical_array3 (value, root, domain, error)
      logical, dimension(:,:,:), intent(inout) :: value
      integer, intent(in) :: root
      integer, intent(in), optional :: domain
      integer, intent(out), optional :: error
      logical, dimension(size(value)) :: buffer
      buffer = reshape (value, shape(buffer))
      call mpi90_broadcast_logical_array (buffer, root, domain, error)
      value = reshape (buffer, shape(value))
    end subroutine mpi90_broadcast_logical_array3
```

—M—
IDEAS

M.1   Toolbox for Interactive Optimization

Idea: Provide a OpenGL interface to visualize the grid optimization.

Motivation: Would help multi channel developers.

Implementation: Coding is straightforward, but interface design is hard.

M.2   Partially Non-Factorized Importance Sampling

Idea: Allow non-factorized grid optimization in two- or three-dimensional subspaces.

Motivation: Handle nastiest subspaces. Non-factorized approaches are impossible in higher than three dimensions (and probably only realistic in two dimensions), but there are cases that are best handled by including non-factorized optimization in two dimensions.

Implementation: The problem is that the present `vamp_sample_grid0` can't accomodate this, because other auxiliary information has to be collected, but a generalization is straightforward. Work has to start from an extended `divisions` module.

M.3   Correlated Importance Sampling (?)

Idea: Is it possible to include *some* correlations in a mainly factorized context?

Motivation: Would be nice . . .

Implementation: First, I have to think about the maths . . .

M.4   Align Coordinate System (i.e. the grid) with Singularities (or the hot region)

Idea: Solve `vegas`' nastiest problem by finding the direction(s) along which singularities are aligned.

Motivation: Automatically choose proper coordinate system in generator generators and separate wild and smooth directions.

Implementation: Diagonalize the covariance matrix $\text{cov}(x_i x_j)$ to find better axes. Caveats:

- damp rotations (rotate only if eigenvalues are spread out sufficiently).

- be careful about blow up of the integration volume, which is $V' = V d^{d/2}$ in the worst case for hypercubes and can be even worse for stretched cubes. (An adaptive grid can help, since we will have more smooth directions!)

Maybe try non-linear transformations as well.

M.5   Automagic Multi Channel

Idea: Find and extract one singularity after the other.

Motivation: Obvious.

Implementation: Either use multiple of `vegas`' $p(x)$ for importance sampling. Or find hot region(s) and split the integration region (á la signal/background).

—N—
CROSS REFERENCES

N.1   Identifiers

abs_evec: <u>128b</u>, <u>128c</u>, 129a, 129d, 130c, 131a

accuracy: <u>94d</u>, 97a, 104, 120b, 140c, 141, 142c, 170, 176, 180a

adaptive_division: 57a, <u>57f</u>

average: 109, 110c, 134c, 292b, <u>292c</u>, 293a, 293d, 293e

avg_chi2: <u>94d</u>, 95, <u>96c</u>, 104, 106c, 108a, 109, 110c, 120b, 124b, 125d, 140c, 141, 142c, 162a, 163, 166b, 170, 176, <u>179f</u>

boost_many_momentum: 325b, 325c, <u>327b</u>

boost_many_velocity: 325b, 325c, <u>326b</u>, 327b

boost_momentum: 228f, 325b, <u>325c</u>, 329c, 329d, 335

boost_one_momentum: 325b, 325c, <u>327a</u>

boost_one_velocity: 325b, 325c, <u>326a</u>, 326b

boost_velocity: 325b, <u>325c</u>, 327a

buffer_end: 261e, 261g, 262d, 263a, 264h, 266d, 266e, 270d, 271b, 272b, 272d, 275a, 275d, 275e, 276a, <u>276b</u>, 276c, 277c, 277d, 278a, 278b, 278c, 278d, 279a, 279b, 279c, 279d, 281i, 282b

BUFFER_SIZE: 59b, <u>60a</u>, 109, <u>110a</u>, 110b, 110c, 266d

calls: 24d, 76b, <u>84a</u>, 84b, 89a, 99b, 101b, 106c, 107d, 107e, 108a, 109, 110c, 125d, 136a, 140c, 141, 142c, 144d, 146b, 151c, 153b, 158b, 160b, 162a, 163, 164, 166b, 239, 242a, 242b, 243, 244

calls_per_cell: 76b, <u>84a</u>, 84b, 88b, 90a, 98a, 99b, 99c, 144d, 146b, 151c, 153b, 158b, 160b, 164

cartesian_to_spherical: 339c, <u>341a</u>

cartesian_to_spherical_2: 339c, <u>339d</u>, 341a, 341b

cartesian_to_spherical_cos: 195a, 342c, <u>343</u>

cartesian_to_spherical_cos_2: 197b, 342c, <u>342d</u>, 343, 344a

cartesian_to_spherical_cos_j: 195b, 342c, <u>344a</u>

cartesian_to_spherical_j: 339c, <u>341b</u>

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N.2   Refinements

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Acknowledgements

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