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

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Abstract

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

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Contents

1 Introduction 1

2 Algorithms 3
- *2.1 Importance Sampling* 4
- *2.2 Stratified Sampling* 5
- *2.3 Vegas* 6
  - *2.3.1 Vegas' Inflexibility* 6
  - *2.3.2 Vegas' Dark Side* 7
- *2.4 Multi Channel Sampling* 7
- *2.5 Revolving* 8
- *2.6 Parallelization* 8
  - *2.6.1 Multilinear Structure of the Sampling Algorithm* 8
  - *2.6.2 State and Message Passing* 13
  - *2.6.3 Random Numbers* 13
  - *2.6.4 Practice* 14

3 Design Trade Offs 19
- *3.1 Programming Language* 20

4 Usage 21
- *4.1 Basic Usage* 21
  - *4.1.1 Basic Example* 22
- *4.2 Advanced Usage* 24
  - *4.2.1 Types* 25
  - *4.2.2 Shared Arguments* 25
  - *4.2.3 Single Channel Procedures* 27
  - *4.2.4 Inout/Output and Marshling* 28
  - *4.2.5 Multi Channel Procedures* 31
  - *4.2.6 Event Generation* 34
  - *4.2.7 Parallelization* 34
  - *4.2.8 Diagnostics* 35

4.2.9 *Other Procedures* 36
4.2.10 *(Currently) Undocumented Procedures* 36

5 Implementation 37
5.1 *The Abstract Datatype `division`* 37
5.1.1 *Creation, Manipulation & Injection* 38
5.1.2 *Grid Refinement* 44
5.1.3 *Probability Density* 48
5.1.4 *Quadrupole* 49
5.1.5 *Forking and Joining* 49
5.1.6 *Inquiry* 57
5.1.7 *Diagnostics* 58
5.1.8 *I/O* 61
5.1.9 *Marshaling* 66
5.1.10 *Boring Copying and Deleting of Objects* 69
5.2 *The Abstract Datatype `vamp_grid`* 70
5.2.1 *Initialization* 77
5.2.2 *Sampling* 85
5.2.3 *Forking and Joining* 95
5.2.4 *Parallel Execution* 102
5.2.5 *Diagnostics* 105
5.2.6 *Multi Channel* 111
5.2.7 *Mapping* 125
5.2.8 *Event Generation* 133
5.2.9 *Convenience Routines* 138
5.2.10 *I/O* 142
5.2.11 *Marshaling* 156
5.2.12 *Boring Copying and Deleting of Objects* 162
5.3 *Interface to MPI* 165
5.3.1 *Parallel Execution* 166
5.3.2 *Event Generation* 180
5.3.3 *I/O* 182
5.3.4 *Communicating Grids* 184

6 Self Test 190
6.1 *No Mapping Mode* 190
6.1.1 *Serial Test* 190
6.1.2 *Parallel Test* 200
6.1.3 *Output* 202
6.2 *Mapped Mode* 202
6.2.1 *Serial Test* 202

6.2.2 *Parallel Test* . . . 218
6.2.3 *Output* . . . 219

7 APPLICATION 220
7.1 *Cross section* . . . 220

A CONSTANTS 243
A.1 *Kinds* . . . 243
A.2 *Mathematical and Physical Constants* . . . 243

B ERRORS AND EXCEPTIONS 245

C THE ART OF RANDOM NUMBERS 249
C.1 *Application Program Interface* . . . 249
C.2 *Low Level Routines* . . . 252
C.2.1 *Generation of 30-bit Random Numbers* . . . 252
C.2.2 *Initialization of 30-bit Random Numbers* . . . 253
C.2.3 *Generation of 52-bit Random Numbers* . . . 257
C.2.4 *Initialization of 52-bit Random Numbers* . . . 258
C.3 *The State* . . . 260
C.3.1 *Creation* . . . 261
C.3.2 *Destruction* . . . 262
C.3.3 *Copying* . . . 263
C.3.4 *Flushing* . . . 264
C.3.5 *Input and Output* . . . 264
C.3.6 *Marshaling and Unmarshaling* . . . 269
C.4 *High Level Routines* . . . 272
C.4.1 *Single Random Numbers* . . . 274
C.4.2 *Arrays of Random Numbers* . . . 275
C.4.3 *Procedures With Explicit `tao_random_state`* . . . 277
C.4.4 *Static Procedures* . . . 278
C.4.5 *Generic Procedures* . . . 279
C.4.6 *Luxury* . . . 280
C.5 *Testing* . . . 282
C.5.1 *30-bit* . . . 282
C.5.2 *52-bit* . . . 284
C.5.3 *Test Program* . . . 285

D SPECIAL FUNCTIONS 286
D.1 *Test* . . . 288

E STATISTICS 291

F Histogramming 294

G Miscellaneous Utilities 304
G.1 Memory Management . . . 304
G.2 Sorting . . . 307
G.3 Mathematics . . . 310
G.4 I/O . . . 312

H Linear Algebra 313
H.1 LU Decomposition . . . 313
H.2 Determinant . . . 316
H.3 Diagonalization . . . 316
H.4 Test . . . 321

I Products 323

J Kinematics 324
J.1 Lorentz Transformations . . . 324
J.2 Massive Phase Space . . . 326
J.3 Massive 3-Particle Phase Space Revisited . . . 329
J.4 Massless n-Particle Phase Space: RAMBO . . . 332
J.5 Tests . . . 333

K Coordinates 336
K.1 Angular Spherical Coordinates . . . 336
K.2 Trigonometric Spherical Coordinates . . . 339
K.3 Surface of a Sphere . . . 342

L Idiomatic Fortran90 Interface for MPI 343
L.1 Basics . . . 343
L.2 Point to Point . . . 346
L.3 Collective Communication . . . 352

M Poor Man's Elemental Procedures 357
M.1 m4 Macros . . . 357
M.2 Miscellaneous Utilities . . . 358
M.3 Errors and Exceptions . . . 360
M.4 The Abstract Datatype division . . . 360
M.5 The Abstract Datatype vamp_grid . . . 368

N Ideas 373
N.1 Toolbox for Interactive Optimization 373
N.2 Partially Non-Factorized Importance Sampling 373
N.3 Correlated Importance Sampling (?) 373
N.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region) 374
N.5 Automagic Multi Channel 374

O Cross References 375
O.1 Identifiers 375
O.2 Refinements 395

Program Summary:

- **Title of program:** VAMP, Version 1.0 (October 1999)
- **Program obtainable** by anonymous `ftp` from the host `crunch.ikp.physik.th-darmstadt.de` in the directory `pub/ohl/vamp`.
- **Licensing provisions:** Free software under the GNU General Public License.
- **Programming language used:** Fortran95 [8] (Fortran90 [7] and F [13] versions available as well)
- **Number of program lines in distributed program, including test data, etc.:** $\approx$ 4300 (excluding comments)
- **Computer/Operating System:** Any with a Fortran95 (or Fortran90 or F) programming environment.
- **Memory required to execute with typical data:** Negligible on the scale of typical applications calling the library.
- **Typical running time:** A small fraction (typically a few percent) of the running time of applications calling the library.
- **Purpose of program:**
- **Nature of physical problem:**
- **Method of solution:**
- **Keywords:** adaptive integration, event generation, parallel processing

—1—
Introduction

We present a reimplementation of the classic Vegas [1, 2] algorithm for adaptive multi-dimensional integration in Fortran95 [8, 12][1] 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 [16, 17, 18], which is almost identical to [2].

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[1]Fully functional versions conforming to preceeding Fortran standard [7], High Performance Fortran (HPF) [9, 10, 14], and to the Fortran90 subset F [13] are available as well. A translation to the obsolete FORTRAN77 standard [6] is possible in principle, but extremely tedious and error prone if the full functionality shall be preserved.

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—2—
Algorithms

The notation has to be synchronized with [3]!

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

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

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

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

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

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, 19]. The most popular technique for this will be discussed below in section 2.3.

2.2 *Stratified Sampling*

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

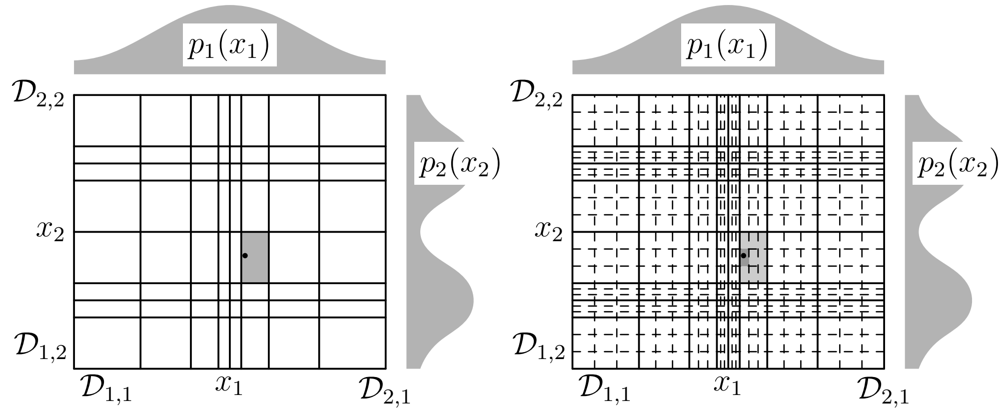


Figure 2.1: `vegas` grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.

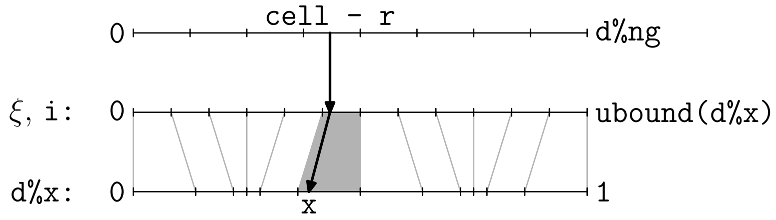


Figure 2.2: One-dimensional illustration of the `vegas` grid structure for pseudo stratified sampling, which is used in high dimensions.

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.

One small step along this line is implemented in Version 5.0 of the package BASES/SPRING [19], where one set of "wild" variables is separated from "smooth" variables [20].

The present 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

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

where we have used the damped standard deviation

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

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 [21].

2.6.1 Multilinear Structure of the Sampling Algorithm

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

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

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

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

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

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

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

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

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

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:

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

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.

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

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.

[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 [21], 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 [11]. More general paradigms can not be supported since the separation of the state for the processors is not explicit (it is implicit in the separated address space of the PVM or MPI processes).

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

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

and decompositions of the D^j induce decompositions of G

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

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)

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

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

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

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

Now it remains to find a decomposition

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

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

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

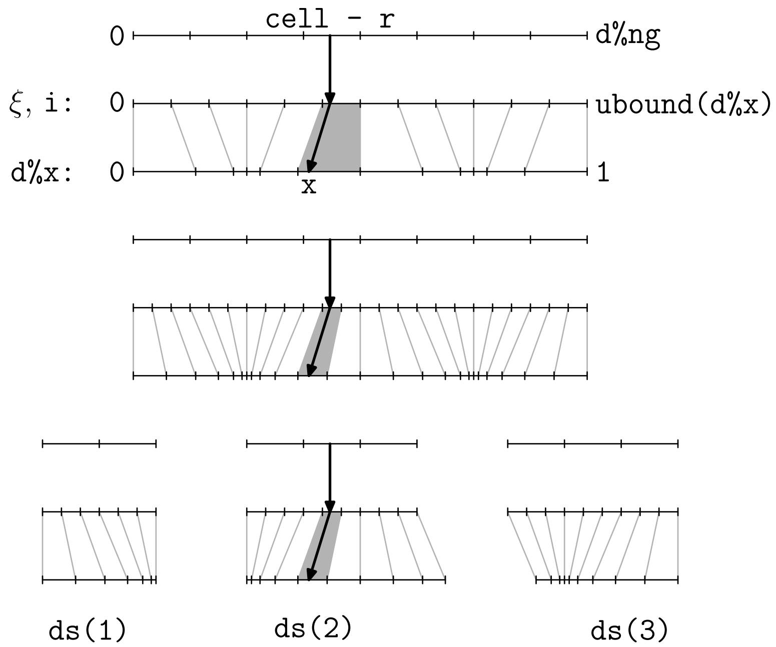


Figure 2.3: Forking one dimension `d` of a grid into three parts `ds(1)`, `ds(2)`, and `ds(3)`. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 2.2).

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

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

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

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

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

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

2.6.4 Practice

In this section we show three implementations of S_n: one serial, and two parallel, based on HPF [9, 10, 14] and MPI [11], respectively. From these examples, it should be obvious how to adapt VAMP to other parallel computing paradigms.

Serial

Here is a bare bones 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 [15] is most convenient and is included with VAMP (see the example on page 16). Before each S_0, the procedure `vamp_distribute_work` determines a good decomposition of the grid `d` into `size(rng)` pieces. This decomposition is encoded in the array `d` where `d(1,:)` holds the dimensions along which to split the grid and `d(2,:)` holds the 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 ⟨*Parallel implementation of* $S_n = S_0(rS_0)^n$ *(HPF)* 15⟩≡

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

```
      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 [15] and will fail with other approaches.

16 ⟨*Parallel usage of* $S_n = S_0(rS_0)^n$ *(HPF)* 16⟩≡

```
type(tao_random_state), dimension(:), allocatable :: rngs
!hpf$ processors p(number_of_processors())
!hpf$ distribute gs(cyclic(1)) onto p
integer :: i, seed
! ...
allocate (rngs(number_of_processors()))
seed = 42 ! can be read from a file, of course ...
!hpf$ independent
do i = 1, size (rngs)
   call tao_random_create (rngs(i), seed + i)
end do
! ...
call vamp_sample_grid_hpf (rngs, g, 6, func)
! ...
```

MPI

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

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

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

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

3.1 Programming Language

We have chosen to implement VAMP in Fortran90/95, which some might consider a questionable choice today. Nevertheless, we are convinced that Fortran90/95 (with all 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, 8] 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

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

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

`subroutine vamp_delete_grid` (`g` [, `exc`])

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

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

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

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

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

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

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

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

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

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

22 ⟨*Interface declaration for* `func` 22⟩≡

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

4.1.1 Basic Example

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

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

23a ⟨basic.f90 23a⟩≡

```
module basic_fct
  use kinds
  implicit none
  private
  public :: fct
contains
  function fct (x, weights, channel) result (f_x)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    real(kind=default) :: f_x
    f_x = exp (-0.5 * sum (x*x))
  end function fct
end module basic_fct
```

In the main program, we need to import five modules. The customary module **kinds** defines **double** as the kind for double precision floating point numbers. The model **exceptions** provides simple error handling support (parallelizable routines are not allowed to issue error messages 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⟩+≡

```
program basic
  use kinds
  use exceptions
  use tao_random_numbers
  use vamp
  use basic_fct
  implicit none
```

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

23c ⟨basic.f90 23a⟩+≡

```
  type(exception) :: exc
  type(tao_random_state) :: rng
  type(vamp_grid) :: grid
  real(kind=default), dimension(2,7) :: domain
  real(kind=default) :: integral, error, chi2
  domain(1,:) = -1.0
  domain(2,:) =  1.0
```

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

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

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

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

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

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

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

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

4.2 Advanced Usage

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

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

4.2.1 Types

`type(vamp_grid)`

`type(vamp_grids)`

`type(vamp_history)`

`type(exception)`

(from module `exceptions`)

4.2.2 Shared Arguments

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

`real, intent(in) :: accuracy`

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

```
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!

`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`.

`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 [11]

29 ⟨*MPI communication example* 29⟩≡

```
call vamp_marshal_grid_size (g, isize, dsize)
```

```
allocate (ibuf(isize), dbuf(dsize))
call mpi_comm_rank (MPI_COMM_WORLD, proc_id, errno)
select case (proc_id)
   case (0)
      call vamp_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

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

31a ⟨*Interface declaration for* `phi` 31a⟩≡

```
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⟩≡

```
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⟩≡

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

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

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

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

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

`function vamp_multi_channel0` (`func`, `phi`, `jacobian`, `x`, `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

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

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

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

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

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

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

4.2.8 Diagnostics

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.2.9 Other Procedures

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

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

`function vamp_get_covariance` (g, [, ...])

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

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

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

`function vamp_get_variance` (g, [, ...])

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

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

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

4.2.10 (Currently) Undocumented Procedures

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

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

—5— Implementation

5.1 The Abstract Datatype `division`

37a ⟨divisions.f90 37a⟩≡

```
! divisions.f90 --
⟨Copyleft notice 1⟩
module divisions
  use kinds
  use exceptions
  use vamp_stat
  use utils
  use iso_fortran_env
  implicit none
  private
  ⟨Declaration of divisions procedures 38a⟩
  ⟨Interfaces of divisions procedures 61b⟩
  ⟨Variables in divisions 46a⟩
  ⟨Declaration of divisions types 37b⟩
  ⟨Constants in divisions 65a⟩
  character(len=*), public, parameter :: DIVISIONS_RCS_ID = &
       "$Id: divisions.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of divisions procedures 38b⟩
end module divisions
```

`vamp_apply_equivalences` from `vamp` accesses `%variance` …

37b ⟨Declaration of divisions types 37b⟩≡

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

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

5.1.1 Creation, Manipulation & Injection

38a ⟨*Declaration of* `divisions` *procedures* 38a⟩≡

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

38b ⟨*Implementation of* `divisions` *procedures* 38b⟩≡

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

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

39a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

39b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

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

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

39c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

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

40a ⟨*Set* `m` *to* $(1, 1, \ldots)$ *or to rebinning weights from* `d%variance` 40a⟩≡

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

40b ⟨*Resize arrays, iff necessary* 40b⟩≡

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

Genuinely stratified sampling will superimpose an equidistant grid on the adaptive grid, as shown in figure 5.2. Obviously, this is only possible when the number of cells of the stratification grid is large enough, specifically when $n_g \geq n_{\text{div}}^{\text{min}} = n_{\text{div}}^{\text{max}}/2 = 25$). 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

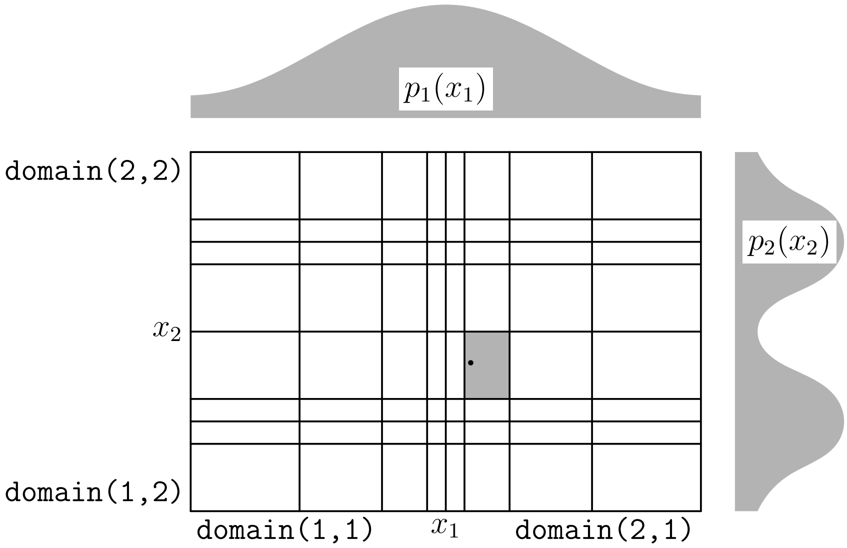


Figure 5.1: `vegas` grid structure for non-stratified sampling. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.

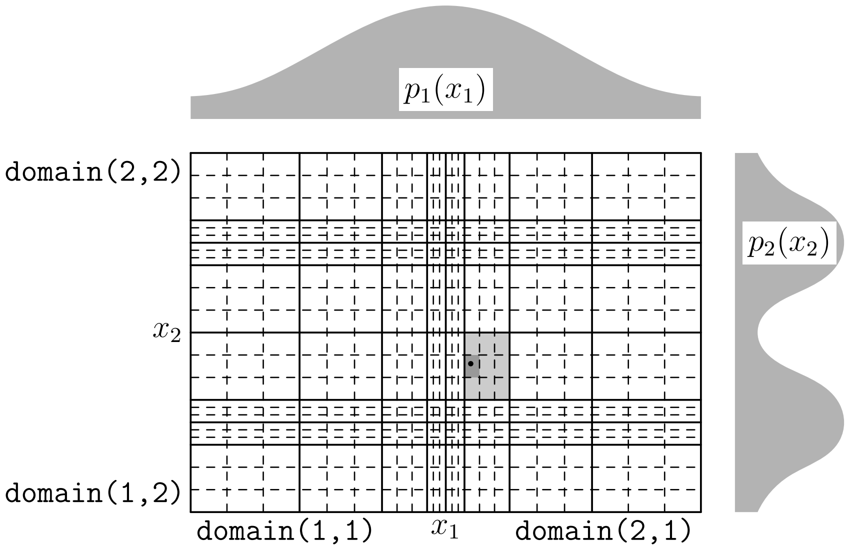


Figure 5.2: `vegas` grid structure for genuinely stratified sampling, which is used in low dimensions. N.B.: the grid and the weight functions $p_{1,2}$ are only in qualitative agreement.

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⟩≡

```
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
```

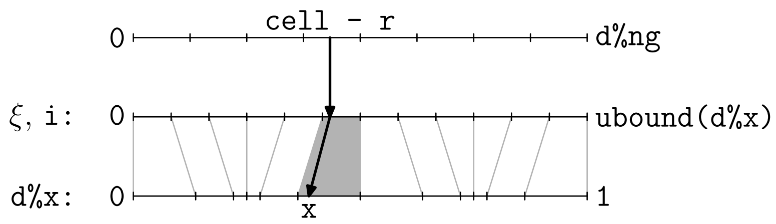


Figure 5.3: One-dimensional illustration of the `vegas` grid structure for pseudo stratified sampling, which is used in high dimensions.

```
      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.

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

43a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

```
  public :: inject_division, inject_division_short
```

43b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
  elemental subroutine inject_division (d, r, cell, x, x_mid, idx, wgt)
    type(division_t), intent(in) :: d
    real(kind=default), intent(in) :: r
    integer, intent(in) :: cell
    real(kind=default), intent(out) :: x, x_mid
    integer, intent(out) :: idx
    real(kind=default), intent(out) :: wgt
    real(kind=default) :: delta_x, xi
    integer :: i
    xi = (cell - r) * d%dxg + 1.0
```

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

44a ⟨*Set* i, delta_x, x, *and* wgt *from* xi 44a⟩≡

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

44b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

5.1.2 *Grid Refinement*

44c ⟨*Declaration of* divisions *procedures* 38a⟩+≡

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

44d ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

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

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

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

45d ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
public :: refine_division
```

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

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

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

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

46a ⟨*Variables in* `divisions` 46a⟩≡

```
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⟩+≡

```
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.

```
      m = 1.0_default
   else
      smooth_d = smooth_d / sum (smooth_d)
      where (smooth_d < tiny (1.0_default))
         smooth_d = tiny (1.0_default)
      end where
      where (smooth_d /= 1._default)
         m = ((smooth_d - 1.0) / (log (smooth_d)))**ALPHA
      elsewhere
         m = 1.0_default
      endwhere
   end if
end function rebinning_weights
```

47a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

```
private :: rebinning_weights
```

The `NaN` test is probably not portable:

47b ⟨*Bail out if* `any (d == NaN)` 47b⟩≡

```
if (any (d /= d)) then
   m = 1.0
   return
end if
```

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

47c ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
pure function rebin (m, x, num_div) result (x_new)
  real(kind=default), dimension(:), intent(in) :: m
  real(kind=default), dimension(0:), intent(in) :: x
  integer, intent(in) :: num_div
  real(kind=default), dimension(0:num_div) :: x_new
  integer :: i, k
  real(kind=default) :: step, delta
  step = sum (m) / num_div
  k = 0
  delta = 0.0
  x_new(0) = x(0)
  do i = 1, num_div - 1
     ⟨Increment k until ∑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
```

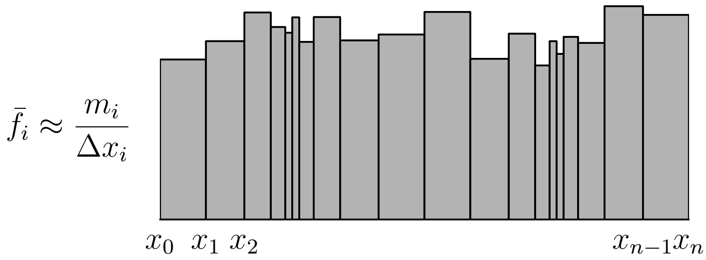


Figure 5.4: Typical weights used in the rebinning algorithm.

48a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡
```
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⟩≡
```
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⟩≡
```
x_new(i) = x(k) - (x(k) - x(k-1)) * delta / m(k)
```

5.1.3 Probability Density

48d ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡
```
public :: probability
```
$$\xi = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \in [0, 1] \tag{5.6}$$
and
$$\int_{x_{\min}}^{x_{\max}} \mathrm{d}x\, p(x) = 1 \tag{5.7}$$

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

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

5.1.4 Quadrupole

49a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

```
  public :: quadrupole_division
```

49b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
  elemental function quadrupole_division (d) result (q)
    type(division_t), intent(in) :: d
    real(kind=default) :: q
    !!!   q = value_spread_percent (rebinning_weights (d%variance))
    q = standard_deviation_percent (rebinning_weights (d%variance))
  end function quadrupole_division
```

5.1.5 Forking and Joining

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

49c ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

```
  public :: fork_division, join_division, sum_division
```

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

50a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

50b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

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

Importance Sampling

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

51a ⟨*Fork an importance sampling division* 51a⟩≡

```
if (d%stratified) then
   call raise_exception (exc, EXC_FATAL, FN, &
                              "ng == 1 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⟩≡

```
call sum_division (d, ds)
```

Note, however, that this is only legitimate as long as `d%ng == 1` implies `d%stratified == .false.`, because otherwise the sampling code would be incorrect (cf. `var_f` on page 88).

Stratified Sampling

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

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

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

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

```
⟨Setup to fork a pure stratified sampling division 52a⟩
do i = 1, num_forks
   call copy_array_pointer (ds(i)%x, d%x(n0(i):n1(i)), lb = 0)
   call copy_array_pointer (ds(i)%integral, d%integral(n0(i)+1:n1(i)))
   call copy_array_pointer (ds(i)%variance, d%variance(n0(i)+1:n1(i)))
!  call copy_array_pointer (ds(i)%efficiency, d%efficiency(n0(i)+1:n1(i)))
   ds(i)%x = (ds(i)%x - ds(i)%x(0)) / (d%x(n1(i)) - d%x(n0(i)))
end do
ds%x_min = d%x_min + d%dx * d%x(n0)
ds%x_max = d%x_min + d%dx * d%x(n1)
ds%dx = ds%x_max - ds%x_min
ds%x_min_true = d%x_min_true
ds%x_max_true = d%x_max_true
ds%stratified = d%stratified
ds%ng = (d%ng * (n1 - n0)) / num_div
num_calls = sum_calls ! this is a misnomer, it remains “calls per cell” here
ds%dxg = real (n1 - n0, kind=default) / ds%ng
```

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

52c ⟨*Join pure stratified sampling divisions* 52c⟩≡

```
⟨Setup to fork a pure stratified sampling division 52a⟩
do i = 1, num_forks
   d%integral(n0(i)+1:n1(i)) = ds(i)%integral
   d%variance(n0(i)+1:n1(i)) = ds(i)%variance
!  d%efficiency(n0(i)+1:n1(i)) = ds(i)%efficiency
end do
```

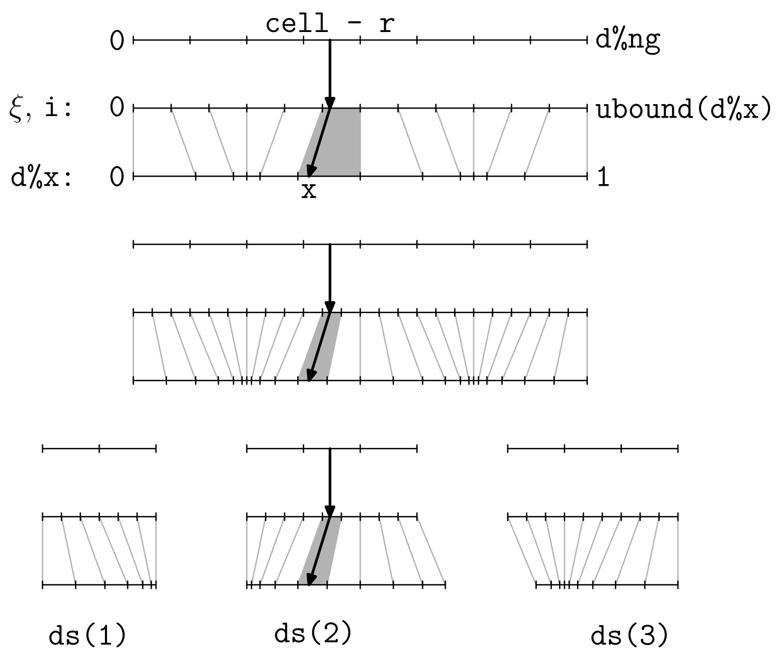


Figure 5.5: Forking one dimension `d` of a grid into three parts `ds(1)`, `ds(2)`, and `ds(3)`. The picture illustrates the most complex case of pseudo stratified sampling (cf. fig. 5.3).

Pseudo Stratified Sampling

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

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

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*⟩≡

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

54a ⟨*Fork a pseudo stratified sampling division* 54a⟩≡

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

54b ⟨*Join pseudo stratified sampling divisions* 54b⟩≡

```
⟨Setup to fork a pseudo stratified sampling division 53⟩
allocate (d_x(0:nx), d_integral(nx), d_variance(nx))
! allocate (d_efficiency(nx))
do i = 1, num_forks
   d_integral(n0(i)+1:n1(i)) = ds(i)%integral
   d_variance(n0(i)+1:n1(i)) = ds(i)%variance
!  d_efficiency(n0(i)+1:n1(i)) = ds(i)%efficiency
end do
call collect (d%integral, d_integral)
call collect (d%variance, d_variance)
! call collect (d%efficiency, d_efficiency)
deallocate (d_x, d_integral, d_variance)
! deallocate (d_efficiency)
```

54c ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
private :: subdivide
private :: distribute
```

```
  private :: collect
```

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

```
  pure subroutine subdivide (x, x0)
    real(kind=default), dimension(0:), intent(inout) :: x
    real(kind=default), dimension(0:), intent(in) :: x0
    integer :: i, n, n0
    n0 = ubound (x0, dim=1)
    n = ubound (x, dim=1) / n0
    x(0) = x0(0)
    do i = 1, n
       x(i::n) = x0(0:n0-1) * real (n - i) / n + x0(1:n0) * real (i) / n
    end do
  end subroutine subdivide
```

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

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

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

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

Trivia

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

```
  pure subroutine sum_division (d, ds)
    type(division_t), intent(inout) :: d
    type(division_t), dimension(:), intent(in) :: ds
    integer :: i
```

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

56a ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  public :: debug_division
  public :: dump_division
```

56b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

56c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

```
end subroutine dump_division
```

5.1.6 Inquiry

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

57a ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

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

57b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

57c ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
elemental function stratified_division (d) result (yorn)
  type(division_t), intent(in) :: d
  logical :: yorn
  yorn = d%stratified
end function stratified_division
```

57d ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
elemental function volume_division (d) result (vol)
  type(division_t), intent(in) :: d
  real(kind=default) :: vol
  vol = d%dx
end function volume_division
```

57e ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
elemental function rigid_division (d) result (n)
  type(division_t), intent(in) :: d
  integer :: n
  n = d%ng
end function rigid_division
```

57f ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
elemental function adaptive_division (d) result (n)
  type(division_t), intent(in) :: d
  integer :: n
  n = ubound (d%x, dim=1)
end function adaptive_division
```

5.1.7 Diagnostics

58a ⟨*Declaration of* divisions *types* 37b⟩+≡
```
type, public :: div_history
   private
   logical :: stratified
   integer :: ng, num_div
   real(kind=default) :: x_min, x_max, x_min_true, x_max_true
   real(kind=default) :: &
        spread_f_p, stddev_f_p, spread_p, stddev_p, spread_m, stddev_m
end type div_history
```

58b ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
public :: copy_history, summarize_division
```

58c ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
elemental function summarize_division (d) result (s)
  type(division_t), intent(in) :: d
  type(div_history) :: s
  real(kind=default), dimension(:), allocatable :: p, m
  allocate (p(ubound(d%x,dim=1)), m(ubound(d%x,dim=1)))
  p = probabilities (d%x)
  m = rebinning_weights (d%variance)
  s%ng = d%ng
  s%num_div = ubound (d%x, dim=1)
  s%stratified = d%stratified
  s%x_min = d%x_min
  s%x_max = d%x_max
  s%x_min_true = d%x_min_true
  s%x_max_true = d%x_max_true
  s%spread_f_p = value_spread_percent (d%integral)
  s%stddev_f_p = standard_deviation_percent (d%integral)
  s%spread_p = value_spread_percent (p)
  s%stddev_p = standard_deviation_percent (p)
  s%spread_m = value_spread_percent (m)
  s%stddev_m = standard_deviation_percent (m)
  deallocate (p, m)
end function summarize_division
```

58d ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
private :: probabilities
```

58e ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure function probabilities (x) result (p)
  real(kind=default), dimension(0:), intent(in) :: x
  real(kind=default), dimension(ubound(x,dim=1)) :: p
```

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

59a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  subroutine print_history (h, tag)
    type(div_history), dimension(:), intent(in) :: h
    character(len=*), intent(in), optional :: tag
    call write_history (output_unit, h, tag)
    flush (output_unit)
  end subroutine print_history
```

59b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  subroutine write_history (u, h, tag)
    integer, intent(in) :: u
    type(div_history), dimension(:), intent(in) :: h
    character(len=*), intent(in), optional :: tag
    character(len=BUFFER_SIZE) :: pfx
    character(len=1) :: s
    integer :: i
    if (present (tag)) then
       pfx = tag
    else
       pfx = "[vamp]"
    end if
    if ((minval (h%x_min) == maxval (h%x_min)) &
         .and. (minval (h%x_max) == maxval (h%x_max))) then
       write (u, "(1X,A11,1X,2X,1X,2(E10.3,A4,E10.3,A7))") pfx, &
            h(1)%x_min, " <= ", h(1)%x_min_true, &
            " < x < ", h(1)%x_max_true, " <= ", h(1)%x_max
    else
       do i = 1, size (h)
          write (u, "(1X,A11,1X,I2,1X,2(E10.3,A4,E10.3,A7))") pfx, &
               i, h(i)%x_min, " <= ", h(i)%x_min_true, &
               " < x < ", h(i)%x_max_true, " <= ", h(i)%x_max
       end do
    end if
    write (u, "(1X,A11,1X,A2,2(1X,A3),A1,6(1X,A8))") pfx, &
         "it", "nd", "ng", "", &
         "spr(f/p)", "dev(f/p)", "spr(m)", "dev(m)", "spr(p)", "dev(p)"
    iterations: do i = 1, size (h)
       if (h(i)%stratified) then
          s = "*"
```

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

60a ⟨*Variables in* `divisions` 46a⟩+≡

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

60b ⟨*Declaration of* `divisions` *procedures* 38a⟩+≡

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

60c ⟨*Declaration of* `divisions` *procedures (removed from WHIZARD)* 60c⟩≡

```
 public :: division_x, division_integral
 public :: division_variance, division_efficiency
```

60d ⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩+≡

```
 pure subroutine division_x (x, d)
   real(kind=default), dimension(:), pointer :: x
   type(division_t), intent(in) :: d
   call copy_array_pointer (x, d%x, 0)
 end subroutine division_x
```

60e ⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩+≡

```
 pure subroutine division_integral (integral, d)
   real(kind=default), dimension(:), pointer :: integral
   type(division_t), intent(in) :: d
   call copy_array_pointer (integral, d%integral)
 end subroutine division_integral
```

60f ⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩+≡

```
 pure subroutine division_variance (variance, d)
   real(kind=default), dimension(:), pointer :: variance
   type(division_t), intent(in) :: d
   call copy_array_pointer (variance, d%variance, 0)
 end subroutine division_variance
```

60g ⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩+≡

```
 pure subroutine division_efficiency (eff, d)
   real(kind=default), dimension(:), pointer :: eff
   type(division_t), intent(in) :: d
```

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

5.1.8 I/O

61a ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
  public :: write_division
  private :: write_division_unit, write_division_name
  public :: read_division
  private :: read_division_unit, read_division_name
  public :: write_division_raw
  private :: write_division_raw_unit, write_division_raw_name
  public :: read_division_raw
  private :: read_division_raw_unit, read_division_raw_name
```

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

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

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

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

62a ⟨*Variables in* divisions 46a⟩+≡

```
  character(len=*), parameter, private :: &
       descr_fmt =         "(1x,a)", &
       integer_fmt =       "(1x,a15,1x,i15)", &
       logical_fmt =       "(1x,a15,1x,l1)", &
       double_fmt =        "(1x,a15,1x,e30.22)", &
       double_array_fmt = "(1x,i15,1x,3(e30.22))"
```

62b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

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

What happened to `d%efficiency`?

63a ⟨*Insure that* `ubound (d%x, dim=1) == num_div` 63a⟩≡

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

63b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

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

64a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

64b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

65a ⟨*Constants in* divisions 65a⟩≡

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

65b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

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

66a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

66b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

5.1.9 Marshaling

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

66c ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  public :: marshal_division_size, marshal_division, unmarshal_division
```

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

```
  pure subroutine marshal_division (d, ibuf, dbuf)
    type(division_t), intent(in) :: d
```

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

67a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

67b ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

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

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

68a ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  public :: marshal_div_history_size, marshal_div_history, unmarshal_div_history
```

68b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

68c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine marshal_div_history_size (h, iwords, dwords)
    type(div_history), intent(in) :: h
    integer, intent(out) :: iwords, dwords
    iwords = 3
    dwords = 10
  end subroutine marshal_div_history_size
```

68d ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine unmarshal_div_history (h, ibuf, dbuf)
```

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

5.1.10 Boring Copying and Deleting of Objects

69 ⟨*Implementation of* divisions *procedures* 38b⟩+≡

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

```
  ! end if
    lhs%dx = rhs%dx
    lhs%dxg = rhs%dxg
    lhs%x_min = rhs%x_min
    lhs%x_max = rhs%x_max
    lhs%x_min_true = rhs%x_min_true
    lhs%x_max_true = rhs%x_max_true
    lhs%ng = rhs%ng
    lhs%stratified = rhs%stratified
  end subroutine copy_division
```

70a ⟨*Implementation of* `divisions` *procedures* 38b⟩+≡

```
  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⟩+≡

```
  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⟩≡

```
! 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⟩+≡
```
module vamp_grid_type
  use kinds
  use divisions
  private
  ⟨Declaration of vamp_grid_type types 76b⟩
end module vamp_grid_type
```

By WK for WHIZARD.

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

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

72a ⟨*Declaration of* vamp_equivalences *types* 71c⟩+≡

```
type, public :: vamp_equivalences_t
   type(vamp_equivalence_t), dimension(:), allocatable :: eq
   integer :: n_eq, n_ch
   integer, dimension(:), allocatable :: pointer
   logical, dimension(:), allocatable :: independent
   integer, dimension(:), allocatable :: equivalent_to_ch
   integer, dimension(:), allocatable :: multiplicity
   integer, dimension(:), allocatable :: symmetry
   logical, dimension(:,:), allocatable :: div_is_invariant
end type vamp_equivalences_t
```

72b ⟨*Constants in* vamp_equivalences 72b⟩≡

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

72c ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩≡

```
subroutine vamp_equivalence_init (eq, n_dim)
  type(vamp_equivalence_t), intent(inout) :: eq
  integer, intent(in) :: n_dim
  allocate (eq%permutation(n_dim), eq%mode(n_dim))
end subroutine vamp_equivalence_init
```

72d ⟨*Declaration of* vamp_equivalences *procedures* 72d⟩≡

```
public :: vamp_equivalences_init
```

72e ⟨*Implementation of* vamp_equivalences *procedures* 72c⟩+≡

```
subroutine vamp_equivalences_init (eq, n_eq, n_ch, n_dim)
  type(vamp_equivalences_t), intent(inout) :: eq
  integer, intent(in) :: n_eq, n_ch, n_dim
  integer :: i
  eq%n_eq = n_eq
  eq%n_ch = n_ch
  allocate (eq%eq(n_eq))
  allocate (eq%pointer(n_ch+1))
  do i=1, n_eq
     call vamp_equivalence_init (eq%eq(i), n_dim)
  end do
  allocate (eq%independent(n_ch), eq%equivalent_to_ch(n_ch))
  allocate (eq%multiplicity(n_ch), eq%symmetry(n_ch))
  allocate (eq%div_is_invariant(n_ch, n_dim))
  eq%independent = .true.
  eq%equivalent_to_ch = 0
  eq%multiplicity = 0
  eq%symmetry = 0
  eq%div_is_invariant = .false.
```

```
  end subroutine vamp_equivalences_init
```

73a ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalence_final (eq)
    type(vamp_equivalence_t), intent(inout) :: eq
    deallocate (eq%permutation, eq%mode)
  end subroutine vamp_equivalence_final
```

73b ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡

```
  public :: vamp_equivalences_final
```

73c ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalences_final (eq)
    type(vamp_equivalences_t), intent(inout) :: eq
  ! integer :: i
  ! do i=1, eq%n_eq
  !    call vamp_equivalence_final (eq%eq(i))
  ! end do
    if (allocated (eq%eq))  deallocate (eq%eq)
    if (allocated (eq%pointer))  deallocate (eq%pointer)
    if (allocated (eq%multiplicity))  deallocate (eq%multiplicity)
    if (allocated (eq%symmetry))  deallocate (eq%symmetry)
    if (allocated (eq%independent))  deallocate (eq%independent)
    if (allocated (eq%equivalent_to_ch))  deallocate (eq%equivalent_to_ch)
    if (allocated (eq%div_is_invariant))  deallocate (eq%div_is_invariant)
    eq%n_eq = 0
    eq%n_ch = 0
  end subroutine vamp_equivalences_final
```

73d ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalence_write (eq, unit)
    integer, intent(in), optional :: unit
    integer :: u
    type(vamp_equivalence_t), intent(in) :: eq
    u = 6;  if (present (unit))  u = unit
    write (u, "(1x,A,2(1x,I4))") "Equivalent channels:", eq%left, eq%right
    write (u, "(1x,A,25(1x,I2))") "  Permutation:", eq%permutation
    write (u, "(1x,A,25(1x,I2))") "  Mode:       ", eq%mode
  end subroutine vamp_equivalence_write
```

73e ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡

```
  public :: vamp_equivalences_write
```

73f ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalences_write (eq, unit)
    type(vamp_equivalences_t), intent(in) :: eq
    integer, intent(in), optional :: unit
```

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

74a ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡

```
  public :: vamp_equivalence_set
```

74b ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalence_set (eq, i, left, right, perm, mode)
    type(vamp_equivalences_t), intent(inout) :: eq
    integer, intent(in) :: i
    integer, intent(in) :: left, right
    integer, dimension(:), intent(in) :: perm, mode
    eq%eq(i)%left = left
    eq%eq(i)%right = right
    eq%eq(i)%permutation = perm
    eq%eq(i)%mode = mode
  end subroutine vamp_equivalence_set
```

74c ⟨*Declaration of* `vamp_equivalences` *procedures* 72d⟩+≡

```
  public :: vamp_equivalences_complete
```

74d ⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩+≡

```
  subroutine vamp_equivalences_complete (eq)
    type(vamp_equivalences_t), intent(inout) :: eq
    integer :: i, ch
    ch = 0
    do i=1, eq%n_eq
```

```
        if (ch /= eq%eq(i)%left) then
           ch = eq%eq(i)%left
           eq%pointer(ch) = i
        end if
     end do
     eq%pointer(ch+1) = eq%n_eq + 1
     do ch=1, eq%n_ch
        call set_multiplicities (eq%eq(eq%pointer(ch):eq%pointer(ch+1)-1))
     end do
  ! call write (6, eq)
  contains
     subroutine set_multiplicities (eq_ch)
       type(vamp_equivalence_t), dimension(:), intent(in) :: eq_ch
       integer :: i
       if (.not. all(eq_ch%left == ch) .or. eq_ch(1)%right > ch) then
          do i = 1, size (eq_ch)
             call vamp_equivalence_write (eq_ch(i))
          end do
          stop "VAMP: Equivalences: Something's wrong with equivalence ordering"
       end if
       eq%symmetry(ch) = count (eq_ch%right == ch)
       if (mod (size(eq_ch), eq%symmetry(ch)) /= 0) then
          do i = 1, size (eq_ch)
             call vamp_equivalence_write (eq_ch(i))
          end do
          stop "VAMP: Equivalences: Something's wrong with permutation count"
       end if
       eq%multiplicity(ch) = size (eq_ch) / eq%symmetry(ch)
       eq%independent(ch) = all (eq_ch%right >= ch)
       eq%equivalent_to_ch(ch) = eq_ch(1)%right
       eq%div_is_invariant(ch,:) = eq_ch(1)%mode == VEQ_INVARIANT
     end subroutine set_multiplicities
  end subroutine vamp_equivalences_complete
```

75 ⟨vamp.f90 70c⟩+≡

```
  module vamp_rest
     use kinds
     use utils
     use exceptions
     use divisions
     use tao_random_numbers
     use vamp_stat
     use linalg
     use iso_fortran_env
```

```
    use vamp_grid_type !NODEP!
    use vamp_equivalences !NODEP!
    implicit none
    private
    ⟨Declaration of vamp procedures 77a⟩
    ⟨Interfaces of vamp procedures 94c⟩
    ⟨Constants in vamp 151a⟩
    ⟨Declaration of vamp types 105a⟩
    ⟨Variables in vamp 78a⟩
    character(len=*), public, parameter :: VAMP_RCS_ID = &
         "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
  contains
    ⟨Implementation of vamp procedures 77c⟩
  end module vamp_rest
```

76a ⟨vamp.f90 70c⟩+≡

```
  module vamp
    use vamp_grid_type    !NODEP!
    use vamp_rest         !NODEP!
    use vamp_equivalences !NODEP!
    public
  end module vamp
```

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

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 $\{+1, -1\}$.

76b ⟨*Declaration of* `vamp_grid_type` *types* 76b⟩≡

```
  type, public :: vamp_grid
     ! private ! forced by use association in interface
     type(division_t), dimension(:), pointer :: div => null ()
     real(kind=default), dimension(:,:), pointer :: map => null ()
     real(kind=default), dimension(:), pointer :: mu_x => null ()
     real(kind=default), dimension(:), pointer :: sum_mu_x => null ()
     real(kind=default), dimension(:,:), pointer :: mu_xx => null ()
     real(kind=default), dimension(:,:), pointer :: sum_mu_xx => null ()
     real(kind=default), dimension(2) :: mu
     real(kind=default) :: sum_integral, sum_weights, sum_chi2
```

```
    real(kind=default) :: calls, dv2g, jacobi
    real(kind=default) :: f_min, f_max
    real(kind=default) :: mu_gi, sum_mu_gi
    integer, dimension(:), pointer :: num_div => null ()
    integer :: num_calls, calls_per_cell
    logical :: stratified = .true.
    logical :: all_stratified = .true.
    logical :: quadrupole = .false.
    logical :: independent
    integer :: equivalent_to_ch, multiplicity
 end type vamp_grid
```

77a ⟨*Declaration of* `vamp` *procedures* 77a⟩≡

```
 public :: vamp_copy_grid, vamp_delete_grid
```

5.2.1 Initialization

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

```
 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`.

77c ⟨*Implementation of* `vamp` *procedures* 77c⟩≡

```
 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.

78a ⟨*Variables in* `vamp` 78a⟩≡

```
  integer, private, parameter :: NUM_DIV_DEFAULT = 20
```

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

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

78b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
  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:

79a ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine map_domain (map, true_xmin, true_xmax, xmin, xmax)
  real(kind=default), dimension(:,:), intent(in) :: map
  real(kind=default), dimension(:), intent(in) :: true_xmin, true_xmax
  real(kind=default), dimension(:), intent(out) :: xmin, xmax
  real(kind=default), dimension(2**size(xmin),size(xmin)) :: corners
  integer, dimension(size(xmin)) :: zero_to_n
  integer :: j, ndim, perm
  ndim = size (xmin)
  zero_to_n = (/ (j, j=0,ndim-1) /)
  do perm = 1, 2**ndim
     corners (perm,:) = &
          merge (true_xmin, true_xmax, btest (perm-1, zero_to_n))
  end do
  corners = matmul (corners, map)
  xmin = minval (corners, dim=1)
  xmax = maxval (corners, dim=1)
end subroutine map_domain
```

79b ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
elemental subroutine vamp_create_empty_grid (g)
  type(vamp_grid), intent(inout) :: g
  nullify (g%div, g%num_div, g%map, g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
end subroutine vamp_create_empty_grid
```

79c ⟨*Declaration of* vamp *procedures* 77a⟩+≡
```
public :: vamp_discard_integral
```

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

79d ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine vamp_discard_integral &
     (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
    & independent, equivalent_to_ch, multiplicity)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole, covariance
  type(exception), intent(inout), optional :: exc
  logical, intent(in), optional :: independent
  integer, intent(in), optional :: equivalent_to_ch, multiplicity
  character(len=*), parameter :: FN = "vamp_discard_integral"
```

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

80a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
private :: set_grid_options
```

80b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

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

Setting Up the Initial Grid

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

81 ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
  pure subroutine vamp_reshape_grid_internal &
       (g, num_calls, num_div, &
        stratified, quadrupole, covariance, exc, use_variance, &
        independent, equivalent_to_ch, multiplicity)
    type(vamp_grid), intent(inout) :: g
    integer, intent(in), optional :: num_calls
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole, covariance
    type(exception), intent(inout), optional :: exc
    logical, intent(in), optional :: use_variance
    logical, intent(in), optional :: independent
    integer, intent(in), optional :: equivalent_to_ch, multiplicity
    integer :: ndim, num_cells
    integer, dimension(size(g%div)) :: ng
    character(len=*), parameter :: FN = "vamp_reshape_grid_internal"
    ndim = size (g%div)
    call set_grid_options &
         (g, num_calls, num_div, stratified, quadrupole, &
        & independent, equivalent_to_ch, multiplicity)
    ⟨Adjust grid and other state for new num_calls 83a⟩
    g%all_stratified = all (stratified_division (g%div))
    if (present (covariance)) then
       ndim = size (g%div)
```

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

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

82a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
 private :: vamp_reshape_grid_internal
 public :: vamp_reshape_grid
```

82b ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

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

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

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

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

83a ⟨*Adjust* grid *and other state for new* num_calls 83a⟩≡

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

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

and

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

83b ⟨*Adjust* grid *and other state for new* num_calls 83a⟩+≡

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

84a ⟨*Adjust* grid *and other state for new* num_calls 83a⟩+≡

```
g%f_min = 1.0
g%f_max = 0.0
```

84b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

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

84c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

84d ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

84e ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

84f ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
elemental function vamp_get_variance (g) result (v)
  type(vamp_grid), intent(in) :: g
  real(kind=default) :: v
  if (abs (g%sum_weights) <= tiny (v)) then
     if (g%sum_mu_gi == 0.0_default) then
        v = 0.0
     else
        v = huge (v)
     end if
  else
     v = g%sum_mu_gi / g%sum_weights
  end if
end function vamp_get_variance
```

85a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
elemental subroutine vamp_nullify_variance (g)
  type(vamp_grid), intent(inout) :: g
  g%sum_mu_gi = 0
end subroutine vamp_nullify_variance
```

5.2.2 Sampling

85b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
public :: vamp_sample_grid
public :: vamp_sample_grid0
public :: vamp_refine_grid
public :: vamp_refine_grids
```

Simple Non-Adaptive Sampling: S_0

85c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_sample_grid0 &
       (rng, g, func, prc_index, channel, weights, grids, exc, &
        negative_weights)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: prc_index
    integer, intent(in), optional :: channel
    real(kind=default), dimension(:), intent(in), optional :: weights
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    type(exception), intent(inout), optional :: exc
    ⟨Interface declaration for func 22⟩
    character(len=*), parameter :: FN = "vamp_sample_grid0"
```

```
    logical, intent(in), optional :: negative_weights
    ⟨Local variables in vamp_sample_grid0 86c⟩
    integer :: ndim
    logical :: neg_w
    ndim = size (g%div)
    neg_w = .false.
    if (present (negative_weights)) neg_w = negative_weights
    ⟨Check optional arguments in vamp_sample_grid0 90a⟩
    ⟨Reset counters in vamp_sample_grid0 86b⟩
    loop_over_cells: do
       ⟨Sample calls_per_cell points in the current cell 87b⟩
       ⟨Collect integration and grid optimization data for current cell 88d⟩
       ⟨Count up cell, exit if done 86a⟩
    end do loop_over_cells
    ⟨Collect results of vamp_sample_grid0 89a⟩
  end subroutine vamp_sample_grid0
```

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

86a ⟨*Count up* `cell`*, exit if done* 86a⟩≡

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

86b ⟨*Reset counters in* `vamp_sample_grid0` 86b⟩≡

```
g%mu = 0.0
cell = 1
call clear_integral_and_variance (g%div)
if (associated (g%mu_x)) then
   g%mu_x = 0.0
   g%mu_xx = 0.0
end if
if (present (channel)) then
   g%mu_gi = 0.0
end if
```

86c ⟨*Local variables in* `vamp_sample_grid0` 86c⟩≡

```
real(kind=default), parameter :: &
     eps =  tiny (1._default) / epsilon (1._default)
```

```
character(len=6) :: buffer
```

87a ⟨*Local variables in* `vamp_sample_grid0` 86c⟩+≡

```
integer :: j, k
integer, dimension(size(g%div)) :: cell
```

87b ⟨*Sample* `calls_per_cell` *points in the current* `cell` 87b⟩≡

```
sum_f = 0.0
sum_f2 = 0.0
do k = 1, g%calls_per_cell
   ⟨Get x in the current cell 87c⟩
   ⟨f = wgt * func (x, weights, channel), iff x inside true_domain 87d⟩
   ⟨Collect integration and grid optimization data for x from f 88a⟩
end do
```

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

87c ⟨*Get* `x` *in the current* `cell` 87c⟩≡

```
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.

87d ⟨`f = wgt * func (x, weights, channel)`, *iff* `x` *inside* `true_domain` 87d⟩≡

```
if (associated (g%map)) then
   if (all (inside_division (g%div, x))) then
      f = wgt * func (x, prc_index, weights, channel, grids)
   else
```

```
      f = 0.0
   end if
else
   f = wgt * func (x, prc_index, weights, channel, grids)
end if
```

88a ⟨*Collect integration and grid optimization data for* `x` *from* `f` 88a⟩≡

```
if (g%f_min > g%f_max) then
   g%f_min = f * g%calls
   g%f_max = f * g%calls
else if (f * g%calls < g%f_min) then
   g%f_min = f * g%calls
else if (f * g%calls > g%f_max) then
   g%f_max = f * g%calls
end if
```

88b ⟨*Collect integration and grid optimization data for* `x` *from* `f` 88a⟩+≡

```
f2 = f * f
sum_f = sum_f + f
sum_f2 = sum_f2 + f2
call record_integral (g%div, ia, f)
! call record_efficiency (g%div, ia, f/g%f_max)
if ((associated (g%mu_x)) .and. (.not. g%all_stratified)) then
   g%mu_x = g%mu_x + x * f
   g%mu_xx = g%mu_xx + outer_product (x, x) * f
end if
if (present (channel)) then
   g%mu_gi = g%mu_gi + f2
end if
```

88c ⟨*Local variables in* `vamp_sample_grid0` 86c⟩+≡

```
real(kind=default) :: wgt, f, f2, sum_f, sum_f2, var_f
real(kind=default), dimension(size(g%div)):: x, x_mid, wgts
real(kind=default), dimension(size(g%div)):: r
integer, dimension(size(g%div)) :: ia
```

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

88d ⟨*Collect integration and grid optimization data for current* `cell` 88d⟩≡

```
var_f = sum_f2 * g%calls_per_cell - sum_f**2
if (var_f <= 0.0) then
   var_f = tiny (1.0_default)
end if
g%mu = g%mu + (/ sum_f, var_f /)
call record_variance (g%div, ia, var_f)
```

```
if ((associated (g%mu_x)) .and. g%all_stratified) then
   if (associated (g%map)) then
      x_mid = matmul (g%map, x_mid)
   end if
   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
```

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

where the N^2_{calls} cancels the corresponding factor in the Jacobian and the N^{-2}_{cells} is the result of stratification.

89a ⟨*Collect results of* `vamp_sample_grid0` 89a⟩≡

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

89b ⟨*Collect results of* `vamp_sample_grid0` 89a⟩+≡

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

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

90a ⟨*Check optional arguments in* vamp_sample_grid0 90a⟩≡

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

90b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
 public :: vamp_probability
```

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

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

%variance should be private to division

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

```
subroutine vamp_apply_equivalences (g, eq)
  type(vamp_grids), intent(inout) :: g
  type(vamp_equivalences_t), intent(in) :: eq
  integer :: n_ch, n_dim, nb, i, ch, ch_src, dim, dim_src
  integer, dimension(:,:), allocatable :: n_bin
  real(kind=default), dimension(:,:,:), allocatable :: var_tmp
  n_ch = size (g%grids)
  if (n_ch == 0)  return
  n_dim = size (g%grids(1)%div)
  allocate (n_bin(n_ch, n_dim))
  do ch = 1, n_ch
     do dim = 1, n_dim
        n_bin(ch, dim) = size (g%grids(ch)%div(dim)%variance)
     end do
  end do
  allocate (var_tmp (maxval(n_bin), n_dim, n_ch))
  var_tmp = 0
  do i=1, eq%n_eq
     ch = eq%eq(i)%left
     ch_src = eq%eq(i)%right
     do dim=1, n_dim
        nb = n_bin(ch_src, dim)
        dim_src = eq%eq(i)%permutation(dim)
        select case (eq%eq(i)%mode(dim))
        case (VEQ_IDENTITY)
           var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
                & + g%grids(ch_src)%div(dim_src)%variance
        case (VEQ_INVERT)
           var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
                & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)
        case (VEQ_SYMMETRIC)
           var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
                & + g%grids(ch_src)%div(dim_src)%variance / 2 &
                & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)/2
        case (VEQ_INVARIANT)
           var_tmp(:nb,dim,ch) = 1
        end select
     end do
  end do
  do ch=1, n_ch
     do dim=1, n_dim
```

```
        g%grids(ch)%div(dim)%variance = var_tmp(:n_bin(ch, dim),dim,ch)
     end do
  end do
  deallocate (var_tmp)
  deallocate (n_bin)
end subroutine vamp_apply_equivalences
```

Grid Refinement: r

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

where

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

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

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

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

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

92c ⟨*Variables in* vamp 78a⟩+≡

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

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

```
pure subroutine vamp_sample_grid &
     (rng, g, func, prc_index, iterations, &
      integral, std_dev, avg_chi2, accuracy, &
      channel, weights, grids, exc, history)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: prc_index
  integer, intent(in) :: iterations
  real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
  real(kind=default), intent(in), optional :: accuracy
  integer, intent(in), optional :: channel
  real(kind=default), dimension(:), intent(in), optional :: weights
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  type(exception), intent(inout), optional :: exc
  type(vamp_history), dimension(:), intent(inout), optional :: history
  ⟨Interface declaration for func 22⟩
  character(len=*), parameter :: FN = "vamp_sample_grid"
  real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
  integer :: iteration, ndim
  ndim = size (g%div)
  iterate: do iteration = 1, iterations
     call vamp_sample_grid0 &
          (rng, g, func, prc_index, channel, weights, grids, exc)
     call vamp_average_iterations &
          (g, iteration, local_integral, local_std_dev, local_avg_chi2)
     ⟨Trace results of vamp_sample_grid 105b⟩
     ⟨Exit iterate if accuracy has been reached 95b⟩
     if (iteration < iterations) call vamp_refine_grid (g)
  end do iterate
  ⟨Copy results of vamp_sample_grid to dummy variables 95a⟩
end subroutine vamp_sample_grid
```

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

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

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

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

94a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

94b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

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

94c ⟨*Interfaces of* vamp *procedures* 94c⟩≡

```
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:

95a ⟨*Copy results of* `vamp_sample_grid` *to dummy variables* 95a⟩≡
```
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
```

95b ⟨*Exit* `iterate` *if* `accuracy` *has been reached* 95b⟩≡
```
if (present (accuracy)) then
   if (local_std_dev <= accuracy * local_integral) then
      call raise_exception (exc, EXC_INFO, FN, &
           "requested accuracy reached")
      exit iterate
   end if
end if
```

5.2.3 Forking and Joining

95c ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡
```
public :: vamp_fork_grid
private :: vamp_fork_grid_single, vamp_fork_grid_multi
public :: vamp_join_grid
private :: vamp_join_grid_single, vamp_join_grid_multi
```

95d ⟨*Interfaces of* `vamp` *procedures* 94c⟩+≡
```
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.

96a ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
pure subroutine vamp_fork_grid_single (g, gs, d, exc)
  type(vamp_grid), intent(in) :: g
  type(vamp_grid), dimension(:), intent(inout) :: gs
  integer, intent(in) :: d
  type(exception), intent(inout), optional :: exc
  character(len=*), parameter :: FN = "vamp_fork_grid_single"
  type(division_t), dimension(:), allocatable :: d_tmp
  integer :: i, j, num_grids, num_div, ndim, num_cells
  num_grids = size (gs)
  ndim = size (g%div)
  ⟨Allocate or resize the divisions 98c⟩
  do j = 1, ndim
     if (j == d) then
        ⟨call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 97d⟩
     else
        ⟨call copy_division (gs%div(j), g%div(j)) 98b⟩
     end if
  end do
  if (d == 0) then
     ⟨Handle g%calls_per_cell for d == 0 96b⟩
  end if
  ⟨Copy the rest of g to the gs 96c⟩
end subroutine vamp_fork_grid_single
```

Divide the sampling points among identical grids

96b ⟨*Handle* `g%calls_per_cell` *for* `d == 0` 96b⟩≡

```
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
```

96c ⟨*Copy the rest of* `g` *to the* `gs` 96c⟩≡

```
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

97a ⟨*Copy the rest of* g *to the* gs 96c⟩+≡

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

97b ⟨*Copy the rest of* g *to the* gs 96c⟩+≡

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

97c ⟨*Copy the rest of* g *to the* gs 96c⟩+≡

```
   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.

97d ⟨`call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...)` 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 98a⟩
```

98a ⟨*Bail out if exception* `exc` *raised* 98a⟩≡

```
  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.

98b ⟨`call copy_division (gs%div(j), g%div(j))` 98b⟩≡

```
  do i = 1, num_grids
     call copy_division (gs(i)%div(j), g%div(j))
  end do
```

98c ⟨*Allocate or resize the divisions* 98c⟩≡

```
  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
```

98d ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
  pure subroutine vamp_join_grid_single (g, gs, d, exc)
    type(vamp_grid), intent(inout) :: g
    type(vamp_grid), dimension(:), intent(inout) :: gs
    integer, intent(in) :: d
    type(exception), intent(inout), optional :: exc
    type(division_t), dimension(:), allocatable :: d_tmp
    integer :: i, j, num_grids
    num_grids = size (gs)
    do j = 1, size (g%div)
```

```
      if (j == d) then
         ⟨call join_division (g%div(j), gs%div(j)) 99a⟩
      else
         ⟨call sum_division (g%div(j), gs%div(j)) 99b⟩
      end if
   end do
   ⟨Combine the rest of gs onto g 99c⟩
end subroutine vamp_join_grid_single
```

99a ⟨call join_division (g%div(j), gs%div(j)) 99a⟩≡

```
allocate (d_tmp(num_grids))
do i = 1, num_grids
   d_tmp(i) = gs(i)%div(j)
end do
call join_division (g%div(j), d_tmp, exc)
deallocate (d_tmp)
⟨Bail out if exception exc raised 98a⟩
```

99b ⟨call sum_division (g%div(j), gs%div(j)) 99b⟩≡

```
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)
```

99c ⟨*Combine the rest of* gs *onto* g 99c⟩≡

```
g%f_min = minval (gs%f_min * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
g%f_max = maxval (gs%f_max * (g%jacobi * g%calls) / (gs%jacobi * gs%calls))
g%mu(1) = sum (gs%mu(1))
g%mu(2) = sum (gs%mu(2))
g%mu_gi = sum (gs%mu_gi)
g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
g%sum_integral = g%sum_integral + g%mu(1) / g%mu(2)
g%sum_chi2 = g%sum_chi2 + g%mu(1)**2 / g%mu(2)
g%sum_weights = g%sum_weights + 1.0 / g%mu(2)
if (associated (g%mu_x)) then
   do i = 1, num_grids
      g%mu_x = g%mu_x + gs(i)%mu_x
      g%mu_xx = g%mu_xx + gs(i)%mu_xx
   end do
   g%sum_mu_x = g%sum_mu_x + g%mu_x / g%mu(2)
   g%sum_mu_xx = g%sum_mu_xx + g%mu_xx / g%mu(2)
end if
```

The following is made a little bit hairy by the fact that `vamp_fork_grid` can't join grids onto a non-existing grid[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.

100a ⟨*Idioms* 100a⟩≡

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

100b ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

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

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

```
        end do
    end select
  end subroutine vamp_fork_grid_multi
```

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

```
  public :: vamp_fork_grid_joints
```

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

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

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

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

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

```
            joints_offset = joints_offset + joints_stride
         end do
         call vamp_join_grid_single (g, gx(1:d(2,1)), d(1,1), exc)
         call vamp_delete_grid (gx(1:d(2,1)))
    end select
  end subroutine vamp_join_grid_multi
```

5.2.4 Parallel Execution

102a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

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

HPF [9, 10, 14]:

102b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  subroutine vamp_sample_grid_parallel &
       (rng, g, func, prc_index, iterations, &
        integral, std_dev, avg_chi2, accuracy, &
        channel, weights, grids, exc, history)
    type(tao_random_state), dimension(:), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: prc_index
    integer, intent(in) :: iterations
    real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
    real(kind=default), intent(in), optional :: accuracy
    integer, intent(in), optional :: channel
    real(kind=default), dimension(:), intent(in), optional :: weights
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    type(exception), intent(inout), optional :: exc
    type(vamp_history), dimension(:), intent(inout), optional :: history
    ⟨Interface declaration for func 22⟩
    character(len=*), parameter :: FN = "vamp_sample_grid_parallel"
    real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
    type(exception), dimension(size(rng)) :: excs
    type(vamp_grid), dimension(:), allocatable :: gs, gx
    !hpf$ processors p(number_of_processors())
    !hpf$ distribute gs(cyclic(1)) onto p
    integer, dimension(:,:), pointer :: d
    integer :: iteration, i
    integer :: num_workers
    nullify (d)
    call clear_exception (excs)
    iterate: do iteration = 1, iterations
```

```
      call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
      num_workers = max (1, product (d(2,:)))
      if (num_workers > 1) then
         allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
         call vamp_create_empty_grid (gs)
         ! vamp_fork_grid is certainly not local. Speed freaks might
         ! want to tune it to the processor topology, but the gain will be small.
         call vamp_fork_grid (g, gs, gx, d, exc)
         !hpf$ independent
         do i = 1, num_workers
            call vamp_sample_grid0 &
                 (rng(i), gs(i), func, prc_index, &
                  channel, weights, grids, exc)
         end do
         ⟨Gather exceptions in vamp_sample_grid_parallel 103a⟩
         call vamp_join_grid (g, gs, gx, d, exc)
         call vamp_delete_grid (gs)
         deallocate (gs, gx)
      else
         call vamp_sample_grid0 &
              (rng(1), g, func, prc_index, channel, weights, grids, exc)
      end if
      ⟨Bail out if exception exc raised 98a⟩
      call vamp_average_iterations &
           (g, iteration, local_integral, local_std_dev, local_avg_chi2)
      ⟨Trace results of vamp_sample_grid 105b⟩
      ⟨Exit iterate if accuracy has been reached 95b⟩
      if (iteration < iterations) call vamp_refine_grid (g)
   end do iterate
   deallocate (d)
   ⟨Copy results of vamp_sample_grid to dummy variables 95a⟩
end subroutine vamp_sample_grid_parallel
```

103a ⟨*Gather exceptions in* `vamp_sample_grid_parallel` 103a⟩≡

```
if ((present (exc)) .and. (any (excs(1:num_workers)%level > 0))) then
   call gather_exceptions (exc, excs(1:num_workers))
end if
```

We could sort d such that (5.23) is minimized

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

but the gain will be negligible.

103b ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
pure subroutine vamp_distribute_work (num_workers, ng, d)
```

```
  integer, intent(in) :: num_workers
  integer, dimension(:), intent(in) :: ng
  integer, dimension(:,:), pointer :: d
  integer, dimension(32) :: factors
  integer :: n, num_factors, i, j
  integer, dimension(size(ng)) :: num_forks
  integer :: nfork
  try: do n = num_workers, 1, -1
     call factorize (n, factors, num_factors)
     num_forks = 1
     do i = num_factors, 1, -1
        j = sum (maxloc (ng / num_forks))
        nfork = num_forks(j) * factors(i)
        if (nfork <= ng(j)) then
           num_forks(j) = nfork
        else
           cycle try
        end if
     end do
     ⟨Accept distribution among n workers 104a⟩
  end do try
end subroutine vamp_distribute_work
```

104a ⟨*Accept distribution among* `n` *workers* 104a⟩≡

```
j = count (num_forks > 1)
if (associated (d)) then
   if (size (d, dim = 2) /= j) then
      deallocate (d)
      allocate (d(2,j))
   end if
else
   allocate (d(2,j))
end if
```

104b ⟨*Accept distribution among* `n` *workers* 104a⟩+≡

```
j = 1
do i = 1, size (ng)
   if (num_forks(i) > 1) then
      d(:,j) = (/ i, num_forks(i) /)
      j = j + 1
   end if
end do
return
```

5.2.5 *Diagnostics*

105a ⟨*Declaration of* vamp *types* 105a⟩≡
```
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
```

105b ⟨*Trace results of* vamp_sample_grid 105b⟩≡
```
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
```

105c ⟨*Declaration of* vamp *procedures* 77a⟩+≡
```
public :: vamp_create_history, vamp_copy_history, vamp_delete_history
public :: vamp_terminate_history
public :: vamp_get_history, vamp_get_history_single
```

105d ⟨*Interfaces of* vamp *procedures* 94c⟩+≡
```
interface vamp_get_history
   module procedure vamp_get_history_single
end interface
```

105e ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
elemental subroutine vamp_create_history (h, ndim, verbose)
  type(vamp_history), intent(out) :: h
  integer, intent(in), optional :: ndim
  logical, intent(in), optional :: verbose
  if (present (verbose)) then
     h%verbose = verbose
  else
     h%verbose = .false.
  end if
  h%calls = 0.0
```

```
    if (h%verbose .and. (present (ndim))) then
       if (associated (h%div)) then
          deallocate (h%div)
       end if
       allocate (h%div(ndim))
    end if
  end subroutine vamp_create_history
```

106a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  elemental subroutine vamp_terminate_history (h)
    type(vamp_history), intent(inout) :: h
    h%calls = 0.0
  end subroutine vamp_terminate_history
```

106b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_get_history_single (h, g, integral, std_dev, avg_chi2)
    type(vamp_history), intent(inout) :: h
    type(vamp_grid), intent(in) :: g
    real(kind=default), intent(in) :: integral, std_dev, avg_chi2
    h%calls = g%calls
    h%stratified = g%all_stratified
    h%integral = g%mu(1)
    h%std_dev = sqrt (g%mu(2))
    h%avg_integral = integral
    h%avg_std_dev = std_dev
    h%avg_chi2 = avg_chi2
    h%f_min = g%f_min
    h%f_max = g%f_max
    if (h%verbose) then
       ⟨Adjust h%div iff necessary 106c⟩
       call copy_history (h%div, summarize_division (g%div))
    end if
  end subroutine vamp_get_history_single
```

106c ⟨*Adjust* h%div *iff necessary* 106c⟩≡

```
  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
```

106d ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  public :: vamp_print_history, vamp_write_history
```

```
  private :: vamp_print_one_history, vamp_print_histories
  ! private :: vamp_write_one_history, vamp_write_histories
```

107a ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
  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
```

107b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

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

108a ⟨*Variables in* vamp 78a⟩+≡

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

108b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  subroutine vamp_print_histories (h, tag)
    type(vamp_history), dimension(:,:), intent(in) :: h
    character(len=*), intent(in), optional :: tag
    character(len=BUFFER_SIZE) :: pfx
    integer :: i
    print "(1X,A78)", repeat ("=", 78)
    channels: do i = 1, size (h, dim=2)
       if (present (tag)) then
          write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
       else
          write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
       end if
       call vamp_print_one_history (h(:,i), pfx)
    end do channels
    print "(1X,A78)", repeat ("=", 78)
    flush (output_unit)
  end subroutine vamp_print_histories
```

WK

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

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

```
          do i = 1, imax
             call copy_history (h_tmp(i), h(i)%div(j))
          end do
          if (present (tag)) then
             write (unit = pfx, fmt = "(A,A1,I2.2)") &
                  trim (tag(1:min(len_trim(tag),8))), "#", j
          else
             write (unit = pfx, fmt = "(A,A1,I2.2)") "[vamp]", "#", j
          end if
          call write_history (u, h_tmp, tag = pfx)
          print "(1X,A78)", repeat ("-", 78)
       end do dimensions
       deallocate (h_tmp)
    end if
  end if
  flush (u)
end subroutine vamp_write_one_history_unit
subroutine vamp_write_histories_unit (u, h, tag)
  integer, intent(in) :: u
  type(vamp_history), dimension(:,:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  character(len=BUFFER_SIZE) :: pfx
  integer :: i
  write (u, "(1X,A78)") repeat ("=", 78)
  channels: do i = 1, size (h, dim=2)
     if (present (tag)) then
        write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i
     else
        write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i
     end if
     call vamp_write_one_history_unit (u, h(:,i), pfx)
  end do channels
  write (u, "(1X,A78)") repeat ("=", 78)
  flush (u)
end subroutine vamp_write_histories_unit
```

5.2.6 Multi Channel

[22]

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

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

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

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

Therefore...

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

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

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

111a ⟨*Declaration of* `vamp` *types* 105a⟩+≡

```
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
```

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

111b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

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

112a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure function vamp_multi_channel &
     (func, prc_index, phi, ihp, jacobian, x, weights, channel, grids) result (w_x)
  integer, intent(in) :: prc_index
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in) :: channel
  type(vamp_grid), dimension(:), intent(in) :: grids
  ⟨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, prc_index, i)
  end do
  w_x = func (phi_x, prc_index, weights, channel, grids) &
       / dot_product (weights, g_phi_x)
end function vamp_multi_channel
```

112b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure function vamp_multi_channel0 &
     (func, prc_index, phi, jacobian, x, weights, channel) result (w_x)
  integer, intent(in) :: prc_index
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in) :: channel
  ⟨Interface declaration for func 22⟩
  ⟨Interface declaration for phi 31a⟩
  ⟨Interface declaration for jacobian 31c⟩
  real(kind=default) :: w_x
  real(kind=default), dimension(size(x)) :: x_prime
  real(kind=default), dimension(size(weights)) :: g_phi_x
```

```
    integer :: i
    x_prime = phi (x, channel)
    do i = 1, size (weights)
       g_phi_x(i) = jacobian (x_prime, prc_index, i)
    end do
    w_x = func (x_prime, prc_index) / dot_product (weights, g_phi_x)
  end function vamp_multi_channel0
```

WK

113a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

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

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

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

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

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

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

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

```
  end subroutine vamp_check_jacobian
```

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

115a ⟨*Declaration of* vamp *procedures (removed from WHIZARD)* 115a⟩≡

```
  private :: numeric_jacobian
```

115b ⟨*Implementation of* vamp *procedures (removed from WHIZARD)* 115b⟩≡

```
  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
```

115c ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  public :: vamp_create_grids, vamp_create_empty_grids
```

```
public :: vamp_copy_grids, vamp_delete_grids
```

The rules for optional arguments forces us to handle special cases, because we can't just pass a array section of an optional array as an actual argument (cf. 12.4.1.5(4) in [8]) even if the dummy argument is optional itself.

116a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

116b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_create_empty_grids (g)
  type(vamp_grids), intent(inout) :: g
  nullify (g%grids, g%weights, g%num_calls)
end subroutine vamp_create_empty_grids
```

117a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
public :: vamp_discard_integrals
```

117b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_discard_integrals &
     (g, num_calls, num_div, stratified, quadrupole, exc, eq)
  type(vamp_grids), intent(inout) :: g
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole
  type(exception), intent(inout), optional :: exc
  type(vamp_equivalences_t), intent(in), optional :: eq
  integer :: ch
  character(len=*), parameter :: FN = "vamp_discard_integrals"
  g%sum_integral = 0.0
  g%sum_weights = 0.0
  g%sum_chi2 = 0.0
  do ch = 1, size (g%grids)
     call vamp_discard_integral (g%grids(ch))
  end do
  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
```

117c ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
public :: vamp_update_weights
```

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

117d ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_update_weights &
     (g, weights, num_calls, num_div, stratified, quadrupole, exc)
  type(vamp_grids), intent(inout) :: g
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole
  type(exception), intent(inout), optional :: exc
  character(len=*), parameter :: FN = "vamp_update_weights"
  if (sum (weights) > 0) then
     g%weights = weights / sum (weights)
  else
     g%weights = 1._default / size(g%weights)
```

```
    end if
    if (present (num_calls)) then
       call vamp_discard_integrals (g, num_calls, num_div, &
                                    stratified, quadrupole, exc)
    else
       call vamp_discard_integrals (g, sum (g%num_calls), num_div, &
                                    stratified, quadrupole, exc)
    end if
  end subroutine vamp_update_weights
```

118a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
  public :: vamp_reshape_grids
```

118b ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

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

```
         end if
      else
         g%num_calls(ch) = 0
      end if
   end do
 end subroutine vamp_reshape_grids
```

119a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
 public :: vamp_sample_grids
```

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

119b ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
   pure subroutine vamp_sample_grids &
        (rng, g, func, prc_index, iterations, integral, std_dev, avg_chi2, &
         accuracy, history, histories, exc, eq, warn_error, negative_weights)
     type(tao_random_state), intent(inout) :: rng
     type(vamp_grids), intent(inout) :: g
     integer, intent(in) :: prc_index
     integer, intent(in) :: iterations
     real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
     real(kind=default), intent(in), optional :: accuracy
     type(vamp_history), dimension(:), intent(inout), optional :: history
     type(vamp_history), dimension(:,:), intent(inout), optional :: histories
     type(exception), intent(inout), optional :: exc
     type(vamp_equivalences_t), intent(in), optional :: eq
     logical, intent(in), optional :: warn_error, negative_weights
     ⟨Interface declaration for func 22⟩
     integer :: ch, iteration
     logical :: neg_w
     type(exception), dimension(size(g%grids)) :: excs
     logical, dimension(size(g%grids)) :: active
     real(kind=default), dimension(size(g%grids)) :: weights, integrals, std_devs
     real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
     character(len=*), parameter :: FN = "vamp_sample_grids"
     integrals = 0
     std_devs = 0
     neg_w = .false.
     if (present (negative_weights)) neg_w = negative_weights
     active = (g%num_calls >= 2)
     where (active)
        weights = g%num_calls
     elsewhere
        weights = 0.0
```

```
      endwhere
      if (sum (weights) /= 0)  weights = weights / sum (weights)
      call clear_exception (excs)
      iterate: do iteration = 1, iterations
         do ch = 1, size (g%grids)
            if (active(ch)) then
               call vamp_discard_integral (g%grids(ch))
               ⟨Sample the grid g%grids(ch) 120⟩
            else
               call vamp_nullify_variance (g%grids(ch))
               call vamp_nullify_covariance (g%grids(ch))
            end if
         end do
         if (present(eq))  call vamp_apply_equivalences (g, eq)
         if (iteration < iterations) then
            do ch = 1, size (g%grids)
               active(ch) = (integrals(ch) /= 0)
               if (active(ch)) then
                  call vamp_refine_grid (g%grids(ch))
                end if
            end do
         end if
         if (present (exc) .and. (any (excs%level > 0))) then
            call gather_exceptions (exc, excs)
!           return
         end if
         call vamp_reduce_channels (g, integrals, std_devs, active)
         call vamp_average_iterations &
              (g, iteration, local_integral, local_std_dev, local_avg_chi2)
         ⟨Trace results of vamp_sample_grids 123b⟩
         ⟨Exit iterate if accuracy has been reached 95b⟩
      end do iterate
      ⟨Copy results of vamp_sample_grid to dummy variables 95a⟩
    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`:

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

```
  call vamp_sample_grid0 &
       (rng, g%grids(ch), func, prc_index, &
        ch, weights, g%grids, excs(ch), neg_w)
  if (present (exc) .and. present (warn_error)) then
     if (warn_error) call handle_exception (excs(ch))
```

```
  end if
  call vamp_average_iterations &
       (g%grids(ch), iteration, integrals(ch), std_devs(ch), local_avg_chi2)
  if (present (histories)) then
     if (iteration <= ubound (histories, dim=1)) then
        call vamp_get_history &
             (histories(iteration,ch), g%grids(ch), &
              integrals(ch), std_devs(ch), local_avg_chi2)
     else
        call raise_exception (exc, EXC_WARN, FN, "history too short")
     end if
     call vamp_terminate_history (histories(iteration+1:,ch))
  end if
```

121a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  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.

121b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

```
    else
       this_integral = 0
    end if
    total_variance = sum ((g%num_calls*std_devs)**2, mask=active)
    if (total_variance > 0) then
       this_weight = total_calls**2 / total_variance
    else
       this_weight = 0
    end if
    g%sum_weights = g%sum_weights + this_weight
    g%sum_integral = g%sum_integral + this_weight * this_integral
    g%sum_chi2 = g%sum_chi2 + this_weight * this_integral**2
  end subroutine vamp_reduce_channels
```

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

```
  public :: vamp_refine_weights
```

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

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

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

```
  private :: vamp_average_iterations_grids
```

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

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

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

123a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

123b ⟨*Trace results of* vamp_sample_grids 123b⟩≡

```
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
```

123c ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
private :: vamp_get_history_multi
```

123d ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
interface vamp_get_history
   module procedure vamp_get_history_multi
end interface
```

123e ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_get_history_multi (h, g, integral, std_dev, avg_chi2)
  type(vamp_history), intent(inout) :: h
  type(vamp_grids), intent(in) :: g
  real(kind=default), intent(in) :: integral, std_dev, avg_chi2
  h%calls = sum (g%grids%calls)
  h%stratified = all (g%grids%all_stratified)
  h%integral = 0.0
  h%std_dev = 0.0
```

```
    h%avg_integral = integral
    h%avg_std_dev = std_dev
    h%avg_chi2 = avg_chi2
    h%f_min = 0.0
    h%f_max = huge (h%f_max)
    if (h%verbose) then
       h%verbose = .false.
       if (associated (h%div)) then
          deallocate (h%div)
       end if
    end if
  end subroutine vamp_get_history_multi
```

WK

124a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  public :: vamp_sum_channels
```

124b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

5.2.7 Mapping

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

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

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.

125a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

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

125b ⟨*Set* `iv` *to the index of the optimal eigenvector* 125b⟩≡

```
if (num_pancake > 0) then
   print *, "FORCED PANCAKE: ", num_pancake
   iv = sum (minloc (evals))
else if (num_cigar > 0) then
   print *, "FORCED CIGAR: ", num_cigar
```

```
      iv = sum (maxloc (evals))
   else
      call more_pancake_than_cigar (evals, like_pancake)
      if (like_pancake) then
         iv = sum (minloc (evals))
      else
         iv = sum (maxloc (evals))
      end if
   end if
```

126a ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

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

126b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
private :: more_pancake_than_cigar
```

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

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

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

127a ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane* 127a⟩≡
```
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:

127b ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane (broken!)* 127b⟩≡
```
abs_evec = abs (evecs(:,iv))
i(1) = sum (maxloc (abs_evec))
i(2) = sum (maxloc (abs_evec, mask = abs_evec < abs_evec(i(1))))
```

127c ⟨*Set* `i(1)`, `i(2)` *to the axes of the optimal plane* 127a⟩+≡
```
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)
```

127d ⟨*Get* $\cos\theta$ *and* $\sin\theta$ *from* `evecs` 127d⟩≡
```
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
```

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

127e ⟨*Construct* $\hat{R}(\theta;i,j)$ 127e⟩≡
```
call unit (r)
r(i(1),i) = (/  cos_theta, - sin_theta /)
r(i(2),i) = (/  sin_theta,   cos_theta /)
```

127f ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡
```
subroutine select_rotation_axis (cov, r, pancake, cigar)
  real(kind=default), dimension(:,:), intent(in) :: cov
  real(kind=default), dimension(:,:), intent(out) :: r
```

[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.

```
    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 128a⟩
    call diagonalize_real_symmetric (cov, evals, evecs)
    ⟨Set iv to the index of the optimal eigenvector 125b⟩
    ⟨Set i(1), i(2) to the axes of the optimal plane 127a⟩
    ⟨Get cos θ and sin θ from evecs 127d⟩
    ⟨Construct R̂(θ; i, j) 127e⟩
  end subroutine select_rotation_axis
```

128a ⟨*Handle optional* pancake *and* cigar 128a⟩≡

```
  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:

128b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

128c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
subroutine select_subspace_guess (cov, r, ndim, pancake, cigar)
  real(kind=default), dimension(:,:), intent(in) :: cov
  real(kind=default), dimension(:,:), intent(out) :: r
  integer, intent(in) :: ndim
  integer, intent(in), optional :: pancake, cigar
  integer :: num_pancake, num_cigar
  logical :: like_pancake
  real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evecs
  real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
  integer :: iv, i
  integer, dimension(ndim) :: subspace
  ⟨Handle optional pancake and cigar 128a⟩
  call diagonalize_real_symmetric (cov, evals, evecs)
  ⟨Set iv to the index of the optimal eigenvector 125b⟩
  ⟨Set subspace to the axes of the optimal plane 129a⟩
  call select_subspace_explicit (cov, r, subspace)
end subroutine select_subspace_guess
```

129a ⟨*Set* subspace *to the axes of the optimal plane* 129a⟩≡

```
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
```

129b ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
interface select_rotation_subspace
   module procedure select_subspace_explicit, select_subspace_guess
end interface
```

129c ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
private :: select_subspace_explicit
private :: select_subspace_guess
```

129d ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
public :: vamp_print_covariance
```

129e ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
subroutine vamp_print_covariance (cov)
  real(kind=default), dimension(:,:), intent(in) :: cov
  real(kind=default), dimension(size(cov,dim=1)) :: &
       evals, abs_evals, tmp
  real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: &
       evecs, abs_evecs
  integer, dimension(size(cov,dim=1)) :: idx
```

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

Condensing Eigenvalues

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

130 ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
  ! 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!

131a ⟨*Initialize clusters* 131a⟩≡

```
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

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

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

$$d_\alpha(x,y) = |x^\alpha - y^\alpha| \tag{5.37c}$$

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.

131b ⟨*Join closest clusters* 131b⟩≡

```
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)
```

131c ⟨*Join closest clusters* 131b⟩+≡

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

131d ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
subroutine condense (x, cluster_pos, clusters, linear)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(out) :: cluster_pos
  integer, dimension(:,:), intent(out) :: clusters
  logical, intent(in), optional :: linear
```

```
    logical :: linear_metric
    real(kind=default), dimension(size(x)) :: cl_pos
    real(kind=default) :: wgt0, wgt1
    integer :: cl_num
    integer, dimension(size(x),2) :: cl
    integer :: i, gap
    linear_metric = .false.
    if (present (linear)) then
       linear_metric = linear
    end if
    ⟨Initialize clusters 131a⟩
    do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
       ⟨Join closest clusters 131b⟩
       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
```

132a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  ! private :: condense_action
  public :: condense_action
```

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

132b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  function condense_action (positions, clusters) result (s)
    real(kind=default), dimension(:), intent(in) :: positions
    integer, dimension(:,:), intent(in) :: clusters
    real(kind=default) :: s
    integer :: i
    integer, parameter :: POWER = 2
    s = 0
    do i = 1, size (clusters, dim = 1)
       s = s + standard_deviation (positions(clusters(i,1) &
                                             :clusters(i,2))) ** POWER
    end do
  end function condense_action
```

132c ⟨ctest.f90 132c⟩≡

```
  program ctest
    use kinds
    use utils
    use vamp_stat
    use tao_random_numbers
```

```
  use vamp
  implicit none
  integer, parameter :: N = 16, NC = 2
  real(kind=default), dimension(N) :: eval
  real(kind=default), dimension(NC) :: cluster_pos
  integer, dimension(NC,2) :: clusters
  integer :: i
  call tao_random_number (eval)
  call sort (eval)
  print *, eval
  eval(1:N/2) = 0.95*eval(1:N/2)
  eval(N/2+1:N) = 1.0 - 0.95*(1.0 - eval(N/2+1:N))
  print *, eval
  call condense (eval, cluster_pos, clusters, linear=.true.)
  do i = 1, NC
     print "(I2,A,F5.2,A,I2,A,I2,A,A,F5.2,A,F5.2,A,32F5.2)", &
          i, ": ", cluster_pos(i), &
          " [", clusters(i,1), "-", clusters(i,2), "]", &
          " [", eval(clusters(i,1)), " - ", eval(clusters(i,2)), "]", &
          eval(clusters(i,1)+1:clusters(i,2)) &
            - eval(clusters(i,1):clusters(i,2)-1)
     print *, average (eval(clusters(i,1):clusters(i,2))), "+/-", &
              standard_deviation (eval(clusters(i,1):clusters(i,2)))
  end do
end program ctest
```

5.2.8 *Event Generation*

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

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

```
public :: vamp_next_event
```

133b ⟨*Interfaces of* `vamp` *procedures* 94c⟩+≡

```
interface vamp_next_event
   module procedure vamp_next_event_single, vamp_next_event_multi
end interface
```

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

```
private :: vamp_next_event_single, vamp_next_event_multi
```

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

133d ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
pure subroutine vamp_next_event_single &
     (x, rng, g, func, prc_index, &
      weight, channel, weights, grids, exc)
  real(kind=default), dimension(:), intent(out) :: x
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  real(kind=default), intent(out), optional :: weight
  integer, intent(in) :: prc_index
  integer, intent(in), optional :: channel
  real(kind=default), dimension(:), intent(in), optional :: weights
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  type(exception), intent(inout), optional :: exc
  ⟨Interface declaration for func 22⟩
  character(len=*), parameter :: FN = "vamp_next_event_single"
  real(kind=default), dimension(size(g%div)):: wgts
  real(kind=default), dimension(size(g%div)):: r
  integer, dimension(size(g%div)):: ia
  real(kind=default) :: f, wgt
  real(kind=default) :: r0
  rejection: do
     ⟨Choose a x and calculate f(x) 134a⟩
     if (present (weight)) then
        ⟨Unconditionally accept weighted event 134b⟩
     else
        ⟨Maybe accept unweighted event 134c⟩
     end if
  end do rejection
end subroutine vamp_next_event_single
```

134a ⟨*Choose a* x *and calculate f(*x*)* 134a⟩≡

```
call tao_random_number (rng, r)
call inject_division_short (g%div, real(r, kind=default), x, ia, wgts)
wgt = g%jacobi * product (wgts)
wgt = g%calls * wgt ! the calling procedure will divide by #calls
if (associated (g%map)) then
   x = matmul (g%map, x)
end if
⟨f = wgt * func (x, weights, channel), iff x inside true_domain 87d⟩
! call record_efficiency (g%div, ia, f/g%f_max)
```

134b ⟨*Unconditionally accept weighted event* 134b⟩≡

```
weight = f
exit rejection
```

134c ⟨*Maybe accept unweighted event* 134c⟩≡

```
if (f > g%f_max) then
   g%f_max = f
   call raise_exception (exc, EXC_WARN, FN, "weight > 1")
   exit rejection
end if
call tao_random_number (rng, r0)
if (r0 * g%f_max <= f) then
   exit rejection
end if
```

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

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

with $w(x) = f(x)/g(x) = f(x)/\sum_i \alpha_i g_i(x)$ and $\sum_i \alpha_i = 1$. The non-trivial poblem is that the adaptive grid is diferent in each channel, so we can't just reject on $w(x)$.

135 ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
pure subroutine vamp_next_event_multi &
     (x, rng, g, func, prc_index, phi, weight, excess, exc)
  real(kind=default), dimension(:), intent(out) :: x
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grids), intent(inout) :: g
  integer, intent(in) :: prc_index
  real(kind=default), intent(out), optional :: weight
  real(kind=default), intent(out), optional :: excess
  type(exception), intent(inout), optional :: exc
  ⟨Interface declaration for func 22⟩
  ⟨Interface declaration for phi 31a⟩
  character(len=*), parameter :: FN = "vamp_next_event_multi"
  real(kind=default), dimension(size(x)) :: xi
  real(kind=default) :: r, wgt
  real(kind=default), dimension(size(g%weights)) :: weights
  integer :: channel
  ⟨weights: α_i → w_max,i α_i 136a⟩
  rejection: do
     ⟨Select channel from weights 136b⟩
     call vamp_next_event_single &
          (xi, rng, g%grids(channel), func, prc_index, wgt, &
           channel, g%weights, g%grids, exc)
     if (present (weight)) then
        ⟨Unconditionally accept weighted multi channel event 136c⟩
```

```
      else
         ⟨Maybe accept unweighted multi channel event 136d⟩
      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

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

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.

136a ⟨weights: $\alpha_i \to w_{\max,i}\alpha_i$ 136a⟩≡

```
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)
```

136b ⟨*Select* channel *from* weights 136b⟩≡

```
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
```

136c ⟨*Unconditionally accept weighted multi channel event* 136c⟩≡

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

136d ⟨*Maybe accept unweighted multi channel event* 136d⟩≡

```
if (wgt > g%grids(channel)%f_max) then
   if (present(excess)) then
      excess = wgt/g%grids(channel)%f_max - 1
   else
```

```
!     call raise_exception (exc, EXC_WARN, FN, "weight > 1")
      print *, "weight > 1 (", wgt/g%grids(channel)%f_max, &
           & ") in channel ", channel

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

137a ⟨*Maybe accept unweighted multi channel event (old version)* 137a⟩≡

```
if (wgt > g%grids(channel)%f_max) then
   g%grids(channel)%f_max = wgt
   ⟨weights: αi → wmax,iαi 136a⟩
   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.

137b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
public :: vamp_warmup_grid, vamp_warmup_grids
```

137c ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
pure subroutine vamp_warmup_grid &
     (rng, g, func, prc_index, iterations, exc, history)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: prc_index
  integer, intent(in) :: iterations
  type(exception), intent(inout), optional :: exc
  type(vamp_history), dimension(:), intent(inout), optional :: history
  ⟨Interface declaration for func 22⟩
```

```
  call vamp_sample_grid &
     (rng, g, func, prc_index, &
      iterations - 1, exc = exc, history = history)
  call vamp_sample_grid0 (rng, g, func, prc_index, exc = exc)
end subroutine vamp_warmup_grid
```

WHERE ... END WHERE alert!

138a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

5.2.9 Convenience Routines

138b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
public :: vamp_integrate
private :: vamp_integrate_grid, vamp_integrate_region
```

139a ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
interface vamp_integrate
   module procedure vamp_integrate_grid, vamp_integrate_region
end interface
```

139b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_integrate_grid &
     (rng, g, func, prc_index, calls, integral, std_dev, avg_chi2, num_div, &
      stratified, quadrupole, accuracy, exc, history)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: prc_index
  integer, dimension(:,:), intent(in) :: calls
  real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole
  real(kind=default), intent(in), optional :: accuracy
  type(exception), intent(inout), optional :: exc
  type(vamp_history), dimension(:), intent(inout), optional :: history
  ⟨Interface declaration for func 22⟩
  character(len=*), parameter :: FN = "vamp_integrate_grid"
  integer :: step, last_step, it
  last_step = size (calls, dim = 2)
  it = 1
  do step = 1, last_step - 1
     call vamp_discard_integral (g, calls(2,step), num_div, &
                                 stratified, quadrupole, exc = exc)
     call vamp_sample_grid (rng, g, func, prc_index, calls(1,step), &
                            exc = exc, history = history(it:))
     ⟨Bail out if exception exc raised 98a⟩
     it = it + calls(1,step)
  end do
  call vamp_discard_integral (g, calls(2,last_step), exc = exc)
  call vamp_sample_grid (rng, g, func, prc_index, calls(1,last_step), &
                         integral, std_dev, avg_chi2, accuracy, exc = exc, &
                         history = history(it:))
end subroutine vamp_integrate_grid
```

139c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
pure subroutine vamp_integrate_region &
     (rng, region, func, prc_index, calls, &
      integral, std_dev, avg_chi2, num_div, &
```

```
       stratified, quadrupole, accuracy, map, covariance, exc, history)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, intent(in) :: prc_index
    integer, dimension(:,:), intent(in) :: calls
    real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole
    real(kind=default), intent(in), optional :: accuracy
    real(kind=default), dimension(:,:), intent(in), optional :: map
    real(kind=default), dimension(:,:), intent(out), optional :: covariance
    type(exception), intent(inout), optional :: exc
    type(vamp_history), dimension(:), intent(inout), optional :: history
    ⟨Interface declaration for func 22⟩
    character(len=*), parameter :: FN = "vamp_integrate_region"
    type(vamp_grid) :: g
    call vamp_create_grid &
         (g, region, calls(2,1), num_div, &
          stratified, quadrupole, present (covariance), map, exc)
    call vamp_integrate_grid &
         (rng, g, func, prc_index, calls, &
          integral, std_dev, avg_chi2, num_div, &
          accuracy = accuracy, exc = exc, history = history)
    if (present (covariance)) then
       covariance = vamp_get_covariance (g)
    end if
    call vamp_delete_grid (g)
  end subroutine vamp_integrate_region
```

140a ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡

```
  public :: vamp_integratex
  private :: vamp_integratex_region
```

140b ⟨*Interfaces of* `vamp` *procedures* 94c⟩+≡

```
  interface vamp_integratex
     module procedure vamp_integratex_region
  end interface
```

140c ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
  subroutine vamp_integratex_region &
       (rng, region, func, prc_index, calls, integral, std_dev, avg_chi2, &
        num_div, stratified, quadrupole, accuracy, pancake, cigar, &
        exc, history)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
```

```
integer, intent(in) :: prc_index
integer, dimension(:,:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: pancake, cigar
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
⟨Interface declaration for func 22⟩
real(kind=default), dimension(size(region,dim=2)) :: eval
real(kind=default), dimension(size(region,dim=2),size(region,dim=2)) :: evec
type(vamp_grid) :: g
integer :: step, last_step, it
it = 1
call vamp_create_grid &
     (g, region, calls(2,1,1), num_div, &
      stratified, quadrupole, covariance = .true., exc = exc)
call vamp_integrate_grid &
     (rng, g, func, prc_index, calls(:,:,1), num_div = num_div, &
      exc = exc, history = history(it:))
⟨Bail out if exception exc raised 98a⟩
it = it + sum (calls(1,:,1))
last_step = size (calls, dim = 3)
do step = 2, last_step - 1
   call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
   call sort (eval, evec)
   call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
   call vamp_delete_grid (g)
   call vamp_create_grid &
        (g, region, calls(2,1,step), num_div, stratified, quadrupole, &
         covariance = .true., map = evec, exc = exc)
   call vamp_integrate_grid &
        (rng, g, func, prc_index, calls(:,:,step), num_div = num_div, &
         exc = exc, history = history(it:))
   ⟨Bail out if exception exc raised 98a⟩
   it = it + sum (calls(1,:,step))
end do
call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
call sort (eval, evec)
call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
call vamp_delete_grid (g)
call vamp_create_grid &
```

```
        (g, region, calls(2,1,last_step), num_div, stratified, quadrupole, &
         covariance = .true., map = evec, exc = exc)
   call vamp_integrate_grid &
        (rng, g, func, prc_index, calls(:,:,last_step), &
         integral, std_dev, avg_chi2, &
         num_div = num_div, exc = exc, history = history(it:))
   call vamp_delete_grid (g)
 end subroutine vamp_integratex_region
```

5.2.10 I/O

142a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
 public :: vamp_write_grid
 private :: write_grid_unit, write_grid_name
 public :: vamp_read_grid
 private :: read_grid_unit, read_grid_name
 public :: vamp_write_grids
 private :: write_grids_unit, write_grids_name
 public :: vamp_read_grids
 private :: read_grids_unit, read_grids_name
```

142b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
 public :: vamp_read_grids_raw
 private :: read_grids_raw_unit, read_grids_raw_name
 public :: vamp_read_grid_raw
 private :: read_grid_raw_unit, read_grid_raw_name
 public :: vamp_write_grids_raw
 private :: write_grids_raw_unit, write_grids_raw_name
 public :: vamp_write_grid_raw
 private :: write_grid_raw_unit, write_grid_raw_name
```

142c ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
 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
```

143a ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
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
```

143b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

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

144a ⟨*Variables in* vamp 78a⟩+≡

```
  character(len=*), parameter, private :: &
       descr_fmt =         "(1x,a)", &
       integer_fmt =       "(1x,a17,1x,i15)", &
       integer_array_fmt = "(1x,i17,1x,i15)", &
       logical_fmt =       "(1x,a17,1x,l1)", &
       double_fmt =        "(1x,a17,1x,e30.22)", &
       double_array_fmt =  "(1x,i17,1x,e30.22)", &
       double_array2_fmt =  "(2(1x,i8),1x,e30.22)"
```

144b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  subroutine read_grid_unit (g, unit, read_integrals)
```

```
type(vamp_grid), intent(inout) :: g
integer, intent(in) :: unit
logical, intent(in), optional :: read_integrals
character(len=*), parameter :: FN = "vamp_read_grid"
character(len=80) :: chdum
integer :: ndim, i, j, idum, jdum
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = integer_fmt) chdum, ndim
⟨Insure that size (g%div) == ndim 146a⟩
call create_array_pointer (g%num_div, ndim)
read (unit = unit, fmt = integer_fmt) chdum, g%num_calls
read (unit = unit, fmt = integer_fmt) chdum, g%calls_per_cell
read (unit = unit, fmt = logical_fmt) chdum, g%stratified
read (unit = unit, fmt = logical_fmt) chdum, g%all_stratified
read (unit = unit, fmt = logical_fmt) chdum, g%quadrupole
read (unit = unit, fmt = double_fmt) chdum, g%mu(1)
read (unit = unit, fmt = double_fmt) chdum, g%mu(2)
read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
read (unit = unit, fmt = double_fmt) chdum, g%calls
read (unit = unit, fmt = double_fmt) chdum, g%dv2g
read (unit = unit, fmt = double_fmt) chdum, g%jacobi
read (unit = unit, fmt = double_fmt) chdum, g%f_min
read (unit = unit, fmt = double_fmt) chdum, g%f_max
read (unit = unit, fmt = double_fmt) chdum, g%mu_gi
read (unit = unit, fmt = double_fmt) chdum, g%sum_mu_gi
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
   read (unit = unit, fmt = integer_array_fmt) idum, g%num_div(i)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
do i = 1, size (g%div)
   call read_division (g%div(i), unit, read_integrals)
end do
read (unit = unit, fmt = descr_fmt) chdum
read (unit = unit, fmt = descr_fmt) chdum
if (chdum == "begin g%map") then
   call create_array_pointer (g%map, (/ ndim, ndim /))
   do i = 1, size (g%div)
      do j = 1, size (g%div)
         read (unit = unit, fmt = double_array2_fmt) idum, jdum, g%map(i,j)
```

```
         end do
      end do
      read (unit = unit, fmt = descr_fmt) chdum
   else
      ⟨Insure that associated (g%map) == .false. 146b⟩
   end if
   read (unit = unit, fmt = descr_fmt) chdum
   if (chdum == "begin g%mu_x") then
      call create_array_pointer (g%mu_x, ndim )
      call create_array_pointer (g%sum_mu_x, ndim)
      call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
      call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
      do i = 1, size (g%div)
         read (unit = unit, fmt = double_array_fmt) idum, jdum, g%mu_x(i)
         read (unit = unit, fmt = double_array_fmt) idum, jdum, g%sum_mu_x(i)
         do j = 1, size (g%div)
            read (unit = unit, fmt = double_array2_fmt) &
                 idum, jdum, g%mu_xx(i,j)
            read (unit = unit, fmt = double_array2_fmt) &
                 idum, jdum, g%sum_mu_xx(i,j)
         end do
      end do
      read (unit = unit, fmt = descr_fmt) chdum
   else
      ⟨Insure that associated (g%mu_x) == .false. 147a⟩
   end if
   read (unit = unit, fmt = descr_fmt) chdum
 end subroutine read_grid_unit
```

146a ⟨*Insure that* size (g%div) == ndim 146a⟩≡

```
 if (associated (g%div)) then
    if (size (g%div) /= ndim) then
       call delete_division (g%div)
       deallocate (g%div)
       allocate (g%div(ndim))
       call create_empty_division (g%div)
    end if
 else
    allocate (g%div(ndim))
    call create_empty_division (g%div)
 end if
```

146b ⟨*Insure that* associated (g%map) == .false. 146b⟩≡

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

```
    end if
```

147a ⟨*Insure that* associated (g%mu_x) == .false. 147a⟩≡

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

147b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
    subroutine write_grid_name (g, name, write_integrals)
      type(vamp_grid), intent(inout) :: g
      character(len=*), intent(in) :: name
      logical, intent(in), optional :: write_integrals
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "write", status = "replace", file = name)
      call write_grid_unit (g, unit, write_integrals)
      close (unit = unit)
    end subroutine write_grid_name
```

147c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
    subroutine read_grid_name (g, name, read_integrals)
      type(vamp_grid), intent(inout) :: g
      character(len=*), intent(in) :: name
      logical, intent(in), optional :: read_integrals
      integer :: unit
      call find_free_unit (unit)
      open (unit = unit, action = "read", status = "old", file = name)
      call read_grid_unit (g, unit, read_integrals)
      close (unit = unit)
    end subroutine read_grid_name
```

147d ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
    subroutine write_grids_unit (g, unit, write_integrals)
      type(vamp_grids), intent(in) :: g
      integer, intent(in) :: unit
      logical, intent(in), optional :: write_integrals
      integer :: i
```

```
    write (unit = unit, fmt = descr_fmt) "begin type(vamp_grids) :: g"
    write (unit = unit, fmt = integer_fmt) "size (g%grids) = ", size (g%grids)
    write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
    write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
    write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
    write (unit = unit, fmt = descr_fmt) "begin g%weights"
    do i = 1, size (g%grids)
       write (unit = unit, fmt = double_array_fmt) i, g%weights(i)
    end do
    write (unit = unit, fmt = descr_fmt) "end g%weights"
    write (unit = unit, fmt = descr_fmt) "begin g%num_calls"
    do i = 1, size (g%grids)
       write (unit = unit, fmt = integer_array_fmt) i, g%num_calls(i)
    end do
    write (unit = unit, fmt = descr_fmt) "end g%num_calls"
    write (unit = unit, fmt = descr_fmt) "begin g%grids"
    do i = 1, size (g%grids)
       call write_grid_unit (g%grids(i), unit, write_integrals)
    end do
    write (unit = unit, fmt = descr_fmt) "end g%grids"
    write (unit = unit, fmt = descr_fmt) "end type(vamp_grids)"
  end subroutine write_grids_unit
```

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

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

```
    read (unit = unit, fmt = double_fmt) chdum, g%sum_integral
    read (unit = unit, fmt = double_fmt) chdum, g%sum_weights
    read (unit = unit, fmt = double_fmt) chdum, g%sum_chi2
    read (unit = unit, fmt = descr_fmt) chdum
    do i = 1, nch
       read (unit = unit, fmt = double_array_fmt) idum, g%weights(i)
    end do
    read (unit = unit, fmt = descr_fmt) chdum
    read (unit = unit, fmt = descr_fmt) chdum
    do i = 1, nch
       read (unit = unit, fmt = integer_array_fmt) idum, g%num_calls(i)
    end do
    read (unit = unit, fmt = descr_fmt) chdum
    read (unit = unit, fmt = descr_fmt) chdum
    do i = 1, nch
       call read_grid_unit (g%grids(i), unit, read_integrals)
    end do
    read (unit = unit, fmt = descr_fmt) chdum
    read (unit = unit, fmt = descr_fmt) chdum
  end subroutine read_grids_unit
```

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

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

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

```
  subroutine read_grids_name (g, name, read_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: read_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "read", status = "old", file = name)
    call read_grids_unit (g, unit, read_integrals)
    close (unit = unit)
  end subroutine read_grids_name
```

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

```
subroutine write_grid_raw_unit (g, unit, write_integrals)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: unit
  logical, intent(in), optional :: write_integrals
  integer :: i, j
  write (unit = unit) MAGIC_GRID_BEGIN
  write (unit = unit) size (g%div)
  write (unit = unit) g%num_calls
  write (unit = unit) g%calls_per_cell
  write (unit = unit) g%stratified
  write (unit = unit) g%all_stratified
  write (unit = unit) g%quadrupole
  write (unit = unit) g%mu(1)
  write (unit = unit) g%mu(2)
  write (unit = unit) g%sum_integral
  write (unit = unit) g%sum_weights
  write (unit = unit) g%sum_chi2
  write (unit = unit) g%calls
  write (unit = unit) g%dv2g
  write (unit = unit) g%jacobi
  write (unit = unit) g%f_min
  write (unit = unit) g%f_max
  write (unit = unit) g%mu_gi
  write (unit = unit) g%sum_mu_gi
  do i = 1, size (g%div)
     write (unit = unit) g%num_div(i)
  end do
  do i = 1, size (g%div)
     call write_division_raw (g%div(i), unit, write_integrals)
  end do
  if (associated (g%map)) then
     write (unit = unit) MAGIC_GRID_MAP
     do i = 1, size (g%div)
        do j = 1, size (g%div)
           write (unit = unit) g%map(i,j)
        end do
     end do
  else
     write (unit = unit) MAGIC_GRID_EMPTY
  end if
  if (associated (g%mu_x)) then
     write (unit = unit) MAGIC_GRID_MU_X
```

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

151a ⟨*Constants in* vamp 151a⟩≡

```
 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
```

151b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 subroutine read_grid_raw_unit (g, unit, read_integrals)
   type(vamp_grid), intent(inout) :: g
   integer, intent(in) :: unit
   logical, intent(in), optional :: read_integrals
   character(len=*), parameter :: FN = "vamp_read_raw_grid"
   integer :: ndim, i, j, magic
   read (unit = unit) magic
   if (magic /= MAGIC_GRID_BEGIN) then
      print *, FN, " fatal: expecting magic ", MAGIC_GRID_BEGIN, &
                   ", found ", magic
      stop
   end if
   read (unit = unit) ndim
   ⟨Insure that size (g%div) == ndim 146a⟩
   call create_array_pointer (g%num_div, ndim)
   read (unit = unit) g%num_calls
   read (unit = unit) g%calls_per_cell
   read (unit = unit) g%stratified
   read (unit = unit) g%all_stratified
   read (unit = unit) g%quadrupole
   read (unit = unit) g%mu(1)
   read (unit = unit) g%mu(2)
```

```
read (unit = unit) g%sum_integral
read (unit = unit) g%sum_weights
read (unit = unit) g%sum_chi2
read (unit = unit) g%calls
read (unit = unit) g%dv2g
read (unit = unit) g%jacobi
read (unit = unit) g%f_min
read (unit = unit) g%f_max
read (unit = unit) g%mu_gi
read (unit = unit) g%sum_mu_gi
do i = 1, size (g%div)
   read (unit = unit) g%num_div(i)
end do
do i = 1, size (g%div)
   call read_division_raw (g%div(i), unit, read_integrals)
end do
read (unit = unit) magic
if (magic == MAGIC_GRID_MAP) then
   call create_array_pointer (g%map, (/ ndim, ndim /))
   do i = 1, size (g%div)
      do j = 1, size (g%div)
         read (unit = unit) g%map(i,j)
      end do
   end do
else if (magic == MAGIC_GRID_EMPTY) then
   ⟨Insure that associated (g%map) == .false. 146b⟩
else
   print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
                " or ", MAGIC_GRID_MAP, ", found ", magic
   stop
end if
read (unit = unit) magic
if (magic == MAGIC_GRID_MU_X) then
   call create_array_pointer (g%mu_x, ndim )
   call create_array_pointer (g%sum_mu_x, ndim)
   call create_array_pointer (g%mu_xx, (/ ndim, ndim /))
   call create_array_pointer (g%sum_mu_xx, (/ ndim, ndim /))
   do i = 1, size (g%div)
      read (unit = unit) g%mu_x(i)
      read (unit = unit) g%sum_mu_x(i)
      do j = 1, size (g%div)
         read (unit = unit) g%mu_xx(i,j)
         read (unit = unit) g%sum_mu_xx(i,j)
```

```
      end do
    end do
  else if (magic == MAGIC_GRID_EMPTY) then
    ⟨Insure that associated (g%mu_x) == .false. 147a⟩
  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
```

153a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

153b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
subroutine read_grid_raw_name (g, name, read_integrals)
  type(vamp_grid), intent(inout) :: g
  character(len=*), intent(in) :: name
  logical, intent(in), optional :: read_integrals
  integer :: unit
  call find_free_unit (unit)
  open (unit = unit, action = "read", status = "old", &
        form = "unformatted",  file = name)
  call read_grid_raw_unit (g, unit, read_integrals)
  close (unit = unit)
end subroutine read_grid_raw_name
```

153c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
subroutine write_grids_raw_unit (g, unit, write_integrals)
```

```
    type(vamp_grids), intent(in) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    integer :: i
    write (unit = unit) MAGIC_GRIDS_BEGIN
    write (unit = unit) size (g%grids)
    write (unit = unit) g%sum_integral
    write (unit = unit) g%sum_weights
    write (unit = unit) g%sum_chi2
    do i = 1, size (g%grids)
       write (unit = unit) g%weights(i)
    end do
    do i = 1, size (g%grids)
       write (unit = unit) g%num_calls(i)
    end do
    do i = 1, size (g%grids)
       call write_grid_raw_unit (g%grids(i), unit, write_integrals)
    end do
    write (unit = unit) MAGIC_GRIDS_END
  end subroutine write_grids_raw_unit
```

154a ⟨*Constants in* vamp 151a⟩+≡

```
  integer, parameter, private :: MAGIC_GRIDS = 33333333
  integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1
  integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2
```

154b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  subroutine read_grids_raw_unit (g, unit, read_integrals)
    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: read_integrals
    character(len=*), parameter :: FN = "vamp_read_grids_raw"
    integer :: i, nch, magic
    read (unit = unit) magic
    if (magic /= MAGIC_GRIDS_BEGIN) then
       print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_BEGIN, &
                    " found ", magic
       stop
    end if
    read (unit = unit) nch
    if (associated (g%grids)) then
       if (size (g%grids) /= nch) then
          call vamp_delete_grid (g%grids)
          deallocate (g%grids, g%weights, g%num_calls)
          allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
```

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

155a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

155b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

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

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

5.2.11 Marshaling

156a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  public :: vamp_marshal_grid_size, vamp_marshal_grid, vamp_unmarshal_grid
```

156b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  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
    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
```

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

```
  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
```

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

```
  pure subroutine vamp_unmarshal_grid (g, ibuf, dbuf)
    type(vamp_grid), intent(inout) :: g
    integer, dimension(:), intent(in) :: ibuf
    real(kind=default), dimension(:), intent(in) :: dbuf
    integer :: i, iwords, dwords, iidx, didx, ndim
    g%num_calls = ibuf(1)
    g%calls_per_cell = ibuf(2)
    ndim = ibuf(3)
    g%stratified = ibuf(4) /= 0
    g%all_stratified = ibuf(5) /= 0
    g%quadrupole = ibuf(6) /= 0
    g%mu = dbuf(1:2)
    g%sum_integral = dbuf(3)
    g%sum_weights = dbuf(4)
    g%sum_chi2 = dbuf(5)
    g%calls = dbuf(6)
    g%dv2g = dbuf(7)
    g%jacobi = dbuf(8)
    g%f_min = dbuf(9)
    g%f_max = dbuf(10)
    g%mu_gi = dbuf(11)
    g%sum_mu_gi = dbuf(12)
```

```
    call copy_array_pointer (g%num_div, ibuf(7:6+ndim))
    ⟨Insure that size (g%div) == ndim 146a⟩
    iidx = 7 + ndim
    didx = 13
    do i = 1, ndim
       iwords = ibuf(iidx)
       dwords = ibuf(iidx+1)
       iidx = iidx + 2
       call unmarshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
                                           dbuf(didx:didx-1+dwords))
       iidx = iidx + iwords
       didx = didx + dwords
    end do
    if (ibuf(iidx) > 0) then
       call copy_array_pointer &
            (g%map, reshape (dbuf(didx:didx-1+ibuf(iidx)), (/ ndim, ndim /)))
       didx = didx + ibuf(iidx)
    else
       ⟨Insure that associated (g%map) == .false. 146b⟩
    end if
    iidx = iidx + 1
    if (ibuf(iidx) > 0) then
       call copy_array_pointer (g%mu_x, dbuf(didx:didx-1+ndim))
       didx = didx + ndim
       call copy_array_pointer (g%sum_mu_x, dbuf(didx:didx-1+ndim))
       didx = didx + ndim
       call copy_array_pointer &
            (g%mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
       didx = didx + ndim**2
       call copy_array_pointer &
            (g%sum_mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
       didx = didx + ndim**2
    else
       ⟨Insure that associated (g%mu_x) == .false. 147a⟩
    end if
    iidx = iidx + 1
  end subroutine vamp_unmarshal_grid
```

159a ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  public :: vamp_marshal_history_size, vamp_marshal_history
  public :: vamp_unmarshal_history
```

159b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_marshal_history (h, ibuf, dbuf)
    type(vamp_history), intent(in) :: h
```

```
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=default), dimension(:), intent(inout) :: dbuf
  integer :: j, ndim, iidx, didx, iwords, dwords
  if (h%verbose .and. (associated (h%div))) then
     ndim = size (h%div)
  else
     ndim = 0
  end if
  ibuf(1) = ndim
  ibuf(2) = h%calls
  if (h%stratified) then
     ibuf(3) = 1
  else
     ibuf(3) = 0
  end if
  dbuf(1) = h%integral
  dbuf(2) = h%std_dev
  dbuf(3) = h%avg_integral
  dbuf(4) = h%avg_std_dev
  dbuf(5) = h%avg_chi2
  dbuf(6) = h%f_min
  dbuf(7) = h%f_max
  iidx = 4
  didx = 8
  do j = 1, ndim
     call marshal_div_history_size (h%div(j), iwords, dwords)
     ibuf(iidx) = iwords
     ibuf(iidx+1) = dwords
     iidx = iidx + 2
     call marshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                                         dbuf(didx:didx-1+dwords))
     iidx = iidx + iwords
     didx = didx + dwords
  end do
end subroutine vamp_marshal_history
```

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

```
pure subroutine vamp_marshal_history_size (h, iwords, dwords)
  type(vamp_history), intent(in) :: h
  integer, intent(out) :: iwords, dwords
  integer :: i, ndim, iw, dw
  if (h%verbose .and. (associated (h%div))) then
     ndim = size (h%div)
  else
```

```
      ndim = 0
    end if
    iwords = 3
    dwords = 7
    do i = 1, ndim
      call marshal_div_history_size (h%div(i), iw, dw)
      iwords = iwords + 2 + iw
      dwords = dwords + dw
    end do
  end subroutine vamp_marshal_history_size
```

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

```
  pure subroutine vamp_unmarshal_history (h, ibuf, dbuf)
    type(vamp_history), intent(inout) :: h
    integer, dimension(:), intent(in) :: ibuf
    real(kind=default), dimension(:), intent(in) :: dbuf
    integer :: j, ndim, iidx, didx, iwords, dwords
    ndim = ibuf(1)
    h%calls = ibuf(2)
    h%stratified = ibuf(3) /= 0
    h%integral = dbuf(1)
    h%std_dev = dbuf(2)
    h%avg_integral = dbuf(3)
    h%avg_std_dev = dbuf(4)
    h%avg_chi2 = dbuf(5)
    h%f_min = dbuf(6)
    h%f_max = dbuf(7)
    if (ndim > 0) then
      if (associated (h%div)) then
        if (size (h%div) /= ndim) then
          deallocate (h%div)
          allocate (h%div(ndim))
        end if
      else
        allocate (h%div(ndim))
      end if
      iidx = 4
      didx = 8
      do j = 1, ndim
        iwords = ibuf(iidx)
        dwords = ibuf(iidx+1)
        iidx = iidx + 2
        call unmarshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                                      dbuf(didx:didx-1+dwords))
```

```
        iidx = iidx + iwords
        didx = didx + dwords
     end do
  end if
end subroutine vamp_unmarshal_history
```

5.2.12 Boring Copying and Deleting of Objects

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

```
elemental subroutine vamp_copy_grid (lhs, rhs)
  type(vamp_grid), intent(inout) :: lhs
  type(vamp_grid), intent(in) :: rhs
  integer :: ndim
  ndim = size (rhs%div)
  lhs%mu = rhs%mu
  lhs%sum_integral = rhs%sum_integral
  lhs%sum_weights = rhs%sum_weights
  lhs%sum_chi2 = rhs%sum_chi2
  lhs%calls = rhs%calls
  lhs%num_calls = rhs%num_calls
  call copy_array_pointer (lhs%num_div, rhs%num_div)
  lhs%dv2g = rhs%dv2g
  lhs%jacobi = rhs%jacobi
  lhs%f_min = rhs%f_min
  lhs%f_max = rhs%f_max
  lhs%mu_gi = rhs%mu_gi
  lhs%sum_mu_gi = rhs%sum_mu_gi
  lhs%calls_per_cell = rhs%calls_per_cell
  lhs%stratified = rhs%stratified
  lhs%all_stratified = rhs%all_stratified
  lhs%quadrupole = rhs%quadrupole
  if (associated (lhs%div)) then
     if (size (lhs%div) /= ndim) then
        call delete_division (lhs%div)
        deallocate (lhs%div)
        allocate (lhs%div(ndim))
     end if
  else
     allocate (lhs%div(ndim))
  end if
  call copy_division (lhs%div, rhs%div)
  if (associated (rhs%map)) then
     call copy_array_pointer (lhs%map, rhs%map)
```

```
    else if (associated (lhs%map)) then
       deallocate (lhs%map)
    end if
    if (associated (rhs%mu_x)) then
       call copy_array_pointer (lhs%mu_x, rhs%mu_x)
       call copy_array_pointer (lhs%mu_xx, rhs%mu_xx)
       call copy_array_pointer (lhs%sum_mu_x, rhs%sum_mu_x)
       call copy_array_pointer (lhs%sum_mu_xx, rhs%sum_mu_xx)
    else if (associated (lhs%mu_x)) then
       deallocate (lhs%mu_x, lhs%mu_xx, lhs%sum_mu_x, lhs%sum_mu_xx)
    end if
  end subroutine vamp_copy_grid
```

163a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  elemental subroutine vamp_delete_grid (g)
    type(vamp_grid), intent(inout) :: g
    if (associated (g%div)) then
       call delete_division (g%div)
       deallocate (g%div, g%num_div)
    end if
    if (associated (g%map)) then
       deallocate (g%map)
    end if
    if (associated (g%mu_x)) then
       deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
    end if
  end subroutine vamp_delete_grid
```

163b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  elemental subroutine vamp_copy_grids (lhs, rhs)
    type(vamp_grids), intent(inout) :: lhs
    type(vamp_grids), intent(in) :: rhs
    integer :: nch
    nch = size (rhs%grids)
    lhs%sum_integral = rhs%sum_integral
    lhs%sum_chi2 = rhs%sum_chi2
    lhs%sum_weights = rhs%sum_weights
    if (associated (lhs%grids)) then
       if (size (lhs%grids) /= nch) then
          deallocate (lhs%grids)
          allocate (lhs%grids(nch))
          call vamp_create_empty_grid (lhs%grids(nch))
       end if
    else
```

```
      allocate (lhs%grids(nch))
      call vamp_create_empty_grid (lhs%grids(nch))
   end if
   call vamp_copy_grid (lhs%grids, rhs%grids)
   call copy_array_pointer (lhs%weights, rhs%weights)
   call copy_array_pointer (lhs%num_calls, rhs%num_calls)
 end subroutine vamp_copy_grids
```

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

```
 elemental subroutine vamp_delete_grids (g)
   type(vamp_grids), intent(inout) :: g
   if (associated (g%grids)) then
      call vamp_delete_grid (g%grids)
      deallocate (g%weights, g%grids, g%num_calls)
   end if
 end subroutine vamp_delete_grids
```

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

```
   elemental subroutine vamp_copy_history (lhs, rhs)
     type(vamp_history), intent(inout) :: lhs
     type(vamp_history), intent(in) :: rhs
     lhs%calls = rhs%calls
     lhs%stratified = rhs%stratified
     lhs%verbose = rhs%verbose
     lhs%integral = rhs%integral
     lhs%std_dev = rhs%std_dev
     lhs%avg_integral = rhs%avg_integral
     lhs%avg_std_dev = rhs%avg_std_dev
     lhs%avg_chi2 = rhs%avg_chi2
     lhs%f_min = rhs%f_min
     lhs%f_max = rhs%f_max
     if (rhs%verbose) then
        if (associated (lhs%div)) then
           if (size (lhs%div) /= size (rhs%div)) then
              deallocate (lhs%div)
              allocate (lhs%div(size(rhs%div)))
           end if
        else
           allocate (lhs%div(size(rhs%div)))
        end if
        call copy_history (lhs%div, rhs%div)
     end if
   end subroutine vamp_copy_history
```

165a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
elemental subroutine vamp_delete_history (h)
  type(vamp_history), intent(inout) :: h
  if (associated (h%div)) then
     deallocate (h%div)
  end if
end subroutine vamp_delete_history
```

5.3 Interface to MPI

The module `vamp` makes no specific assumptions about the hardware and software supporting parallel execution. In this section, we present a specific example of a parallel implementation of multi channel sampling using the message passing paradigm.

The modules `vamp_serial_mpi` and `vamp_parallel_mpi` are not intended to be `used` directly by application programs. For this purpose, the module `vampi` is provided. `vamp_serial_mpi` is identical to `vamp`, but some types, procedures and variables are renamed so that `vamp_parallel_mpi` can redefine them:

165b ⟨vampi.f90 165b⟩≡

```
! vampi.f90 --
⟨Copyleft notice 1⟩
module vamp_serial_mpi
  use vamp, &
       ⟨vamp0_* => vamp_* 166c⟩
       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.

165c ⟨vampi.f90 165b⟩+≡

```
module vamp_parallel_mpi
  use kinds
  use utils
  use tao_random_numbers
  use exceptions
  use mpi90
  use divisions
  use vamp_serial_mpi !NODEP!
  use iso_fortran_env
```

```
    implicit none
    private
    ⟨Declaration of vampi procedures 166b⟩
    ⟨Interfaces of vampi procedures 170d⟩
    ⟨Parameters in vampi 167a⟩
    ⟨Declaration of vampi types 171b⟩
    character(len=*), public, parameter :: VAMPI_RCS_ID = &
         "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    ⟨Implementation of vampi procedures 166d⟩
  end module vamp_parallel_mpi
```

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

166a ⟨vampi.f90 165b⟩+≡

```
  module vampi
    use vamp_serial_mpi !NODEP!
    use vamp_parallel_mpi !NODEP!
    public
  end module vampi
```

5.3.1 Parallel Execution

Single Channel

166b ⟨Declaration of vampi procedures 166b⟩≡

```
  public :: vamp_create_grid
  public :: vamp_discard_integral
  public :: vamp_reshape_grid
  public :: vamp_sample_grid
  public :: vamp_delete_grid
```

166c ⟨vamp0_* => vamp_* 166c⟩≡

```
  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, &
```

166d ⟨Implementation of vampi procedures 166d⟩≡

```
  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
```

167a ⟨*Parameters in* vampi 167a⟩≡

```
  integer, public, parameter :: VAMP_ROOT = 0
```

167b ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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
```

167c ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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.

168 ⟨*Implementation of* `vampi` *procedures* 166d⟩+≡

```
  subroutine vamp_sample_grid &
       (rng, g, func, iterations, integral, std_dev, avg_chi2, accuracy, &
        channel, weights, grids, exc, history)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: iterations
    real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
    real(kind=default), intent(in), optional :: accuracy
    integer, intent(in), optional :: channel
    real(kind=default), dimension(:), intent(in), optional :: weights
    type(vamp_grid), dimension(:), intent(inout), optional :: grids
    type(exception), intent(inout), optional :: exc
    type(vamp_history), dimension(:), intent(inout), optional :: history
    ⟨Interface declaration for func 22⟩
    character(len=*), parameter :: FN = "vamp_sample_grid"
    real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
    type(vamp_grid), dimension(:), allocatable :: gs, gx
    integer, dimension(:,:), pointer :: d
    integer :: iteration, i
    integer :: num_proc, proc_id, num_workers
    nullify (d)
    call mpi90_size (num_proc)
    call mpi90_rank (proc_id)
    iterate: do iteration = 1, iterations
       if (proc_id == VAMP_ROOT) then
          call vamp_distribute_work (num_proc, vamp_rigid_divisions (g), d)
          num_workers = max (1, product (d(2,:)))
       end if
       call mpi90_broadcast (num_workers, VAMP_ROOT)
       if ((present (grids)) .and. (num_workers > 1)) then
          call vamp_broadcast_grid (grids, VAMP_ROOT)
       end if
       if (proc_id == VAMP_ROOT) then
          allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
```

```
      call vamp_create_empty_grid (gs)
      call vamp_fork_grid (g, gs, gx, d, exc)
      do i = 2, num_workers
         call vamp_send_grid (gs(i), i-1, 0)
      end do
   else if (proc_id < num_workers) then
      call vamp_receive_grid (g, VAMP_ROOT, 0)
   end if
   if (proc_id == VAMP_ROOT) then
      if (num_workers > 1) then
         call vamp_sample_grid0 &
              (rng, gs(1), func, channel, weights, grids, exc)
      else
         call vamp_sample_grid0 &
              (rng, g, func, channel, weights, grids, exc)
      end if
   else if (proc_id < num_workers) then
      call vamp_sample_grid0 &
           (rng, g, func, channel, weights, grids, exc)
   end if
   if (proc_id == VAMP_ROOT) then
      do i = 2, num_workers
         call vamp_receive_grid (gs(i), i-1, 0)
      end do
      call vamp_join_grid (g, gs, gx, d, exc)
      call vamp0_delete_grid (gs)
      deallocate (gs, gx)
      call vamp_refine_grid (g)
      call vamp_average_iterations &
           (g, iteration, local_integral, local_std_dev, local_avg_chi2)
      if (present (history)) then
         if (iteration <= size (history)) then
            call vamp_get_history &
                 (history(iteration), g, &
                  local_integral, local_std_dev, local_avg_chi2)
         else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
         end if
         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
```

170a ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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
```

170b ⟨*Declaration of* vampi *procedures* 166b⟩+≡

```
public :: vamp_print_history
private :: vamp_print_one_history, vamp_print_histories
```

170c ⟨vamp0_* => vamp_* 166c⟩+≡

```
vamp0_print_history => vamp_print_history, &
```

170d ⟨*Interfaces of* vampi *procedures* 170d⟩≡

```
interface vamp_print_history
   module procedure vamp_print_one_history, vamp_print_histories
end interface
```

170e ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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
```

171a ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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

171b ⟨*Declaration of* vampi *types* 171b⟩≡

```
  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
```

171c ⟨vamp0_* => vamp_* 166c⟩+≡

```
  vamp0_grids => vamp_grids, &
```

Partially duplicate the API of vamp:

171d ⟨*Declaration of* vampi *procedures* 166b⟩+≡

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

171e ⟨vamp0_* => vamp_* 166c⟩+≡

```
  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

172a ⟨*Implementation of* `vampi` *procedures* 166d⟩+≡

```
  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
```

172b ⟨*Implementation of* `vampi` *procedures* 166d⟩+≡

```
  subroutine vamp_discard_integrals &
       (g, num_calls, num_div, stratified, quadrupole, exc)
    type(vamp_grids), intent(inout) :: g
    integer, intent(in), optional :: num_calls
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole
    type(exception), intent(inout), optional :: exc
    integer :: proc_id
    call mpi90_rank (proc_id)
    if (proc_id == VAMP_ROOT) then
       call vamp0_discard_integrals &
```

```
          (g%g0, num_calls, num_div, stratified, quadrupole, exc)
    end if
  end subroutine vamp_discard_integrals
```

173a ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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
```

173b ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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
```

173c ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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.

173d ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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 175b⟩
   else
      ⟨Distribute each grid among processes 179b⟩
   end if
   ⟨Exit iterate if accuracy has been reached (MPI) 178a⟩
end do iterate
```

⟨*Copy results of* `vamp_sample_grids` *to dummy variables* 177e⟩

```
  end subroutine vamp_sample_grids
```

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

175a ⟨*Parameters in* `vampi` 167a⟩+≡

```
  real(kind=default), private, parameter :: VAMP_MAX_WASTE = 1.0
  ! real(kind=default), private, parameter :: VAMP_MAX_WASTE = 0.3
```

175b ⟨*Distribute complete grids among processes* 175b⟩≡

```
  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) 175d⟩
        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:

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

```
  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 176c⟩
        end if
     end if
  end do
```

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

175d ⟨*Sample* `g%g0%grids(ch)` 175d⟩≡

```
  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
```

176a ⟨*Distribute complete grids among processes* 175b⟩+≡

```
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 177a⟩
      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:

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

```
do ch = 1, nch
   if (g%active(ch) .and. (g%proc(ch) /= VAMP_ROOT)) then
      if (proc_id == VAMP_ROOT) then
         call vamp_send_grid &
              (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
      else if (proc_id == g%proc(ch)) then
         call vamp_receive_grid &
              (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
      end if
   end if
end do
```

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

```
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
```

177a ⟨*Receive the result for channel #*`ch` *at the root* 177a⟩≡

```
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
```

177b ⟨*Declaration of* `vampi` *procedures* 166b⟩+≡

```
private :: object
```

177c ⟨*Implementation of* `vampi` *procedures* 166d⟩+≡

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

177d ⟨*Parameters in* `vampi` 167a⟩+≡

```
integer, public, parameter :: &
     TAG_INTEGRAL = 1, &
     TAG_STD_DEV = 2, &
     TAG_GRID = 3, &
     TAG_HISTORY = 6, &
     TAG_NEXT_FREE = 9
```

177e ⟨*Copy results of* `vamp_sample_grids` *to dummy variables* 177e⟩≡

```
if (present (integral)) then
   call mpi90_broadcast (local_integral, VAMP_ROOT)
   integral = local_integral
end if
if (present (std_dev)) then
   call mpi90_broadcast (local_std_dev, VAMP_ROOT)
   std_dev = local_std_dev
end if
if (present (avg_chi2)) then
   call mpi90_broadcast (local_avg_chi2, VAMP_ROOT)
   avg_chi2 = local_avg_chi2
end if
```

178a ⟨*Exit* iterate *if* accuracy *has been reached (MPI)* 178a⟩≡

```
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.

178b ⟨*Declaration of* vampi *procedures* 166b⟩+≡

```
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.

178c ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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 179a⟩
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:

179a ⟨*Estimate* `waste` *of processor time* 179a⟩≡

```
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!

179b ⟨*Distribute each grid among processes* 179b⟩≡

```
do ch = 1, size (g%g0%grids)
   if (g%active(ch)) then
      call vamp_discard_integral (g%g0%grids(ch))
      if (present (histories)) then
         call vamp_sample_grid &
              (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
               channel = ch, weights = weights, grids = g%g0%grids, &
               history = histories(iteration:iteration,ch))
      else
         call vamp_sample_grid &
              (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
               channel = ch, weights = weights, grids = g%g0%grids)
      end if
   else
      if (proc_id == VAMP_ROOT) then
         call vamp_nullify_variance (g%g0%grids(ch))
         call vamp_nullify_covariance (g%g0%grids(ch))
      end if
   end if
end do
if (proc_id == VAMP_ROOT) then
   call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
   call vamp_average_iterations &
        (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
   if (present (history)) then
      if (iteration <= size (history)) then
         call vamp_get_history &
              (history(iteration), g%g0, local_integral, local_std_dev, &
               local_avg_chi2)
```

```
        else
           call raise_exception (exc, EXC_WARN, FN, "history too short")
        end if
        call vamp_terminate_history (history(iteration+1:))
     end if
  end if
```

5.3.2 Event Generation

This is currently only a syntactical translation …

180a ⟨*Declaration of* vampi *procedures* 166b⟩+≡

```
  public :: vamp_warmup_grid
  public :: vamp_warmup_grids
  public :: vamp_next_event
  private :: vamp_next_event_single, vamp_next_event_multi
```

180b ⟨vamp0_* => vamp_* 166c⟩+≡

```
  vamp0_warmup_grid => vamp_warmup_grid, &
  vamp0_warmup_grids => vamp_warmup_grids, &
  vamp0_next_event => vamp_next_event, &
```

180c ⟨*Interfaces of* vampi *procedures* 170d⟩+≡

```
  interface vamp_next_event
     module procedure vamp_next_event_single, vamp_next_event_multi
  end interface
```

180d ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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
```

181a ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

181b ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

181c ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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

182a ⟨*Declaration of* vampi *procedures* 166b⟩+≡
```
public :: vamp_write_grid, vamp_read_grid
private :: write_grid_unit, write_grid_name
private :: read_grid_unit, read_grid_name
```

182b ⟨vamp0_* => vamp_* 166c⟩+≡
```
vamp0_write_grid => vamp_write_grid, &
vamp0_read_grid => vamp_read_grid, &
```

182c ⟨*Interfaces of* vampi *procedures* 170d⟩+≡
```
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
```

182d ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

182e ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

183a ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

183b ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
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
```

183c ⟨*Declaration of* vampi *procedures* 166b⟩+≡
```
public :: vamp_write_grids, vamp_read_grids
private :: write_grids_unit, write_grids_name
private :: read_grids_unit, read_grids_name
```

183d ⟨vamp0_* => vamp_* 166c⟩+≡
```
vamp0_write_grids => vamp_write_grids, &
vamp0_read_grids => vamp_read_grids, &
```

183e ⟨*Interfaces of* vampi *procedures* 170d⟩+≡
```
  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
```

183f ⟨*Implementation of* vampi *procedures* 166d⟩+≡
```
  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
```

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

```
  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
```

184b ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
  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
```

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

```
  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

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

```
  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`:

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

```
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
```

185b ⟨*Implementation of* `vampi` *procedures* 166d⟩+≡

```
subroutine vamp_receive_grid (g, source, tag, domain, status, error)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: source, tag
  integer, intent(in), optional :: domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call mpi90_receive (words, source, tag, domain, status, error)
  allocate (ibuf(words(1)), dbuf(words(2)))
  call mpi90_receive (ibuf, source, tag+1, domain, status, error)
  call mpi90_receive (dbuf, source, tag+2, domain, status, error)
  call vamp_unmarshal_grid (g, ibuf, dbuf)
  deallocate (ibuf, dbuf)
```

```
end subroutine vamp_receive_grid
```

Caveat: the real `vamp_send_grid` uses *two* tags: `tag` and `tag+1`:

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

```
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 . . .

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

```
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.

187a ⟨*Interfaces of* vampi *procedures* 170d⟩+≡
```
interface vamp_broadcast_grid
   module procedure &
        vamp_broadcast_one_grid, vamp_broadcast_many_grids
end interface
```

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

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

188a ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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
```

188b ⟨*Declaration of* vampi *procedures* 166b⟩+≡

```
public :: vamp_send_history
public :: vamp_receive_history
```

188c ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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
```

189 ⟨*Implementation of* vampi *procedures* 166d⟩+≡

```
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 reselt and error estimate.

6.1.1 Serial Test

190a ⟨vamp_test.f90 190a⟩≡

```
! vamp_test.f90 --
⟨Copyleft notice 1⟩
⟨Module vamp_test_functions 190b⟩
⟨Module vamp_tests 194b⟩
```

190b ⟨*Module* vamp_test_functions 190b⟩≡

```
module vamp_test_functions
  use kinds
  use constants, only: PI
  use coordinates
  use vamp, only: vamp_grid, vamp_multi_channel
  implicit none
  private
  public :: f, j, phi, ihp, w
  public :: lorentzian
  private :: lorentzian_normalized
  real(kind=default), public :: width
contains
  ⟨Implementation of vamp_test_functions procedures 191a⟩
end module vamp_test_functions
```

$$\int_{x_1}^{x_2} \mathrm{d}x \, \frac{1}{(x-x_0)^2+a^2} = \frac{1}{a}\left(\operatorname{atan}\left(\frac{x_2-x_0}{a}\right) - \operatorname{atan}\left(\frac{x_1-x_0}{a}\right)\right) = N(x_0,x_1,x_2,a) \tag{6.1}$$

191a ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩≡

```
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
```

$$\int \mathrm{d}^n x \, f(x) = \int \mathrm{d}\Omega_n \, r^{n-1} \mathrm{d}r \, f(x) = 1 \tag{6.2}$$

191b ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩+≡

```
pure function lorentzian (x, x0, x1, x2, r0, a) result (f)
  real(kind=default), dimension(:), intent(in) :: x, x0, x1, x2
  real(kind=default), intent(in) :: r0, a
  real(kind=default) :: f
  real(kind=default) :: r, r1, r2
  integer :: n
  n = size (x)
  if (n > 1) then
     r = sqrt (dot_product (x-x0, x-x0))
     r1 = 0.4_default
     r2 = min (minval (x2-x0), minval (x0-x1))
     if (r1 <= r .and. r <= r2) then
        f = lorentzian_normalized (r, r0, r1, r2, a) * r**(1-n) / surface (n)
     else
        f = 0
     end if
  else
     f = lorentzian_normalized (x(1), x0(1), x1(1), x2(1), a)
  endif
end function lorentzian
```

191c ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩+≡

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

```
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: f_x
    real(kind=default), dimension(size(x)) :: minus_one, plus_one, zero, w_i, f_i
    integer :: n, i
    n = size(x)
    minus_one = -1
    zero = 0
    plus_one = 1
    w_i = 1
    do i = 1, n
       if (all (abs (x(i+1:)) <= 1)) then
          f_i = lorentzian (x(1:i), zero(1:i), minus_one(1:i), plus_one(1:i), &
                            0.7_default, width) &
               / 2.0_default**(n-i)
       else
          f_i = 0
       end if
    end do
    f_x = dot_product (w_i, f_i) / sum (w_i)
  end function f
```

192 ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩+≡

```
  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
```

193a ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩+≡

```
  pure function ihp (x, channel) result (xi)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: channel
    real(kind=default), dimension(size(x)) :: xi
    real(kind=default) :: r, phi
    integer :: n
    n = size(x)
    if (channel == 1) then
       xi = x
    else if (channel == 2) then
       call cartesian_to_spherical_cos (x(1:2), r, phi)
       xi(1) = 2 * r / sqrt (2.0_default) - 1
       xi(2) = phi / PI
       xi(3:) = x(3:)
    else if (channel < n) then
       call cartesian_to_spherical_cos (x(1:channel), r, phi, xi(3:channel))
       xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
       xi(2) = phi / PI
       xi(channel+1:) = x(channel+1:)
    else if (channel == n) then
       call cartesian_to_spherical_cos (x, r, phi, xi(3:))
       xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
       xi(2) = phi / PI
    else
       xi = 0
    end if
  end function ihp
```

193b ⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩+≡

```
  pure function j (x, prc_index, channel) result (j_x)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: prc_index
    integer, intent(in) :: channel
    real(kind=default) :: j_x
    if (channel == 1) then
       j_x = 1
    else if (channel > 1) then
       j_x = 2 / sqrt (real (channel, kind=default)) ! 1/|dr/dξ_1|
       j_x = j_x / PI                                ! 1/|dφ/dξ_2|
```

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

194a ⟨*Implementation of* vamp_test_functions *procedures* 191a⟩+≡

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

194b ⟨*Module* vamp_tests 194b⟩≡

```
module vamp_tests
  use kinds
  use exceptions
  use histograms
  use tao_random_numbers
  use coordinates
  use vamp
  use vamp_test_functions !NODEP!
  implicit none
  private
  ⟨Declaration of procedures in vamp_tests 194c⟩
contains
  ⟨Implementation of procedures in vamp_tests 195a⟩
end module vamp_tests
```

Verification

194c ⟨*Declaration of procedures in* vamp_tests 194c⟩≡

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

194d ⟨*Implementation of procedures in* vamp_tests *(broken?)* 194d⟩≡

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

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

195a ⟨*Implementation of procedures in* `vamp_tests` 195a⟩≡

```
  subroutine check_inverses (rng, region, weights, samples)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
    real(kind=default), dimension(:), intent(in) :: weights
    integer, intent(in) :: samples
    real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx
    real(kind=default) :: dx, dx_max
    integer :: ch, i
    dx_max = 0
    x_dx = 0
    do ch = 1, size(weights)
       do i = 1, samples
          call tao_random_number (rng, x1)
          x2 = ihp (phi (x1, ch), ch)
          dx = sqrt (dot_product (x1-x2, x1-x2))
          if (dx > dx_max) then
             dx_max = dx
             x_dx = x1
          end if
       end do
       print *, "channel", ch, ": |x-x|=", real(dx), ", @x=", real (x_dx)
    end do
  end subroutine check_inverses
```

195b ⟨*Implementation of procedures in* `vamp_tests` 195a⟩+≡

```
  subroutine check_inverses3 (rng, region, samples)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, intent(in) :: samples
    real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx, x_dj
    real(kind=default) :: r, phi, jac, caj, dx, dx_max, dj, dj_max
    real(kind=default), dimension(size(x1)-2) :: cos_theta
    integer :: i
    dx_max = 0
```

```
    x_dx = 0
    dj_max = 0
    x_dj = 0
    do i = 1, samples
       call tao_random_number (rng, x1)
       call cartesian_to_spherical_cos_2 (x1, r, phi, cos_theta, jac)
       call spherical_cos_to_cartesian_2 (r, phi, cos_theta, x2, caj)
       dx = sqrt (dot_product (x1-x2, x1-x2))
       dj = jac*caj - 1
       if (dx > dx_max) then
          dx_max = dx
          x_dx = x1
       end if
       if (dj > dj_max) then
          dj_max = dj
          x_dj = x1
       end if
    end do
    print *, "channel 3 : j*j-1=", real(dj), ", @x=", real (x_dj)
    print *, "channel 3 : |x-x|=", real(dx), ", @x=", real (x_dx)
  end subroutine check_inverses3
```

Integration

196a ⟨*Declaration of procedures in* `vamp_tests` 194c⟩+≡

```
  public :: single_channel, multi_channel
```

196b ⟨*Implementation of procedures in* `vamp_tests` 195a⟩+≡

```
  subroutine single_channel (rng, region, samples, iterations, &
       integral, standard_dev, chi_squared)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: samples, iterations
    real(kind=default), intent(out) :: integral, standard_dev, chi_squared
    type(vamp_grid) :: gr
    type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
    integer, parameter :: PRC_INDEX = 1
    call vamp_create_history (history)
    call vamp_create_grid (gr, region, samples(1))
    call vamp_sample_grid (rng, gr, f, PRC_INDEX, iterations(1), history = history)
    call vamp_discard_integral (gr, samples(2))
    call vamp_sample_grid &
         (rng, gr, f, PRC_INDEX, iterations(2), &
          integral, standard_dev, chi_squared, &
```

```
        history = history(iterations(1)+1:))
  call vamp_write_grid (gr, "vamp_test.grid")
  call vamp_delete_grid (gr)
  call vamp_print_history (history, "single")
  call vamp_delete_history (history)
end subroutine single_channel
```

197a ⟨*Implementation of procedures in* `vamp_tests` 195a⟩+≡

```
subroutine multi_channel (rng, region, weights, samples, iterations, powers, &
     integral, standard_dev, chi_squared)
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), dimension(:,:), intent(in) :: region
  real(kind=default), dimension(:), intent(inout) :: weights
  integer, dimension(:), intent(in) :: samples, iterations
  real(kind=default), dimension(:), intent(in) :: powers
  real(kind=default), intent(out) :: integral, standard_dev, chi_squared
  type(vamp_grids) :: grs
  ⟨Body of multi_channel 197b⟩
end subroutine multi_channel
```

197b ⟨*Body of* `multi_channel` 197b⟩≡

```
type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
     history
type(vamp_history), dimension(size(history),size(weights)) :: histories
integer :: it, nit
integer, parameter :: PRC_INDEX = 1
nit = size (powers)
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weights)
call vamp_sample_grids (rng, grs, w, PRC_INDEX, iterations(1) - 1, &
                        history = history, histories = histories)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
do it = 1, nit
   call vamp_sample_grids (rng, grs, w, PRC_INDEX, 1, &
                           history = history(iterations(1)+it-1:), &
                           histories = histories(iterations(1)+it-1:,:))
   call vamp_print_history (history(iterations(1)+it-1:), "multi")
   call vamp_print_history (histories(iterations(1)+it-1:,:), "multi")
   call vamp_refine_weights (grs, powers(it))
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
     (rng, grs, w, PRC_INDEX, iterations(2), &
```

```
      integral, standard_dev, chi_squared, &
      history = history(iterations(1)+nit:), &
      histories = histories(iterations(1)+nit:,:))
call vamp_print_history (history(iterations(1)+nit:), "multi")
call vamp_print_history (histories(iterations(1)+nit:,:), "multi")
call vamp_write_grids (grs, "vamp_test.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
```

Input/Output

198a ⟨*Declaration of procedures in* vamp_tests 194c⟩+≡

```
public :: print_results
```

198b ⟨*Implementation of procedures in* vamp_tests 195a⟩+≡

```
subroutine print_results (prefix, prev_ticks, &
     integral, std_dev, chi2, acceptable, failures)
  character(len=*), intent(in) :: prefix
  integer, intent(in) :: prev_ticks
  real(kind=default), intent(in) :: integral, std_dev, chi2, acceptable
  integer, intent(inout) :: failures
  integer :: ticks, ticks_per_second
  real(kind=default) :: pull
  call system_clock (ticks, ticks_per_second)
  pull = (integral - 1) / std_dev
  print "(1X,A,A,F6.2,A)", prefix, &
       ": time = ", real (ticks - prev_ticks) / ticks_per_second, " secs"
  print *, prefix, ":    int, err, chi2: ", &
       real (integral), real (std_dev), real (chi2)
  if (abs (pull) > acceptable) then
     failures = failures + 1
     print *, prefix, ": inacceptable pull:", real (pull)
  else
     print *, prefix, ":   acceptable pull:", real (pull)
  end if
end subroutine print_results
```

Main Program

198c ⟨vamp_test.f90 190a⟩+≡

```
program vamp_test
```

```
use kinds
use tao_random_numbers
use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp
use vamp_test_functions !NODEP!
use vamp_tests !NODEP!
implicit none
integer :: start_ticks
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
failures = 0
call tao_random_create (rng, 0)
call system_clock (start_ticks)
call tao_random_seed (rng, start_ticks)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
region(1,:)  = -1.0
region(2,:)  =  1.0
width = 0.0001
print *, "Starting VAMP 1.0 self test..."
print *, "serial code"
print *, VAMP_RCS_ID
print *, DIVISIONS_RCS_ID
call system_clock (start_ticks)
call single_channel (rng, region, samples, iterations, &
        single_integral, single_standard_dev, single_chi_squared)
call print_results ("SINGLE", start_ticks, &
        single_integral, single_standard_dev, single_chi_squared, &
        10*ACCEPTABLE, failures)
weight_vector = 1
powers = 0.25_default
call system_clock (start_ticks)
call multi_channel (rng, region, weight_vector, samples, iterations, &
        powers, multi_integral, multi_standard_dev, multi_chi_squared)
call print_results ("MULTI", start_ticks, &
```

```
              multi_integral, multi_standard_dev, multi_chi_squared, &
             ACCEPTABLE, failures)
  call system_clock (start_ticks)
! call check_jacobians (rng, region, weight_vector, samples(1))
  call check_inverses (rng, region, weight_vector, samples(1))
  call check_inverses3 (rng, region, samples(1))
  if (failures == 0) then
     stop 0
  else if (failures == 1) then
     stop 1
  else
     stop 2
  end if
end program vamp_test
```

6.1.2 Parallel Test

200a ⟨vampi_test.f90 200a⟩≡
```
! vampi_test.f90 --
⟨Copyleft notice 1⟩
⟨Module vamp_test_functions 190b⟩
```

The following is identical to `vamp_tests`, except for `use vampi`:

200b ⟨vampi_test.f90 200a⟩+≡
```
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 194c⟩
contains
  ⟨Implementation of procedures in vamp_tests 195a⟩
end module vampi_tests
```

200c ⟨vampi_test.f90 200a⟩+≡
```
program vampi_test
  use kinds
  use tao_random_numbers
  use coordinates
```

```
use divisions, only: DIVISIONS_RCS_ID
use vamp, only: VAMP_RCS_ID
use vampi
use mpi90
use vamp_test_functions !NODEP!
use vampi_tests !NODEP!
implicit none
integer :: num_proc, proc_id, start_ticks
logical :: perform_io
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
integer :: iostat, command
character(len=72) :: command_line
integer, parameter :: &
     CMD_ERROR = -1, CMD_END = 0, &
     CMD_NOP = 1, CMD_SINGLE = 2, CMD_MULTI = 3, CMD_CHECK = 4
call tao_random_create (rng, 0)
call mpi90_init ()
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
perform_io = (proc_id == 0)
call system_clock (start_ticks)
call tao_random_seed (rng, start_ticks + proc_id)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
samples = (/ 200000, 2000000 /)
region(1,:)  = -1.0
region(2,:)  =  1.0
width = 0.0001
if (perform_io) then
   print *, "Starting VAMP 1.0 self test..."
   if (num_proc > 1) then
      print *, "parallel code running on ", num_proc, " processors"
   else
      print *, "parallel code running serially"
   end if
   print *, VAMP_RCS_ID
   print *, VAMPI_RCS_ID
```

```
      print *, DIVISIONS_RCS_ID
   end if
   command_loop: do
      ⟨Parse the commandline in vamp_test and set command (never defined)⟩
      call mpi90_broadcast (command, 0)
      call system_clock (start_ticks)
      select case (command)
      ⟨Execute command in vamp_test (never defined)⟩
      case (CMD_END)
         exit command_loop
      case (CMD_NOP)
         ! do nothing
      case (CMD_ERROR)
         ! do nothing
      end select
   end do command_loop
   call mpi90_finalize ()
 end program vampi_test
```

6.1.3 Output

202a ⟨vamp_test.out 202a⟩≡

6.2 Mapped Mode

In this chapter we 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

202b ⟨vamp_test0.f90 202b⟩≡

```
 ! vamp_test0.f90 --
 ⟨Copyleft notice 1⟩
 ⟨Module vamp_test0_functions 203⟩
```

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

203 ⟨*Module* `vamp_test0_functions` 203⟩≡

```
module vamp_test0_functions
  use kinds
  use vamp, only: vamp_grid, vamp_multi_channel0
  implicit none
  private
  public :: f, g, phi, w
  public :: create_sample, delete_sample
  private :: f0, psi, g0, f_norm
  real(kind=default), dimension(:), allocatable, private :: c, x_min, x_max
  real(kind=default), dimension(:,:,:), allocatable, public :: x0, gamma
contains
  ⟨Implementation of vamp_test0_functions procedures 204a⟩
end module vamp_test0_functions
```

We start from a model of n_p interfering resonances in one variable (cf. section **??**)

$$f_0(x|x_{\min},x_{\max},x_0,\gamma) = \frac{1}{N(x_{\min},x_{\max},x_0,\gamma)} \left|\sum_{p=1}^{n_p} \frac{1}{x-x_{0,p}+i\gamma_p}\right|^2 \tag{6.3}$$

where

$$N(x_{\min},x_{\max},x_0,\gamma) = \int_{x_{\min}}^{x_{\max}} \mathrm{d}x \left|\sum_{p=1}^{n_p} \frac{1}{x-x_{0,p}+i\gamma_p}\right|^2 \tag{6.4}$$

such that

$$\int_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_0(x|x_{\min},x_{\max},x_0,\gamma) = 1 \tag{6.5}$$

NB: the $N(x_{\min},x_{\max},x_0,\gamma)$ should be calculated once and tabulated to save processing time, but we are lazy here.

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

204a ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩≡

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

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

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

204b ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
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.

205a ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
pure function f (x, prc_index, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: prc_index
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: f_x
  real(kind=default) :: fi_x
  integer :: i, j
  f_x = 0.0
  do i = 1, size (c)
     fi_x = 1.0
     do j = 1, size (x)
        if (all (gamma(:,i,j) > 0)) then
           fi_x = fi_x * f0 (x(j), x_min(j), x_max(j), &
                             x0(:,i,j), gamma(:,i,j))
        else
           fi_x = fi_x / (x_max(j) - x_min(j))
        end if
     end do
     f_x = f_x + c(i) * fi_x
  end do
  f_x = f_x / sum (c)
end function f
```

205b ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

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

205c ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
subroutine create_sample (num_poles, weights, region)
  integer, intent(in) :: num_poles
  real(kind=default), dimension(:), intent(in) :: weights
```

```
    real(kind=default), dimension(:,:), intent(in) :: region
    integer :: nd, nc
    nd = size (region, dim=2)
    nc = size (weights)
    allocate (c(nc), x_min(nd), x_max(nd))
    allocate (x0(num_poles,nc,nd), gamma(num_poles,nc,nd))
    x_min = region(1,:)
    x_max = region(2,:)
    c = weights
  end subroutine create_sample
```

Multi Channel

We start from the usual mapping for Lorentzian peaks

$$\begin{aligned} \psi(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\to [x_{\min}, x_{\max}] \\ \xi \mapsto x &= \psi(\xi | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \tag{6.9}$$

where

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

206 ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
  pure function psi (xi, x_min, x_max, x0, gamma) result (x)
    real(kind=default), intent(in) :: xi, x_min, x_max, x0, gamma
    real(kind=default) :: x
    x = x0 + gamma &
         * tan (((xi - x_min) * atan ((x_max - x0) / gamma) &
                    - (x_max - xi) * atan ((x0 - x_min) / gamma)) &
                 / (x_max - x_min))
  end function psi
```

The inverse mapping is

$$\begin{aligned} \psi^{-1}(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\to [x_{\min}, x_{\max}] \\ x \mapsto \xi &= \psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \tag{6.11}$$

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

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

207a ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
pure function g0 (x, x_min, x_max, x0, gamma) result (g_x)
  real(kind=default), intent(in) :: x, x_min, x_max, x0, gamma
  real(kind=default) :: g_x
  g_x = gamma / (atan ((x_max - x0) / gamma) - atan ((x_min - x0) / gamma)) &
         * (x_max - x_min) / ((x - x0)**2 + gamma**2)
end function g0
```

The function f has $n_c n_p^{n_d}$ peaks and we need a channel for each one, plus a constant function for the background. We encode the position on the grid linearly:

207b ⟨*Decode* `channel` *into* `ch` *and* `p(:)` 207b⟩≡

```
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:

207c ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
pure function phi (xi, channel) result (x)
  real(kind=default), dimension(:), intent(in) :: xi
  integer, intent(in) :: channel
  real(kind=default), dimension(size(xi)) :: x
  integer, dimension(size(xi)) :: p
  integer :: j, ch, np, nch, nd, channels
  np = size (x0, dim = 1)
  nch = size (x0, dim = 2)
  nd = size (x0, dim = 3)
  channels = nch * np**nd
  if (channel >= 1 .and. channel <= channels) then
     ⟨Decode channel into ch and p(:) 207b⟩
     do j = 1, size (xi)
        if (all (gamma(:,ch,j) > 0)) then
           x(j) = psi (xi(j), x_min(j), x_max(j), &
                       x0(p(j),ch,j), gamma(p(j),ch,j))
        else
           x = xi
```

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

similarly for the Jacobians:

208a ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

```
pure recursive function g (x, prc_index, channel) result (g_x)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: prc_index
  integer, intent(in) :: channel
  real(kind=default) :: g_x
  integer, dimension(size(x)) :: p
  integer :: j, ch, np, nch, nd, channels
  np = size (x0, dim = 1)
  nch = size (x0, dim = 2)
  nd = size (x0, dim = 3)
  channels = nch * np**nd
  if (channel >= 1 .and. channel <= channels) then
     ⟨Decode channel into ch and p(:) 207b⟩
     g_x = 1.0
     do j = 1, size (x)
        if (all (gamma(:,ch,j) > 0)) then
           g_x = g_x * g0 (x(j), x_min(j), x_max(j), &
                           x0(p(j),ch,j), gamma(p(j),ch,j))
        end if
     end do
  else if (channel == channels + 1) then
     g_x = 1.0
  else
     g_x = 0
  end if
end function g
```

208b ⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩+≡

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

```
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    w_x = vamp_multi_channel0 (f, prc_index, phi, g, x, weights, channel)
  end function w
```

Driver Routines

209a ⟨vamp_test0.f90 202b⟩+≡

```
  module vamp_tests0
    ⟨Modules used by vamp_tests0 209b⟩
    use vamp
    implicit none
    private
    ⟨Declaration of procedures in vamp_tests0 210a⟩
  contains
    ⟨Implementation of procedures in vamp_tests0 210b⟩
  end module vamp_tests0
```

209b ⟨*Modules used by* vamp_tests0 209b⟩≡

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

Verification

209c ⟨*Declaration of procedures in* vamp_tests0 *(broken?)* 209c⟩≡

```
  public :: check_jacobians
```

209d ⟨*Implementation of procedures in* vamp_tests0 *(broken?)* 209d⟩≡

```
  subroutine check_jacobians (do_print, region, samples, rng)
    logical, intent(in) :: do_print
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: samples
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(size(region,dim=2)) :: x
    real(kind=default) :: d
    integer :: ch
    do ch = 1, size(x0,dim=2) * size(x0,dim=1)**size(x0,dim=3) + 1
       call vamp_check_jacobian (rng, samples(1), g, phi, ch, region, d, x)
       if (do_print) then
          print *, ch, ": ", d, ", x = ", real (x)
       end if
```

```
    end do
  end subroutine check_jacobians
```

Integration

210a ⟨*Declaration of procedures in* vamp_tests0 210a⟩≡

```
  public :: single_channel, multi_channel
```

210b ⟨*Implementation of procedures in* vamp_tests0 210b⟩≡

```
  subroutine single_channel (do_print, region, iterations, samples, rng, &
       acceptable, failures)
    logical, intent(in) :: do_print
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: iterations, samples
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), intent(in) :: acceptable
    integer, intent(inout) :: failures
    type(vamp_grid) :: gr
    type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
    real(kind=default) :: integral, standard_dev, chi_squared, pull
    integer, parameter :: PRC_INDEX = 1
    call vamp_create_history (history)
    call vamp_create_grid (gr, region, samples(1))
    call vamp_sample_grid (rng, gr, f, PRC_INDEX, iterations(1), history = history)
    call vamp_discard_integral (gr, samples(2))
    call vamp_sample_grid &
         (rng, gr, f, PRC_INDEX, iterations(2), &
          integral, standard_dev, chi_squared, &
          history = history(iterations(1)+1:))
    call vamp_write_grid (gr, "vamp_test0.grid")
    call vamp_delete_grid (gr)
    call vamp_print_history (history, "single")
    call vamp_delete_history (history)
    pull = (integral - 1) / standard_dev
    if (do_print) then
       print *, "    int, err, chi2:", integral, standard_dev, chi_squared
    end if
    if (abs (pull) > acceptable) then
       failures = failures + 1
       print *, " unacceptable pull:", pull
    else
       print *, "   acceptable pull:", pull
    end if
  end subroutine single_channel
```

211a ⟨*Implementation of procedures in* vamp_tests0 210b⟩+≡
```
subroutine multi_channel (do_print, region, iterations, samples, rng, &
     acceptable, failures)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:,:), intent(in) :: region
  integer, dimension(:), intent(in) :: iterations, samples
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), intent(in) :: acceptable
  type(vamp_grids) :: grs
  integer, intent(inout) :: failures
  ⟨Body of multi_channel 197b⟩
end subroutine multi_channel
```

211b ⟨*Body of* multi_channel 197b⟩+≡
```
real(kind=default), &
     dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
     weight_vector
type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
real(kind=default) :: integral, standard_dev, chi_squared, pull
integer :: it
integer, parameter :: PRC_INDEX = 1
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, PRC_INDEX, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
   call vamp_sample_grids (rng, grs, w, PRC_INDEX, 1, &
                           history = history(iterations(1)+it-1:), &
                           histories = histories(iterations(1)+it-1:,:))
   call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
     (rng, grs, w, PRC_INDEX, iterations(2), &
      integral, standard_dev, chi_squared, &
      history = history(iterations(1)+5:), &
      histories = histories(iterations(1)+5:,:))
call vamp_write_grids (grs, "vamp_test0.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
```

```
call vamp_delete_history (history)
call vamp_delete_history (histories)
if (do_print) then
   print *, integral, standard_dev, chi_squared
end if
pull = (integral - 1) / standard_dev
if (abs (pull) > acceptable) then
   failures = failures + 1
   print *, " unacceptable pull:", pull
else
   print *, "   acceptable pull:", pull
end if
```

Event Generation

212a ⟨*Declaration of procedures in* `vamp_tests0` 210a⟩+≡

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

212b ⟨*Implementation of procedures in* `vamp_tests0` 210b⟩+≡

```
subroutine single_channel_generator (do_print, region, iterations, samples, rng)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:,:), intent(in) :: region
  integer, dimension(:), intent(in) :: iterations, samples
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid) :: gr
  type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
  type(histogram) :: unweighted, reweighted, weighted, weights
  type(exception) :: exc
  real(kind=default) :: weight, integral, standard_dev
  integer :: i
  real(kind=default), dimension(size(region,dim=2)) :: x
  integer, parameter :: PRC_INDEX = 1
  call vamp_create_grid (gr, region, samples(1))
  call vamp_sample_grid (rng, gr, f, PRC_INDEX, iterations(1), history = history)
  call vamp_discard_integral (gr, samples(2))
  call vamp_warmup_grid &
       (rng, gr, f, PRC_INDEX, iterations(2), history = history(iterations(1)+1:))
  call vamp_print_history (history, "single")
  call vamp_delete_history (history)
  call create_histogram (unweighted, region(1,1), region(2,1), 100)
  call create_histogram (reweighted, region(1,1), region(2,1), 100)
  call create_histogram (weighted, region(1,1), region(2,1), 100)
  call create_histogram (weights, 0.0_default, 10.0_default, 100)
  ! do i = 1, 1000000
```

```
  do i = 1, 100
     call clear_exception (exc)
     call vamp_next_event (x, rng, gr, f, PRC_INDEX, exc = exc)
     call handle_exception (exc)
     call fill_histogram (unweighted, x(1))
     call fill_histogram (reweighted, x(1), 1.0_default / f (x, PRC_INDEX))
  end do
  integral = 0.0
  standard_dev = 0.0
  do i = 1, 10000
     call clear_exception (exc)
     call vamp_next_event (x, rng, gr, f, PRC_INDEX, weight, exc = exc)
     call handle_exception (exc)
     call fill_histogram (weighted, x(1), weight / f (x, PRC_INDEX))
     call fill_histogram (weights, x(1), weight)
     integral = integral + weight
     standard_dev = standard_dev + weight**2
  end do
  if (do_print) then
     print *, integral / (i-1), sqrt (standard_dev) / (i-1)
     call write_histogram (unweighted, "u_s.d")
     call write_histogram (reweighted, "r_s.d")
     call write_histogram (weighted, "w_s.d")
     call write_histogram (weights, "ws_s.d")
  end if
  call delete_histogram (unweighted)
  call delete_histogram (reweighted)
  call delete_histogram (weighted)
  call delete_histogram (weights)
  call vamp_delete_grid (gr)
end subroutine single_channel_generator
```

213 ⟨*Implementation of procedures in* vamp_tests0 210b⟩+≡

```
subroutine multi_channel_generator (do_print, region, iterations, samples, rng)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:,:), intent(in) :: region
  integer, dimension(:), intent(in) :: iterations, samples
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grids) :: grs
  real(kind=default), &
       dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
       weight_vector
  type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
  type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
```

```
type(histogram) :: unweighted, reweighted, weighted, weights
type(exception) :: exc
real(kind=default) :: weight, integral, standard_dev
real(kind=default), dimension(size(region,dim=2)) :: x
character(len=5) :: pfx
integer :: it, i, j
integer, parameter :: PRC_INDEX = 1
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, PRC_INDEX, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
   call vamp_sample_grids (rng, grs, w, PRC_INDEX, 1, &
                           history = history(iterations(1)+it-1:), &
                           histories = histories(iterations(1)+it-1:,:))
   call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_warmup_grids &
     (rng, grs, w, PRC_INDEX, iterations(2), &
      history = history(iterations(1)+5:), &
      histories = histories(iterations(1)+5:,:))
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
!!! do i = 1, size (grs%grids)
!!!    do j = 1, size (grs%grids(i)%div)
!!!       write (pfx, "(I2.2,'/',I2.2)") i, j
!!!       call dump_division (grs%grids(i)%div(j), pfx)
!!!    end do
!!! end do
call create_histogram (unweighted, region(1,1), region(2,1), 100)
call create_histogram (reweighted, region(1,1), region(2,1), 100)
call create_histogram (weighted, region(1,1), region(2,1), 100)
call create_histogram (weights, 0.0_default, 10.0_default, 100)
! do i = 1, 1000000
do i = 1, 100
   call clear_exception (exc)
   call vamp_next_event (x, rng, grs, f, PRC_INDEX, phi, exc = exc)
   call handle_exception (exc)
```

```
      call fill_histogram (unweighted, x(1))
      call fill_histogram (reweighted, x(1), 1.0_default / f (x, PRC_INDEX))
   end do
   integral = 0.0
   standard_dev = 0.0
   do i = 1, 10000
      call clear_exception (exc)
      call vamp_next_event (x, rng, grs, f, PRC_INDEX, phi, weight, exc = exc)
      call handle_exception (exc)
      call fill_histogram (weighted, x(1), weight / f (x, PRC_INDEX))
      call fill_histogram (weights, x(1), weight)
      integral = integral + weight
      standard_dev = standard_dev + weight**2
   end do
   if (do_print) then
      print *, integral / (i-1), sqrt (standard_dev) / (i-1)
      call write_histogram (unweighted, "u_m.d")
      call write_histogram (reweighted, "r_m.d")
      call write_histogram (weighted, "w_m.d")
      call write_histogram (weights, "ws_m.d")
   end if
   call delete_histogram (unweighted)
   call delete_histogram (reweighted)
   call delete_histogram (weighted)
   call delete_histogram (weights)
   call vamp_delete_grids (grs)
 end subroutine multi_channel_generator
```

Main Program

215 ⟨vamp_test0.f90 202b⟩+≡

```
 program vamp_test0
   ⟨Modules used by vamp_test0 217c⟩
   implicit none
   ⟨Variables in vamp_test0 217a⟩
   do_print = .true.
   print *, "Starting VAMP 1.0 self test..."
   print *, "serial code"
   print *, VAMP_RCS_ID
   print *, DIVISIONS_RCS_ID
   call tao_random_create (rng, 0)
   call system_clock (ticks0)
   call tao_random_seed (rng, ticks0)
```

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

216a ⟨*Execute tests in* vamp_test0 216a⟩≡

```
  failures = 0
  call system_clock (ticks0)
  call single_channel (do_print, region, iterations, samples, rng, 10*ACCEPTABLE, failu
  call system_clock (ticks, ticks_per_second)
  print "(1X,A,F6.2,A)", &
       "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

216b ⟨*Execute tests in* vamp_test0 216a⟩+≡

```
  call system_clock (ticks0)
  call single_channel_generator &
         (do_print, region, iterations, samples, rng)
  call system_clock (ticks, ticks_per_second)
  print "(1X,A,F6.2,A)", &
       "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

216c ⟨*Execute tests in* vamp_test0 216a⟩+≡

```
  call system_clock (ticks0)
  call multi_channel (do_print, region, iterations, samples, rng, ACCEPTABLE, failures
  call system_clock (ticks, ticks_per_second)
  print "(1X,A,F6.2,A)", &
       "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

216d ⟨*Execute tests in* vamp_test0 216a⟩+≡

```
  call system_clock (ticks0)
  call multi_channel_generator &
         (do_print, region, iterations, samples, rng)
  call system_clock (ticks, ticks_per_second)
  print "(1X,A,F6.2,A)", &
       "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

216e ⟨*Execute tests in* vamp_test0 216a⟩+≡

```
  call system_clock (ticks0)
  ! call check_jacobians (do_print, region, samples, rng)
```

```
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
       "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
```

217a ⟨*Variables in* `vamp_test0` 217a⟩≡

```
logical :: do_print
```

217b ⟨*Execute* `command` 217b⟩≡

217c ⟨*Modules used by* `vamp_test0` 217c⟩≡

```
use kinds
use tao_random_numbers
use divisions, only: DIVISIONS_RCS_ID
use vamp, only: VAMP_RCS_ID
use vamp_test0_functions !NODEP!
use vamp_tests0 !NODEP!
```

217d ⟨*Variables in* `vamp_test0` 217a⟩+≡

```
integer :: i, j, ticks, ticks_per_second, ticks0
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(:,:), allocatable :: region
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
```

217e ⟨*Set up integrand and region in* `vamp_test0` 217e⟩≡

```
iterations = (/ 4, 3 /)
samples = (/ 10000, 50000 /)
allocate (region(2,2))
region(1,:)  = -1.0
region(2,:)  =  2.0
call create_sample &
     (num_poles = 2, weights = (/ 1.0_default, 2.0_default /), region = region)
do i = 1, size (x0, dim=2)
   do j = 1, size (x0, dim=3)
      call tao_random_number (rng, x0(:,i,j))
   end do
end do
gamma = 0.001
x0(1,:,:) = 0.2
x0(2:,:,:) = 0.8
```

217f ⟨*Cleanup in* `vamp_test0` 217f⟩≡

```
call delete_sample ()
deallocate (region)
```

6.2.2 Parallel Test

218a ⟨vampi_test0.f90 218a⟩≡

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

218b ⟨vampi_test0.f90 218a⟩+≡

```
program vampi_test0
  ⟨Modules used by vamp_test0 217c⟩
  use mpi90
  use vampi, only: VAMPI_RCS_ID
  implicit none
  ⟨Variables in vamp_test0 217a⟩
  integer :: num_proc, proc_id
  call mpi90_init ()
  call mpi90_size (num_proc)
  call mpi90_rank (proc_id)
  if (proc_id == 0) then
     do_print = .true.
     print *, "Starting VAMP 1.0 self test..."
     if (num_proc > 1) then
        print *, "parallel code running on ", num_proc, " processors"
     else
        print *, "parallel code running serially"
     end if
     print *, VAMP_RCS_ID
     print *, VAMPI_RCS_ID
     print *, DIVISIONS_RCS_ID
  else
     do_print = .false.
  end if
  call tao_random_create (rng, 0)
  call system_clock (ticks0)
```

```
call tao_random_seed (rng, ticks0 + proc_id)
⟨Set up integrand and region in vamp_test0 217e⟩
call mpi90_broadcast (x0, 0)
call mpi90_broadcast (gamma, 0)
command_loop: do
   if (proc_id == 0) then
      ⟨Read command line and decode it as command (never defined)⟩
   end if
   call mpi90_broadcast (command, 0)
   call system_clock (ticks0)
   ⟨Execute command 217b⟩
   call system_clock (ticks, ticks_per_second)
   if (proc_id == 0) then
      print "(1X,A,F6.2,A)", &
           "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
   end if
 end do command_loop
 ⟨Cleanup in vamp_test0 217f⟩
 call mpi90_finalize ()
 if (proc_id == 0) then
    print *, "bye."
 end if
end program vampi_test0
```

6.2.3 Output

219 ⟨vamp_test0.out 219⟩≡

—7—
Application

7.1 Cross section

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

220b ⟨Variables in cross_section 220b⟩≡
```
  real(kind=default), private, parameter :: &
       MA_0 = 0.0, &
       MB_0 = 0.0, &
       M1_0 = 0.0, &
       M2_0 = 0.0, &
       M3_0 = 0.0, &
```

```
      S_0 = 200.0 ** 2
```

221a ⟨*XXX Variables in* `cross_section` 221a⟩≡

```
  real(kind=default), private, parameter :: &
       MA_0 = 0.01, &
       MB_0 = 0.01, &
       M1_0 = 0.01, &
       M2_0 = 0.01, &
       M3_0 = 0.01, &
       S_0 = 200.0 ** 2
```

221b ⟨*XXX Variables in* `cross_section` 221a⟩+≡

```
  real(kind=default), private, parameter :: &
       S1_MIN_0 = 0.0 ** 2, &
       S2_MIN_0 = 0.0 ** 2, &
       S3_MIN_0 = 0.0 ** 2, &
       T1_MIN_0 = 0.0 ** 2, &
       T2_MIN_0 = 0.0 ** 2
```

221c ⟨*Variables in* `cross_section` 220b⟩+≡

```
  real(kind=default), private, parameter :: &
       S1_MIN_0 = 1.0 ** 2, &
       S2_MIN_0 = 1.0 ** 2, &
       S3_MIN_0 = 1.0 ** 2, &
       T1_MIN_0 = 10.0 ** 2, &
       T2_MIN_0 = 10.0 ** 2
```

221d ⟨*Declaration of* `cross_section` *procedures* 221d⟩≡

```
  private :: cuts
```

221e ⟨*XXX Implementation of* `cross_section` *procedures* 221e⟩≡

```
  pure function cuts (k1, k2, p1, p2, q) result (inside)
    real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
    logical :: inside
    inside =    (abs (dot (k1 - q, k1 - q)) >= T1_MIN_0) &
         .and. (abs (dot (k2 - q, k2 - q)) >= T2_MIN_0) &
         .and. (abs (dot (p1 + q, p1 + q)) >= S1_MIN_0) &
         .and. (abs (dot (p2 + q, p2 + q)) >= S2_MIN_0) &
         .and. (abs (dot (p1 + p2, p1 + p2)) >= S3_MIN_0)
  end function cuts
```

221f ⟨*Variables in* `cross_section` 220b⟩+≡

```
  real(kind=default), private, parameter :: &
```

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

222a ⟨*Implementation of* cross_section *procedures* 222a⟩≡

```
pure function cuts (k1, k2, p1, p2, q) result (inside)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  logical :: inside
  real(kind=default), dimension(3) :: p1n, p2n, qn
  inside = .false.
  if ((p1(0) < E_MIN) .or. (p2(0) < E_MIN) .or. (q(0) < E_MIN)) then
     return
  end if
  p1n = p1(1:3) / sqrt (dot_product (p1(1:3), p1(1:3)))
  p2n = p2(1:3) / sqrt (dot_product (p2(1:3), p2(1:3)))
  qn = q(1:3) / sqrt (dot_product (q(1:3), q(1:3)))
  if ((abs (qn(3)) > COSTH_BEAM_MAX) &
       .or. (abs (p1n(3)) > COSTH_BEAM_MAX)&
       .or. (abs (p2n(3)) > COSTH_BEAM_MAX)) then
     return
  end if
  if (dot_product (p1n, qn) > COSTH_SEP_MAX) then
     return
  end if
  if (dot_product (p2n, qn) > COSTH_SEP_MAX) then
     return
  end if
  if (dot_product (p1n, p2n) > COSTH_SEP_MAX) then
     return
  end if
  inside = .true.
end function cuts
```

222b ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
function xsect (k1, k2, p1, p2, q) result (xs)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  real(kind=default) :: xs
  complex(kind=default), dimension(-1:1,-1:1,-1:1,-1:1,-1:1) :: amp
  !!! xs = 1.0_double / phase_space_volume (3, k1(0) + k2(0))
  !!! xs = 1.0_double / dot (p1 + q, p1 + q) &
  !!!      + 1.0_double / dot (p2 + q, p2 + q)
  !!! return
  amp = nneeg (k1, k2, p1, p2, q)
```

```
    xs = sum (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2) &
              * conjg (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2)))
  end function xsect
```

223a ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

```
  private :: xsect
```

$$\begin{aligned}\phi : [0,1]^{\otimes 5} \to\ & [(m_2+m_3)^2, (\sqrt{s}-m_1)^2] \otimes [t_1^{\min}(s_2), t_1^{\max}(s_2)] \\ & \otimes [0,2\pi] \otimes [-1,1] \otimes [0,2\pi] \\ (x_1,\ldots,x_5) \mapsto\ & (s_2, t_1, \phi, \cos\theta_3, \phi_3) \\ & = (s_2(x_1), x_2 t_1^{\max}(s_2) + (1-x_2)t_1^{\min}(s_2), 2\pi x_3, 2x_4-1, 2\pi x_5)\end{aligned} \tag{7.1}$$

where

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

223b ⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1,\ldots,x_5)$ 223b⟩≡

```
    ! s2_min = S1_MIN_0
    s2_min = (m2 + m3)**2
    s2_max = (sqrt (s) - m1)**2
    s2 = s2_max * x(1) + s2_min * (1 - x(1))
    t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
         + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
    t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
         - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
    t1 = t1_max * x(2) + t1_min * (1 - x(2))
    phi = 2*PI * x(3)
    cos_theta3 = 2 * x(4) - 1
    phi3 = 2*PI * x(5)
```

223c ⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1,\ldots,x_5)$ *(massless case)* 223c⟩≡

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

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

i.e.

$$J_\phi(x_1,\ldots,x_5) = 8\pi^2 \cdot \left|\frac{\mathrm{d}s_2}{\mathrm{d}x_1}\right| \cdot \left(t_1^{\max}(s_2) - t_1^{\min}(s_2)\right) \tag{7.4}$$

224a ⟨*Adjust Jacobian* 224a⟩≡

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

224b ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
pure function phase_space (x, channel) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: channel
  type(LIPS3) :: p
  real(kind=default) :: &
       ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s = S_0
  ⟨m_a ↔ m_b, m_1 ↔ m_2 for channel #1 224c⟩
  ⟨Set (s_2, t_1, φ, cos θ_3, φ_3) from (x_1, ..., x_5) 223b⟩
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
  ⟨Adjust Jacobian 224a⟩
  ⟨p_1 ↔ p_2 for channel #2 225a⟩
end function phase_space
```

224c ⟨$m_a \leftrightarrow m_b$, $m_1 \leftrightarrow m_2$ *for channel #1* 224c⟩≡

```
select case (channel)
case (1)
   ma = MA_0
   mb = MB_0
   m1 = M1_0
   m2 = M2_0
   m3 = M3_0
case (2)
   ma = MB_0
   mb = MA_0
   m1 = M2_0
   m2 = M1_0
   m3 = M3_0
case (3)
   ma = MA_0
   mb = MB_0
   m1 = M3_0
```

```
      m2 = M2_0
      m3 = M1_0
   case default
      ma = MA_0
      mb = MB_0
      m1 = M1_0
      m2 = M2_0
      m3 = M3_0
   end select
```

225a ⟨$p_1 \leftrightarrow p_2$ *for channel #2* 225a⟩≡

```
   select case (channel)
   case (1)
      ! OK
   case (2)
      call swap (p%p(1,:), p%p(2,:))
   case (3)
      call swap (p%p(1,:), p%p(3,:))
   case default
      ! OK
   end select
```

225b ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

```
  private :: jacobian
```

225c ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  pure function jacobian (k1, k2, p1, p2, q) result (jac)
    real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
    real(kind=default) :: jac
    real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
    real(kind=default) :: s, s2, s2_min, s2_max, t1_min, t1_max
    ma_2 = max (dot (k1, k1), 0.0_double)
    mb_2 = max (dot (k2, k2), 0.0_double)
    m1_2 = max (dot (p1, p1), 0.0_double)
    m2_2 = max (dot (p2, p2), 0.0_double)
    m3_2 = max (dot (q, q), 0.0_double)
    s = dot (k1 + k2, k1 + k2)
    s2 = dot (p2 + q, p2 + q)
    ! s2_min = S1_MIN_0
    s2_min = (sqrt (m2_2) + sqrt (m3_2))**2
    s2_max = (sqrt (s) - sqrt (m1_2))**2
    t1_min = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
         + sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
    t1_max = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
         - sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
```

```
    jac = 1.0 / ((2*PI)**5 * 32 * s2) &
         * sqrt (lambda (s2, m2_2, m3_2) / lambda (s, ma_2, mb_2)) &
         * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
  end function jacobian
```

226a ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

```
  private :: phase_space, phase_space_massless
```

226b ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  pure function phase_space_massless (x, channel) result (p)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: channel
    type(LIPS3) :: p
    real(kind=default) :: s, t1, s2, phi, cos_theta3, phi3
    real(kind=default) :: s2_min, s2_max, t1_min, t1_max
    s = S_0
    ⟨Set (s2, t1, φ, cos θ3, φ3) from (x1, ..., x5) (massless case) 223c⟩
    p = two_to_three (s, t1, s2, phi, cos_theta3, phi3)
    ⟨Adjust Jacobian 224a⟩
    ⟨p1 ↔ p2 for channel #2 225a⟩
  end function phase_space_massless
```

226c ⟨*Types in* `cross_section` 226c⟩≡

```
    type, public :: LIPS3_m5i2a3
       ! private
       real(kind=default) :: ma, mb, m1, m2, m3
       real(kind=default) :: s, s2, t1
       real(kind=default) :: phi, cos_theta3, phi3
       real(kind=default) :: jacobian
    end type LIPS3_m5i2a3
```

226d ⟨*Types in* `cross_section` 226c⟩+≡

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

226e ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

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

226f ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  pure function invariants_from_p (p, k1, k2) result (q)
    type(LIPS3), intent(in) :: p
```

```
    real(kind=default), dimension(0:), intent(in) :: k1, k2
    type(LIPS3_m5i2a3) :: q
    real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
    real(kind=default), dimension(0:3) :: k1k2, p2p3, k1p1, p3_23
    k1k2 = k1 + k2
    k1p1 = - k1 + p%p(1,:)
    p2p3 = p%p(2,:) + p%p(3,:)
    ma_2 = max (dot (k1, k1), 0.0_double)
    mb_2 = max (dot (k2, k2), 0.0_double)
    m1_2 = max (dot (p%p(1,:), p%p(1,:)), 0.0_double)
    m2_2 = max (dot (p%p(2,:), p%p(2,:)), 0.0_double)
    m3_2 = max (dot (p%p(3,:), p%p(3,:)), 0.0_double)
    q%ma = sqrt (ma_2)
    q%mb = sqrt (mb_2)
    q%m1 = sqrt (m1_2)
    q%m2 = sqrt (m2_2)
    q%m3 = sqrt (m3_2)
    q%s = dot (k1k2, k1k2)
    q%s2 = dot (p2p3, p2p3)
    q%t1 = dot (k1p1, k1p1)
    q%phi = atan2 (p%p(1,2), p%p(1,1))
    if (q%phi < 0) then
       q%phi = q%phi + 2*PI
    end if
    p3_23 = boost_momentum (p%p(3,:), p2p3)
    q%cos_theta3 = p3_23(3) / sqrt (dot_product (p3_23(1:3), p3_23(1:3)))
    q%phi3 = atan2 (p3_23(2), p3_23(1))
    if (q%phi3 < 0) then
       q%phi3 = q%phi3 + 2*PI
    end if
    q%jacobian = 1.0 / ((2*PI)**5 * 32 * q%s2) &
         * sqrt (lambda (q%s2, m2_2, m3_2) / lambda (q%s, ma_2, mb_2))
  end function invariants_from_p
```

227a ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function invariants_to_p (p) result (q)
    type(LIPS3_m5i2a3), intent(in) :: p
    type(LIPS3) :: q
    q = two_to_three (p%s, p%t1, p%s2, p%phi, p%cos_theta3, p%phi3)
    q%jacobian = q%jacobian * p%jacobian
  end function invariants_to_p
```

227b ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
pure function invariants_from_x (x, s, ma, mb, m1, m2, m3) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(in) :: s, ma, mb, m1, m2, m3
  type(LIPS3_m5i2a3) :: p
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  p%ma = ma
  p%mb = mb
  p%m1 = m1
  p%m2 = m2
  p%m3 = m3
  p%s = s
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  p%s2 = s2_max * x(1) + s2_min * (1 - x(1))
  t1_min = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
            + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
               * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
            - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
               * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  p%t1 = t1_max * x(2) + t1_min * (1 - x(2))
  p%phi = 2*PI * x(3)
  p%cos_theta3 = 2 * x(4) - 1
  p%phi3 = 2*PI * x(5)
  p%jacobian = 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_from_x
```

228 ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
pure function invariants_to_x (p) result (x)
  type(LIPS3_m5i2a3), intent(in) :: p
  type(x5) :: x
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  t1_min = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
            + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
               * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
       - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
            - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
```

```
                * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  x%x(1) = (p%s2 - s2_min) / (s2_max - s2_min)
  x%x(2) = (p%t1 - t1_min) / (t1_max - t1_min)
  x%x(3) = p%phi / (2*PI)
  x%x(4) = (p%cos_theta3 + 1) / 2
  x%x(5) = p%phi3 / (2*PI)
  x%jacobian = p%jacobian * 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_to_x
```

229a ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

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

229b ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
function sigma (x, weights, channel, grids) result (xs)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: xs
  real(kind=default), dimension(2,0:3) :: k
  type(LIPS3) :: p
  k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  if (present (channel)) then
     p = phase_space (x, channel)
  else
     p = phase_space (x, 0)
  end if
  if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
     xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
          * jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
          !!! * p%jacobian
  else
     xs = 0.0
  end if
end function sigma
```

229c ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
function sigma_raw (k1, k2, p1, p2, q) result (xs)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  real(kind=default) :: xs
  if (cuts (k1, k2, p1, p2, q)) then
     xs = xsect (k1, k2, p1, p2, q)
```

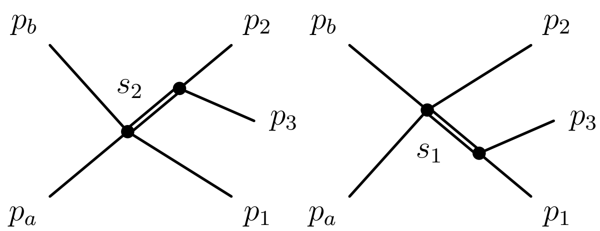
```
    else
       xs = 0.0
    end if
  end function sigma_raw
```

230a ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  function sigma_massless (x, weights, channel, grids) result (xs)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: xs
    real(kind=default), dimension(2,0:3) :: k
    type(LIPS3) :: p
    k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    p = phase_space_massless (x, 0)
    if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
       xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
             * p%jacobian
    else
       xs = 0.0
    end if
  end function sigma_massless
```

230b ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

```
  public :: w
```



230c ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  function w (x, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    real(kind=default), dimension(size(weights)) :: g_x
```

```
    real(kind=default), dimension(2,0:3) :: k
    type(LIPS3) :: p
    integer :: ch
    if (present (channel)) then
       ch = channel
    else
       ch = 0
    end if
    k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    p = phase_space (x, abs (ch))
    g_x(1) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
    g_x(2) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(2,:), p%p(1,:), p%p(3,:))
    g_x(3) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(3,:), p%p(2,:), p%p(1,:))
    if (ch > 0) then
       w_x = sigma_raw (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
              / sum (weights * g_x)
    else if (ch < 0) then
       w_x = g_x(-ch) / sum (weights * g_x)
    else
       w_x = -1
    end if
  end function w
```

231 ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
  function sigma_rambo (x, weights, channel, grids) result (xs)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: xs
    real(kind=default), dimension(2,0:3) :: k
    real(kind=default), dimension(3,0:3) :: p
    k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    p = massless_isotropic_decay (sum (k(:,0)), reshape (x, (/ 3, 4 /)))
    if (cuts (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:))) then
       xs = xsect (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:)) &
             * phase_space_volume (size (p, dim = 1), sum (k(:,0)))
    else
       xs = 0.0
    end if
  end function sigma_rambo
```

232a ⟨*Declaration of* cross_section *procedures* 221d⟩+≡

```
public :: sigma_rambo
```

232b ⟨*Declaration of* cross_section *procedures* 221d⟩+≡

```
public :: check_kinematics
private :: print_LIPS3_m5i2a3
```

232c ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
subroutine check_kinematics (rng)
  type(tao_random_state), intent(inout) :: rng
  real(kind=default), dimension(5) :: x
  real(kind=default), dimension(0:3) :: k1, k2
  type(x5) :: x1, x2
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q, q1, q2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  call tao_random_number (rng, x)
  q = invariants_from_x (x, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
  p1 = invariants_to_p (q)
  q1 = invariants_from_p (p1, k1, k2)
  p2 = phase_space (x, 1)
  q2 = invariants_from_p (p2, k1, k2)
  x1 = invariants_to_x (q1)
  x2 = invariants_to_x (q2)
  print *, p1%jacobian, p2%jacobian, x1%jacobian, x2%jacobian
  call print_lips3_m5i2a3 (q)
  call print_lips3_m5i2a3 (q1)
  call print_lips3_m5i2a3 (q2)
end subroutine check_kinematics
```

232d ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
subroutine print_LIPS3_m5i2a3 (p)
  type(LIPS3_m5i2a3), intent(in) :: p
  print "(1x,5('m',a1,'=',e9.2,' '))", &
       'a', p%ma, 'b', p%mb, '1', p%m1, '2', p%m2, '3', p%m3
  print "(1x,'s=',e9.2,' s2=',e9.2,' t1=',e9.2)", &
       p%s, p%s2, p%t1
  print "(1x,'phi=',e9.2,' cos(th3)=',e9.2,' phi2=',e9.2)", &
       p%phi, p%cos_theta3, p%phi3
  print "(1x,'j=',e9.2)", &
       p%jacobian
end subroutine print_LIPS3_m5i2a3
```

233a ⟨*Declaration of* `cross_section` *procedures* 221d⟩+≡

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

233b ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
pure function phi12 (x1, dummy) result (x2)
  real(kind=default), dimension(:), intent(in) :: x1
  integer, intent(in) :: dummy
  real(kind=default), dimension(size(x1)) :: x2
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x52
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
  p1 = invariants_to_p (q1)
  p2%p(1,:) = p1%p(2,:)
  p2%p(2,:) = p1%p(1,:)
  p2%p(3,:) = p1%p(3,:)
  if (dummy < 0) then
     q2 = invariants_from_p (p2, k2, k1)
  else
     q2 = invariants_from_p (p2, k1, k2)
  end if
  x52 = invariants_to_x (q2)
  x2 = x52%x
end function phi12
```

233c ⟨*Implementation of* `cross_section` *procedures* 222a⟩+≡

```
pure function phi21 (x2, dummy) result (x1)
  real(kind=default), dimension(:), intent(in) :: x2
  integer, intent(in) :: dummy
  real(kind=default), dimension(size(x2)) :: x1
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x51
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
  p2 = invariants_to_p (q2)
  p1%p(1,:) = p2%p(2,:)
  p1%p(2,:) = p2%p(1,:)
```

```
    p1%p(3,:) = p2%p(3,:)
    if (dummy < 0) then
       q1 = invariants_from_p (p1, k2, k1)
    else
       q1 = invariants_from_p (p1, k1, k2)
    end if
    x51 = invariants_to_x (q1)
    x1 = x51%x
  end function phi21
```

234a ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function phi1 (x1) result (p1)
    real(kind=default), dimension(:), intent(in) :: x1
    type(LIPS3) :: p1
    type(LIPS3_m5i2a3) :: q1
    q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
    p1 = invariants_to_p (q1)
  end function phi1
```

234b ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function phi2 (x2) result (p2)
    real(kind=default), dimension(:), intent(in) :: x2
    type(LIPS3) :: p2
    type(LIPS3_m5i2a3) :: q2
    q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
    p2 = invariants_to_p (q2)
  end function phi2
```

234c ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function g12 (x1) result (g)
    real(kind=default), dimension(:), intent(in) :: x1
    real(kind=default) :: g
    type(LIPS3) :: p1, p2
    type(LIPS3_m5i2a3) :: q1, q2
    type(x5) :: x52
    real(kind=default), dimension(0:3) :: k1, k2
    k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
    p1 = invariants_to_p (q1)
    p2%p(1,:) = p1%p(2,:)
    p2%p(2,:) = p1%p(1,:)
```

```
    p2%p(3,:) = p1%p(3,:)
    q2 = invariants_from_p (p2, k2, k1)
    x52 = invariants_to_x (q2)
    g = x52%jacobian / p1%jacobian
  end function g12
```

235a ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function g21 (x2) result (g)
    real(kind=default), dimension(:), intent(in) :: x2
    real(kind=default) :: g
    type(LIPS3) :: p1, p2
    type(LIPS3_m5i2a3) :: q1, q2
    type(x5) :: x51
    real(kind=default), dimension(0:3) :: k1, k2
    k1 = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
    p2 = invariants_to_p (q2)
    p1%p(1,:) = p2%p(2,:)
    p1%p(2,:) = p2%p(1,:)
    p1%p(3,:) = p2%p(3,:)
    q1 = invariants_from_p (p1, k2, k1)
    x51 = invariants_to_x (q1)
    g = x51%jacobian / p2%jacobian
  end function g21
```

235b ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function g1 (x1) result (g)
    real(kind=default), dimension(:), intent(in) :: x1
    real(kind=default) :: g
    type(LIPS3) :: p1
    type(LIPS3_m5i2a3) :: q1
    q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
    p1 = invariants_to_p (q1)
    g = 1 / p1%jacobian
  end function g1
```

235c ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  pure function g2 (x2) result (g)
    real(kind=default), dimension(:), intent(in) :: x2
    real(kind=default) :: g
    type(LIPS3) :: p2
```

```
    type(LIPS3_m5i2a3) :: q2
    q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
    p2 = invariants_to_p (q2)
    g = 1 / p2%jacobian
  end function g2
```

236a ⟨*Declaration of* cross_section *procedures* 221d⟩+≡

```
  public :: wx
```

236b ⟨*Implementation of* cross_section *procedures* 222a⟩+≡

```
  function wx (x, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in) :: weights
    integer, intent(in) :: channel
    type(vamp_grid), dimension(:), intent(in) :: grids
    real(kind=default) :: w_x
    real(kind=default), dimension(size(weights)) :: g_x, p_q
    real(kind=default), dimension(size(x)) :: x1, x2
    real(kind=default), dimension(2,0:3) :: k
    type(LIPS3) :: q
    k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double,  100.0_double /)
    k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    select case (abs (channel))
    case (1)
       x1 = x
       x2 = phi12 (x, 0)
       q = phi1 (x1)
    case (2)
       x1 = phi21 (x, 0)
       x2 = x
       q = phi2 (x2)
    end select
    p_q(1) = vamp_probability (grids(1), x1)
    p_q(2) = vamp_probability (grids(2), x2)
    g_x(1) = p_q(1) * g1 (x1)
    g_x(2) = p_q(2) * g2 (x2)
    g_x = g_x / p_q(abs(channel))
    if (channel > 0) then
       w_x = sigma_raw (k(1,:), k(2,:), q%p(1,:), q%p(2,:), q%p(3,:)) &
            / dot_product (weights, g_x)
    else if (channel < 0) then
       w_x = vamp_probability (grids(-channel), x) / dot_product (weights, g_x)
    else
       w_x = 0
```

```
    end if
  end function wx
```

237 ⟨application.f90 220a⟩+≡

```
program application
  use kinds
  use utils
  use vampi
  use mpi90
  use linalg
  use exceptions
  use kinematics, only: phase_space_volume
  use cross_section !NODEP!
  use tao_random_numbers
  implicit none
  type(vamp_grid) :: gr
  type(vamp_grids) :: grs
  real(kind=default), dimension(:,:), allocatable :: region
  real(kind=default) :: integral, standard_dev, chi_squared
  real(kind=default) :: &
       single_integral, single_standard_dev, &
       rambo_integral, rambo_standard_dev
  real(kind=default), dimension(2) :: weight_vector
  integer, dimension(2) :: calls, iterations
  type(vamp_history), dimension(100) :: history
  type(vamp_history), dimension(100,size(weight_vector)) :: histories
  type(exception) :: exc
  type(tao_random_state) :: rng
  real(kind=default), dimension(5) :: x
  real(kind=default) :: jac
  integer :: i
  integer :: num_proc, proc_id, ticks, ticks0, ticks_per_second, command
  character(len=72) :: command_line
  integer, parameter :: &
       CMD_SINGLE = 1, &
       CMD_MULTI = 2, &
       CMD_ROTATING = 3, &
       CMD_RAMBO = 4, &
       CMD_COMPARE = 5, &
       CMD_MASSLESS = 6, &
       CMD_ERROR = 0
  call mpi90_init ()
  call mpi90_size (num_proc)
```

```
call mpi90_rank (proc_id)
call system_clock (ticks0)
call tao_random_create (rng, 0)
call tao_random_seed (rng, ticks0 + proc_id)
!!! call tao_random_seed (rng, proc_id)
call vamp_create_history (history, verbose = .true.)
call vamp_create_history (histories, verbose = .true.)
iterations = (/ 3, 4 /)
calls =  (/  10000, 100000 /)
if (proc_id == 0) then
   read *, command_line
   if (command_line == "single") then
      command = CMD_SINGLE
   else if (command_line == "multi") then
      command = CMD_MULTI
   else if (command_line == "rotating") then
      command = CMD_ROTATING
   else if (command_line == "rambo") then
      command = CMD_RAMBO
   else if (command_line == "compare") then
      command = CMD_COMPARE
   else if (command_line == "massless") then
      command = CMD_MASSLESS
   else
      command = CMD_ERROR
   end if
end if
call mpi90_broadcast (command, 0)
call system_clock (ticks0)
select case (command)
case (CMD_SINGLE)
   ⟨Application in single channel mode 240a⟩
case (CMD_MASSLESS)
   ⟨Application in massless single channel mode 240b⟩
case (CMD_MULTI)
   ⟨Application in multi channel mode 241⟩
case (CMD_ROTATING)
   allocate (region(2,5))
   region(1,:) =  0.0
   region(2,:) =  1.0
   if (proc_id == 0) then
      print *, "rotating N/A yet ..."
   end if
```

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

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

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

```
allocate (region(2,5))
region(1,:) =  0.0
region(2,:) =  1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
     (rng, gr, sigma, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
     (rng, gr, sigma, iterations(2), &
      integral, standard_dev, chi_squared, &
      history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "single")
if (proc_id == 0) then
   print *, "SINGLE: ", integral, standard_dev, chi_squared
end if
call vamp_write_grid (gr, "application.grid")
call vamp_delete_grid (gr)
deallocate (region)
```

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

```
allocate (region(2,5))
```

```
region(1,:) =  0.0
region(2,:) =  1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
     (rng, gr, sigma_massless, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
     (rng, gr, sigma_massless, iterations(2), &
      integral, standard_dev, chi_squared, &
      history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "single")
if (proc_id == 0) then
   print *, "M=0:    ", integral, standard_dev, chi_squared
end if
call vamp_write_grid (gr, "application.grid")
call vamp_delete_grid (gr)
deallocate (region)
```

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

```
allocate (region(2,5))
region(1,:) =  0.0
region(2,:) =  1.0
weight_vector = 1.0
if (proc_id == 0) then
   read *, weight_vector
end if
call mpi90_broadcast (weight_vector, 0)
weight_vector = weight_vector / sum (weight_vector)
call vamp_create_grids (grs, region, calls(1), weight_vector)
do i = 1, 3
   call clear_exception (exc)
   call vamp_sample_grids &
        (rng, grs, wx, iterations(1), &
         history = history(1+(i-1)*iterations(1):), &
         histories = histories(1+(i-1)*iterations(1):,:), exc = exc)
   call handle_exception (exc)
   call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, calls(2))
call vamp_sample_grids &
     (rng, grs, wx, iterations(2), &
```

```
      integral, standard_dev, chi_squared, &
      history = history(3*iterations(1)+1:), &
      histories = histories(3*iterations(1)+1:,:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
if (proc_id == 0) then
   print *, "MULTI:  ", integral, standard_dev, chi_squared
end if
call vamp_write_grids (grs, "application.grids")
call vamp_delete_grids (grs)
deallocate (region)
```

242 ⟨*Application in Rambo mode* 242⟩≡

```
allocate (region(2,12))
region(1,:) =  0.0
region(2,:) =  1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
     (rng, gr, sigma_rambo, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
     (rng, gr, sigma_rambo, iterations(2), &
      integral, standard_dev, chi_squared, &
      history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "rambo")
if (proc_id == 0) then
   print *, "RAMBO:  ", integral, standard_dev, chi_squared
end if
call vamp_delete_grid (gr)
deallocate (region)
```

—A— Constants

A.1 Kinds

This borders on overkill, but it is the most portable way to get double precision in standard Fortran without relying on `kind (1.0D0)` Currently, it is possible to change `double` to any other supported real kind. The MPI interface is a potential trouble source for such things, however.

243a ⟨vamp_kinds.f90 243a⟩≡
```
! vamp_kinds.f90 --
⟨Copyleft notice 1⟩
module kinds
  implicit none
  integer, parameter, private :: single = &
       & selected_real_kind (precision(1.0), range(1.0))
  integer, parameter, private :: double = &
       & selected_real_kind (precision(1.0_single) + 1, range(1.0_single) + 1)
  integer, parameter, private :: quadruple = &
       & selected_real_kind (precision (1.0_double) + 1, range (1.0_double))
  integer, parameter, public :: default = double
  character(len=*), public, parameter :: KINDS_RCS_ID = &
       "$Id: kinds.nw 314 2010-04-17 20:32:33Z ohl $"
end module kinds
```

A.2 Mathematical and Physical Constants

243b ⟨constants.f90 243b⟩≡
```
! constants.f90 --
⟨Copyleft notice 1⟩
```

```
module constants
  use kinds
  implicit none
  private
  real(kind=default), public, parameter :: &
       PI = 3.1415926535897932384626433832795028841972_default
  character(len=*), public, parameter :: CONSTANTS_RCS_ID = &
       "$Id: constants.nw 314 2010-04-17 20:32:33Z ohl $"
end module constants
```

—B— Errors and Exceptions

Fortran95 does not allow *any* I/O in `pure` and `elemental` procedures, not even output to the unit `*`. A `stop` statement is verboten as well. Therefore we have to use condition codes

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

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

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

```
       EXC_ERROR = 3, &
       EXC_FATAL = 4
```

246a ⟨*Variables in* exceptions 245c⟩+≡

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

246b ⟨*Declaration of* exceptions *procedures* 246b⟩≡

```
  public :: handle_exception
```

246c ⟨*Implementation of* exceptions *procedures* 246c⟩≡

```
  subroutine handle_exception (exc)
    type(exception), intent(inout) :: exc
    character(len=10) :: name
    if (exc%level > 0) then
       select case (exc%level)
          case (EXC_NONE)
             name = "(none)"
          case (EXC_INFO)
             name = "info"
          case (EXC_WARN)
             name = "warning"
          case (EXC_ERROR)
             name = "error"
          case (EXC_FATAL)
             name = "fatal"
          case default
             name = "invalid"
       end select
       print *, trim (exc%origin), ": ", trim(name), ": ", trim (exc%message)
       if (exc%level >= EXC_FATAL) then
          print *, "terminated."
          stop
       end if
    end if
  end subroutine handle_exception
```

246d ⟨*Declaration of* exceptions *procedures* 246b⟩+≡

```
  public :: raise_exception, clear_exception, gather_exceptions
```

Raise an exception, but don't overwrite the messages in `exc` if it holds a more severe exception. This way we can accumulate error codes across procedure calls. We have `exc` optional to simplify life for the cslling procedures, which might have it optional themselves.

246e ⟨*Implementation of* exceptions *procedures* 246c⟩+≡

```
  elemental subroutine raise_exception (exc, level, origin, message)
```

```
    type(exception), intent(inout), optional :: exc
    integer, intent(in), optional :: level
    character(len=*), intent(in), optional :: origin, message
    integer :: local_level
    if (present (exc)) then
       if (present (level)) then
          local_level = level
       else
          local_level = EXC_DEFAULT
       end if
       if (exc%level < local_level) then
          exc%level = local_level
          if (present (origin)) then
             exc%origin = origin
          else
             exc%origin = "[vamp]"
          end if
          if (present (message)) then
             exc%message = message
          else
             exc%message = "[vamp]"
          end if
       end if
    end if
  end subroutine raise_exception
```

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

```
  elemental subroutine clear_exception (exc)
    type(exception), intent(inout) :: exc
    exc%level = 0
    exc%message = ""
    exc%origin = ""
  end subroutine clear_exception
```

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

```
  pure subroutine gather_exceptions (exc, excs)
    type(exception), intent(inout) :: exc
    type(exception), dimension(:), intent(in) :: excs
    integer :: i
    i = sum (maxloc (excs%level))
    if (exc%level < excs(i)%level) then
       call raise_exception (exc, excs(i)%level, excs(i)%origin, &
                             excs(i)%message)
    end if
  end subroutine gather_exceptions
```

Here's how to use `gather_exceptions`. `elemental_procedure`

248 ⟨*Idioms* 100a⟩+≡

```
call clear_exception (excs)
call elemental_procedure_1 (y, x, excs)
call elemental_procedure_2 (b, a, excs)
if (any (excs%level > 0)) then
   call gather_exceptions (exc, excs)
   return
end if
```

—C— The Art Of Random Numbers

Volume two of Donald E. Knuth' *The Art of Computer Programming* [15] has always been celebrated as the prime reference for random number generation. Recently, the third edition has been published and it contains a gem of a *portable* random number generator. It generates 30-bit integers with the following desirable properties

- they pass all the tests from George Marsaglia's "diehard" suite of tests for random number generators [23] (but see [15] for a caveat regarding the "birthday-spacing" test)
- they can be generated with portable signed 32-bit arithmetic (Fortran can't do unsigned arithmetic)
- it is faster than other lagged Fibonacci generators
- it can create at least $2^{30} - 2$ independent sequences

C.1 Application Program Interface

A function returning single reals and integers. Note that the static version without the `tao_random_state` argument does not require initialization. It will behave as if `call tao_random_seed(0)` had been executed. On the other hand, the parallelizable version with the explicit `tao_random_state` will fail if none of the `tao_random_create` have been called for the state. (This is a deficiency of Fortran90 that can be fixed in Fortran95).

249 ⟨*API documentation* 249⟩≡

```
call tao_random_number (r)
call tao_random_number (s, r)
```

The state of the random number generator comes in two 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.

250a ⟨*API documentation* 249⟩+≡
```
type(tao_random_state) :: s
type(tao_random_raw_state) :: rs
```
Subroutines filling arrays of reals and integers:

250b ⟨*API documentation* 249⟩+≡
```
call tao_random_number (a, num = n)
call tao_random_number (s, a, num = n)
```
Subroutine for changing the seed:

250c ⟨*API documentation* 249⟩+≡
```
call tao_random_seed (seed = seed)
call tao_random_seed (s, seed = seed)
```
Subroutine for changing the luxury. Per default, use all random numbers:

250d ⟨*API documentation* 249⟩+≡
```
call tao_random_luxury ()
call tao_random_luxury (s)
```
With an integer argument, use the first `n` of each fill of the buffer:

250e ⟨*API documentation* 249⟩+≡
```
call tao_random_luxury (n)
call tao_random_luxury (s, n)
```
With a floating point argument, use that fraction of each fill of the buffer:

250f ⟨*API documentation* 249⟩+≡
```
call tao_random_luxury (x)
call tao_random_luxury (s, x)
```
Create a `tao_random_state`

250g ⟨*API documentation* 249⟩+≡
```
call tao_random_create (s, seed, buffer_size = buffer_size)
call tao_random_create (s, raw_state, buffer_size = buffer_size)
call tao_random_create (s, state)
```
Create a `tao_random_raw_state`

250h ⟨*API documentation* 249⟩+≡
```
call tao_random_create (rs, seed)
call tao_random_create (rs, raw_state)
call tao_random_create (rs, state)
```
Destroy a `tao_random_state` or `tao_random_raw_state`

250i ⟨*API documentation* 249⟩+≡
```
call tao_random_destroy (s)
```

Copy tao_random_state and tao_random_raw_state in all four combinations

251a ⟨*API documentation* 249⟩+≡
```
call tao_random_copy (lhs, rhs)
lhs = rhs
```

251b ⟨*API documentation* 249⟩+≡
```
call tao_random_flush (s)
```

251c ⟨*API documentation* 249⟩+≡
```
call tao_random_read (s, unit)
call tao_random_write (s, unit)
```

251d ⟨*API documentation* 249⟩+≡
```
call tao_random_test (name = name)
```

Here is a sample application of random number states:

251e ⟨*API documentation* 249⟩+≡
```
subroutine threads (args, y, state)
  real, dimension(:), intent(in) :: args
  real, dimension(:), intent(out) :: y
  type(tao_random_state) :: state
  integer :: seed
  type(tao_random_raw_state), dimension(size(y)) :: states
  integer :: s
  call tao_random_number (state, seed)
  call tao_random_create (states, (/ (s, s=seed,size(y)-1) /))
  y = thread (args, states)
end function thread
```

In this example, we could equivalently pass an integer seed, instead of raw_state. But in more complicated cases it can be beneficial to have the option of reusing raw_state in the calling routine.

251f ⟨*API documentation* 249⟩+≡
```
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 $L = 37$.

252a ⟨*Parameters in* `tao_random_numbers` 252a⟩≡

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

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

252b ⟨*Parameters in* `tao_random_numbers` *(alternatives)* 252b⟩≡

```
integer, parameter, private :: K =  55, L =  24
integer, parameter, private :: K =  89, L =  38
integer, parameter, private :: K = 100, L =  37
integer, parameter, private :: K = 127, L =  30
integer, parameter, private :: K = 258, L =  83
integer, parameter, private :: K = 378, L = 107
integer, parameter, private :: K = 607, L = 273
```

A modulus of 2^{30} is the largest we can handle in *portable* (i.e. *signed*) 32-bit arithmetic

252c ⟨*Variables in 30-bit* `tao_random_numbers` 252c⟩≡

```
integer(kind=tao_i32), parameter, private :: M = 2**30
```

`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:

252d ⟨*Parameters in* `tao_random_numbers` 252a⟩+≡

```
integer, parameter, private :: DEFAULT_BUFFER_SIZE = 1009
```

Since users are not expected to call `generate` directly, we do *not* check for $n \geq K$ and assume that the caller knows what (s)he's doing ...

253a ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩≡
```
pure subroutine generate (a, state)
  integer(kind=tao_i32), dimension(:), intent(inout) :: a, state
  integer :: j, n
  n = size (a)
  ⟨Load a and refresh state 253c⟩
end subroutine generate
```

253b ⟨*Declaration of* `tao_random_numbers` 253b⟩≡
```
private :: generate
```

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

253c ⟨*Load* `a` *and refresh* `state` 253c⟩≡
```
a(1:K) = state(1:K)
```

The remaining $n-K$ random numbers can be gotten directly from the recursion (C.1). Note that Fortran90's new `modulo` intrinsic does the right thing, since it guarantees (unlike Fortran77's `mod`) that $0 \leq \mathtt{modulo}(a,m) < a$ if $m > 0$):

253d ⟨*Load* `a` *and refresh* `state` 253c⟩+≡
```
do j = K+1, n
   a(j) = modulo (a(j-K) - a(j-L), M)
end do
```

Do the recursion (C.1) K more times to prepare `state(1:K)` for the next invokation of `generate`.

253e ⟨*Load* `a` *and refresh* `state` 253c⟩+≡
```
state(1:L) = modulo (a(n+1-K:n+L-K) - a(n+1-L:n), M)
do j = L+1, K
   state(j) = modulo (a(n+j-K) - state(j-L), M)
end do
```

C.2.2 Initialization of 30-bit Random Numbers

The non-trivial and most beautiful part is the algorithm to initialize the random number generator state `state` with the first K numbers. I haven't studied algebra over finite fields in sufficient depth to consider the mathematics behind it straightforward. The commentary below is rather verbose and reflects my understanding of DEK's rather terse remarks (solution to exercise 3.6-9 [15]).

253f ⟨*Implementation of* `tao_random_numbers` 253f⟩≡
```
subroutine seed_static (seed)
```

```
    integer, optional, intent(in) :: seed
    call seed_stateless (s_state, seed)
    s_virginal = .false.
    s_last = size (s_buffer)
  end subroutine seed_static
```

The static version of `tao_random_raw_state`:

254a ⟨*Variables in 30-bit* `tao_random_numbers` 252c⟩+≡

```
  integer(kind=tao_i32), dimension(K), save, private :: s_state
  logical, save, private :: s_virginal = .true.
```

254b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  elemental subroutine seed_raw_state (s, seed)
    type(tao_random_raw_state), intent(inout) :: s
    integer, optional, intent(in) :: seed
    call seed_stateless (s%x, seed)
  end subroutine seed_raw_state
```

254c ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  elemental subroutine seed_state (s, seed)
    type(tao_random_state), intent(inout) :: s
    integer, optional, intent(in) :: seed
    call seed_raw_state (s%state, seed)
    s%last = size (s%buffer)
  end subroutine seed_state
```

This incarnation of the procedure is `pure`.

254d ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine seed_stateless (state, seed)
    integer(kind=tao_i32), dimension(:), intent(out) :: state
    integer, optional, intent(in) :: seed
    ⟨Parameters local to tao_random_seed 255a⟩
    integer :: seed_value, j, s, t
    integer(kind=tao_i32), dimension(2*K-1) :: x
    ⟨Set up seed_value from seed or DEFAULT_SEED 255c⟩
    ⟨Bootstrap the x buffer 255d⟩
    ⟨Set up s and t 255f⟩
    do
       ⟨p(z) → p(z)^2 (modulo 2 and z^K + z^L + 1) 256a⟩
       ⟨p(z) → zp(z) (modulo 2 and z^K + z^L + 1) 257a⟩
       ⟨Shift s or t and exit if t ≤ 0 257b⟩
    end do
    ⟨Fill state from x 257c⟩
  end subroutine seed_stateless
```

Any default will do

255a ⟨*Parameters local to* `tao_random_seed` 255a⟩≡
```
integer, parameter :: DEFAULT_SEED = 0
```
These must not be changed:

255b ⟨*Parameters local to* `tao_random_seed` 255a⟩+≡
```
integer, parameter :: MAX_SEED = 2**30 - 3
integer, parameter :: TT = 70
```

255c ⟨*Set up* `seed_value` *from* `seed` *or* `DEFAULT_SEED` 255c⟩≡
```
if (present (seed)) then
   seed_value = seed
else
   seed_value = DEFAULT_SEED
end if
if (seed_value < 0 .or. seed_value > MAX_SEED) then
   !!! print *, "tao_random_seed: seed (", seed_value, &
   !!!       ") not in [ 0,", MAX_SEED, "]!"
   seed_value = modulo (abs (seed_value), MAX_SEED + 1)
   !!! print *, "tao_random_seed: seed set to ", seed_value, "!"
end if
```
Fill the array $x_1, \ldots, x_K$ with even integers, shifted cyclically by 29 bits.

255d ⟨*Bootstrap the* `x` *buffer* 255d⟩≡
```
s = seed_value - modulo (seed_value, 2) + 2
do j = 1, K
   x(j) = s
   s = 2*s
   if (s >= M) then
      s = s - M + 2
   end if
end do
x(K+1:2*K-1) = 0
```
Make x_2 (and only x_2) odd:

255e ⟨*Bootstrap the* `x` *buffer* 255d⟩+≡
```
x(2) = x(2) + 1
```

255f ⟨*Set up* `s` *and* `t` 255f⟩≡
```
s = seed_value
t = TT - 1
```
Consider the polynomial

$$p(z) = \sum_{n=1}^{K} x_n z^{n-1} = x_K z^{K-1} + \ldots + x_2 z + x_1 \qquad \text{(C.2)}$$

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 $\mod 2$ below.

256a $\langle p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1)$ 256a$\rangle\equiv$
```
x(3:2*K-1:2) = x(2:K)
```
The coefficients of the odd powers (those with the even indices) have not been changed yet. Set them to a flipped version of the other coefficients with the least significant bit set to 0.

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

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

256b $\langle p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1)$ 256a$\rangle{+}\equiv$
```
x(2:K+L-1:2) = x(2*K-1:K-L+2:-2) - modulo (x(2*K-1:K-L+2:-2), 2_tao_i32)
```
The Fortran program in [15] reads

256c $\langle p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1)$ *(DEK, Fortran)* 256c$\rangle\equiv$
```
do j = 2*K-1, K-L+1, -2
   x(2*K+1-j) = x(j) - mod (x(j), 2)
end do
```
i.e.

256d $\langle p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1)$ *(alternative)* 256d$\rangle\equiv$
```
x(2:K+L:2) = x(2*K-1:K-L+1:-2) - modulo (x(2*K-1:K-L+1:-2), 2)
```
which is equivalent, as long as $K + L$ is odd. This is the case most of the time. The version used above is the direct translation of the C version

256e $\langle p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1)$ *(DEK, C)* 256e$\rangle\equiv$
```
for (j = 2*K-2; j > K-L; j -= 2)
  x[2*K-1-j] = evenize (x[j]);
```

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

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

256f ⟨$p(z) \to p(z)^2$ *(modulo* 2 *and* $z^K + z^L + 1$*)* 256a⟩+≡

```
do j= 2*K-1, K+1, -1
   if (modulo (x(j), int(2, tao_i32)) == 1) then
      x(j-(K-L)) = modulo (x(j-(K-L)) - x(j), M)
      x(j-K) = modulo (x(j-K) - x(j), M)
   end if
end do
```

257a ⟨$p(z) \to zp(z)$ *(modulo* 2 *and* $z^K + z^L + 1$*)* 257a⟩≡

```
if (modulo (s, 2) == 1) then
   x(2:K+1) = x(1:K)
   x(1) = x(K+1)
   if (modulo (x(K+1), 2_tao_i32) == 1) then
      x(L+1) = modulo (x(L+1) - x(K+1), M)
   end if
end if
```

257b ⟨*Shift* `s` *or* `t` *and exit if* `t` ≤ 0 257b⟩≡

```
if (s /= 0) then
   s = s / 2
else
   t = t - 1
end if
if (t <= 0) then
   exit
end if
```

257c ⟨*Fill* `state` *from* `x` 257c⟩≡

```
state(K-L+1:K) = x(1:L)
state(1:K-L) = x(L+1:K)
```

257d ⟨*Interfaces of* `tao_random_numbers` 257d⟩≡

```
interface tao_random_seed
   module procedure ⟨Specific procedures for tao_random_seed 257f⟩
end interface
```

257e ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
private :: ⟨Specific procedures for tao_random_seed 257f⟩
```

257f ⟨*Specific procedures for* `tao_random_seed` 257f⟩≡

```
seed_static, seed_state, seed_raw_state
```

C.2.3 Generation of 52-bit Random Numbers

$$X_j = (X_{j-K} + X_{j-L}) \mod 1 \tag{C.4}$$

257g ⟨*Variables in 52-bit* `tao_random_numbers` 257g⟩≡

```
real(kind=tao_r64), parameter, private :: M = 1.0_tao_r64
```

The state of the internal routines

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

258b ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩≡
```
pure subroutine generate (a, state)
  real(kind=tao_r64), dimension(:), intent(inout) :: a
  real(kind=tao_r64), dimension(:), intent(inout) :: state
  integer :: j, n
  n = size (a)
  ⟨Load 52-bit a and refresh state 258c⟩
end subroutine generate
```

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

258c ⟨*Load 52-bit* `a` *and refresh* `state` 258c⟩≡
```
a(1:K) = state(1:K)
do j = K+1, n
   a(j) = modulo (a(j-K) + a(j-L), M)
end do
state(1:L) = modulo (a(n+1-K:n+L-K) + a(n+1-L:n), M)
do j = L+1, K
   state(j) = modulo (a(n+j-K) + state(j-L), M)
end do
```

C.2.4 Initialization of 52-bit Random Numbers

This incarnation of the procedure is `pure`.

258d ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡
```
pure subroutine seed_stateless (state, seed)
  real(kind=tao_r64), dimension(:), intent(out) :: state
  integer, optional, intent(in) :: seed
  ⟨Parameters local to tao_random_seed 255a⟩
  ⟨Variables local to 52-bit tao_random_seed 259b⟩
  ⟨Set up seed_value from seed or DEFAULT_SEED 255c⟩
  ⟨Bootstrap the x and xl buffers 259d⟩
  ⟨Set up s and t 255f⟩
  do
     ⟨52-bit p(z) → p(z)^2 (modulo 2 and z^K + z^L + 1) 259g⟩
     ⟨52-bit p(z) → zp(z) (modulo 2 and z^K + z^L + 1) 260a⟩
     ⟨Shift s or t and exit if t ≤ 0 257b⟩
  end do
  ⟨Fill state from x 257c⟩
```

```
end subroutine seed_stateless
```

259a ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
private :: seed_stateless
```

259b ⟨*Variables local to 52-bit* `tao_random_seed` 259b⟩≡

```
real(kind=tao_r64), parameter :: ULP = 2.0_tao_r64**(-52)
```

259c ⟨*Variables local to 52-bit* `tao_random_seed` 259b⟩+≡

```
real(kind=tao_r64), dimension(2*K-1) :: x, xl
real(kind=tao_r64) :: ss
integer :: seed_value, t, s, j
```

259d ⟨*Bootstrap the* `x` *and* `xl` *buffers* 259d⟩≡

```
xl = 0
xl(2) = ULP
```

259e ⟨*Bootstrap the* `x` *and* `xl` *buffers* 259d⟩+≡

```
ss = 2*ULP * (seed_value + 2)
do j = 1, K
   x(j) = ss
   ss = 2*ss
   if (ss >= 1) then
      ss = ss - 1 + 2*ULP
   end if
end do
x(K+1:2*K-1) = 0.0
```

259f ⟨*Bootstrap the* `x` *and* `xl` *buffers* 259d⟩+≡

```
x(2) = x(2) + ULP
```

259g ⟨*52-bit* $p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) 259g⟩≡

```
xl(3:2*K-1:2) = xl(2:K)
x(3:2*K-1:2) = x(2:K)
```

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

259h ⟨*52-bit* $p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) 259g⟩+≡

```
xl(2:K+L-1:2) = 0.0
x(2:K+L-1:2) = x(2*K-1:K-L+2:-2) - xl(2*K-1:K-L+2:-2)
do j = 2*K-1, K+1, -1
   if (xl(j) /= 0) then
      xl(j-(K-L)) = ULP - xl(j-(K-L))
      x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
      xl(j-K) = ULP - xl(j-K)
      x(j-K) = modulo (x(j-K) + x(j), M)
   end if
end do
```

260a ⟨*52-bit* $p(z) \to zp(z)$ (*modulo* 2 *and* $z^K + z^L + 1$) 260a⟩≡

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

C.3 The State

260b ⟨*Declaration of 30-bit* `tao_random_numbers` *types* 260b⟩≡

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

260c ⟨*Declaration of 30-bit* `tao_random_numbers` *types* 260b⟩+≡

```
type, public :: tao_random_state
   private
   type(tao_random_raw_state) :: state
   integer(kind=tao_i32), dimension(:), pointer :: buffer => null ()
   integer :: buffer_end, last
end type tao_random_state
```

260d ⟨*Declaration of 52-bit* `tao_random_numbers` *types* 260d⟩≡

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

260e ⟨*Declaration of 52-bit* `tao_random_numbers` *types* 260d⟩+≡

```
type, public :: tao_random_state
   private
   type(tao_random_raw_state) :: state
   real(kind=tao_r64), dimension(:), pointer :: buffer => null ()
   integer :: buffer_end, last
end type tao_random_state
```

C.3.1 Creation

261a ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡
```
interface tao_random_create
   module procedure ⟨Specific procedures for tao_random_create 261c⟩
end interface
```

261b ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡
```
private :: ⟨Specific procedures for tao_random_create 261c⟩
```

261c ⟨*Specific procedures for* `tao_random_create` 261c⟩≡
```
create_state_from_seed, create_raw_state_from_seed, &
create_state_from_state, create_raw_state_from_state, &
create_state_from_raw_state, create_raw_state_from_raw_st
```

There are no procedures for copying the state of the static generator to or from an explicit `tao_random_state`. Users needing this functionality can be expected to handle explicit states anyway. Since the direction of the copying can not be obvious from the type of the argument, such functions would spoil the simplicity of the generic procedure interface.

261d ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡
```
elemental subroutine create_state_from_seed (s, seed, buffer_size)
  type(tao_random_state), intent(out) :: s
  integer, intent(in) :: seed
  integer, intent(in), optional :: buffer_size
  call create_raw_state_from_seed (s%state, seed)
  if (present (buffer_size)) then
     s%buffer_end = max (buffer_size, K)
  else
     s%buffer_end = DEFAULT_BUFFER_SIZE
  end if
  allocate (s%buffer(s%buffer_end))
  call tao_random_flush (s)
end subroutine create_state_from_seed
```

261e ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡
```
elemental subroutine create_state_from_state (s, state)
  type(tao_random_state), intent(out) :: s
  type(tao_random_state), intent(in) :: state
  call create_raw_state_from_raw_st (s%state, state%state)
  allocate (s%buffer(size(state%buffer)))
  call tao_random_copy (s, state)
end subroutine create_state_from_state
```

261f ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡
```
elemental subroutine create_state_from_raw_state &
```

```
    (s, raw_state, buffer_size)
  type(tao_random_state), intent(out) :: s
  type(tao_random_raw_state), intent(in) :: raw_state
  integer, intent(in), optional :: buffer_size
  call create_raw_state_from_raw_st (s%state, raw_state)
  if (present (buffer_size)) then
     s%buffer_end = max (buffer_size, K)
  else
     s%buffer_end = DEFAULT_BUFFER_SIZE
  end if
  allocate (s%buffer(s%buffer_end))
  call tao_random_flush (s)
end subroutine create_state_from_raw_state
```

262a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine create_raw_state_from_seed (s, seed)
  type(tao_random_raw_state), intent(out) :: s
  integer, intent(in) :: seed
  call seed_raw_state (s, seed)
end subroutine create_raw_state_from_seed
```

262b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine create_raw_state_from_state (s, state)
  type(tao_random_raw_state), intent(out) :: s
  type(tao_random_state), intent(in) :: state
  call copy_state_to_raw_state (s, state)
end subroutine create_raw_state_from_state
```

262c ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine create_raw_state_from_raw_st (s, raw_state)
  type(tao_random_raw_state), intent(out) :: s
  type(tao_random_raw_state), intent(in) :: raw_state
  call copy_raw_state (s, raw_state)
end subroutine create_raw_state_from_raw_st
```

C.3.2 Destruction

262d ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡

```
interface tao_random_destroy
   module procedure destroy_state, destroy_raw_state
end interface
```

262e ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
private :: destroy_state, destroy_raw_state
```

263a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine destroy_state (s)
  type(tao_random_state), intent(inout) :: s
  deallocate (s%buffer)
end subroutine destroy_state
```

Currently, this is a no-op, but we might need a non-trivial destruction method in the future

263b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine destroy_raw_state (s)
  type(tao_random_raw_state), intent(inout) :: s
end subroutine destroy_raw_state
```

C.3.3 Copying

263c ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡

```
interface tao_random_copy
   module procedure ⟨Specific procedures for tao_random_copy 263f⟩
end interface
```

263d ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡

```
interface assignment(=)
   module procedure ⟨Specific procedures for tao_random_copy 263f⟩
end interface
```

263e ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
public :: assignment(=)
private :: ⟨Specific procedures for tao_random_copy 263f⟩
```

263f ⟨*Specific procedures for* `tao_random_copy` 263f⟩≡

```
copy_state, copy_raw_state, &
copy_raw_state_to_state, copy_state_to_raw_state
```

263g ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine copy_state (lhs, rhs)
  type(tao_random_state), intent(inout) :: lhs
  type(tao_random_state), intent(in) :: rhs
  call copy_raw_state (lhs%state, rhs%state)
  if (size (lhs%buffer) /= size (rhs%buffer)) then
     deallocate (lhs%buffer)
     allocate (lhs%buffer(size(rhs%buffer)))
  end if
  lhs%buffer = rhs%buffer
  lhs%buffer_end = rhs%buffer_end
  lhs%last = rhs%last
end subroutine copy_state
```

264a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine copy_raw_state (lhs, rhs)
  type(tao_random_raw_state), intent(out) :: lhs
  type(tao_random_raw_state), intent(in) :: rhs
  lhs%x = rhs%x
end subroutine copy_raw_state
```

264b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine copy_raw_state_to_state (lhs, rhs)
  type(tao_random_state), intent(inout) :: lhs
  type(tao_random_raw_state), intent(in) :: rhs
  call copy_raw_state (lhs%state, rhs)
  call tao_random_flush (lhs)
end subroutine copy_raw_state_to_state
```

264c ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine copy_state_to_raw_state (lhs, rhs)
  type(tao_random_raw_state), intent(out) :: lhs
  type(tao_random_state), intent(in) :: rhs
  call copy_raw_state (lhs, rhs%state)
end subroutine copy_state_to_raw_state
```

C.3.4 Flushing

264d ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
elemental subroutine tao_random_flush (s)
  type(tao_random_state), intent(inout) :: s
  s%last = size (s%buffer)
end subroutine tao_random_flush
```

C.3.5 Input and Output

264e ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡

```
interface tao_random_write
   module procedure &
        write_state_unit, write_state_name, &
        write_raw_state_unit, write_raw_state_name
end interface
```

264f ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
private :: write_state_unit, write_state_name
private :: write_raw_state_unit, write_raw_state_name
```

265a ⟨*Interfaces of* tao_random_numbers 257d⟩+≡

```
interface tao_random_read
   module procedure &
        read_state_unit, read_state_name, &
        read_raw_state_unit, read_raw_state_name
end interface
```

265b ⟨*Declaration of* tao_random_numbers 253b⟩+≡

```
private :: read_state_unit, read_state_name
private :: read_raw_state_unit, read_raw_state_name
```

265c ⟨*Implementation of* tao_random_numbers 253f⟩+≡

```
subroutine write_state_unit (s, unit)
  type(tao_random_state), intent(in) :: s
  integer, intent(in) :: unit
  write (unit = unit, fmt = *) "BEGIN TAO_RANDOM_STATE"
  call write_raw_state_unit (s%state, unit)
  write (unit = unit, fmt = "(2(1x,a16,1x,i10/),1x,a16,1x,i10)") &
       "BUFFER_SIZE", size (s%buffer), &
       "BUFFER_END", s%buffer_end, &
       "LAST", s%last
  write (unit = unit, fmt = *) "BEGIN BUFFER"
  call write_state_array (s%buffer, unit)
  write (unit = unit, fmt = *) "END BUFFER"
  write (unit = unit, fmt = *) "END TAO_RANDOM_STATE"
end subroutine write_state_unit
```

265d ⟨*Implementation of* tao_random_numbers 253f⟩+≡

```
subroutine read_state_unit (s, unit)
  type(tao_random_state), intent(inout) :: s
  integer, intent(in) :: unit
  integer :: buffer_size
  read (unit = unit, fmt = *)
  call read_raw_state_unit (s%state, unit)
  read (unit = unit, fmt = "(2(1x,16x,1x,i10/),1x,16x,1x,i10)") &
       buffer_size, s%buffer_end, s%last
  read (unit = unit, fmt = *)
  if (buffer_size /= size (s%buffer)) then
     deallocate (s%buffer)
     allocate (s%buffer(buffer_size))
  end if
  call read_state_array (s%buffer, unit)
  read (unit = unit, fmt = *)
  read (unit = unit, fmt = *)
end subroutine read_state_unit
```

266a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
subroutine write_raw_state_unit (s, unit)
  type(tao_random_raw_state), intent(in) :: s
  integer, intent(in) :: unit
  write (unit = unit, fmt = *) "BEGIN TAO_RANDOM_RAW_STATE"
  call write_state_array (s%x, unit)
  write (unit = unit, fmt = *) "END TAO_RANDOM_RAW_STATE"
end subroutine write_raw_state_unit
```

266b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
subroutine read_raw_state_unit (s, unit)
  type(tao_random_raw_state), intent(inout) :: s
  integer, intent(in) :: unit
  read (unit = unit, fmt = *)
  call read_state_array (s%x, unit)
  read (unit = unit, fmt = *)
end subroutine read_raw_state_unit
```

266c ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
subroutine write_state_array (a, unit)
  integer(kind=tao_i32), dimension(:), intent(in) :: a
  integer, intent(in) :: unit
  integer :: i
  do i = 1, size (a)
     write (unit = unit, fmt = "(1x,i10,1x,i10)") i, a(i)
  end do
end subroutine write_state_array
```

266d ⟨*Declaration of 30-bit* `tao_random_numbers` 266d⟩≡

```
private :: write_state_array
```

266e ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
subroutine read_state_array (a, unit)
  integer(kind=tao_i32), dimension(:), intent(inout) :: a
  integer, intent(in) :: unit
  integer :: i, idum
  do i = 1, size (a)
     read (unit = unit, fmt = *) idum, a(i)
  end do
end subroutine read_state_array
```

266f ⟨*Declaration of 30-bit* `tao_random_numbers` 266d⟩+≡

```
private :: read_state_array
```

Reading and writing 52-bit floating point numbers accurately is beyond most Fortran runtime libraries. Their job is simplified considerably if we rescale by 2^{52} before writing. Then the temptation to truncate will not be as overwhelming as before ...

267a ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡
```
subroutine write_state_array (a, unit)
  real(kind=tao_r64), dimension(:), intent(in) :: a
  integer, intent(in) :: unit
  integer :: i
  do i = 1, size (a)
     write (unit = unit, fmt = "(1x,i10,1x,f30.0)") i, 2.0_tao_r64**52 * a(i)
  end do
end subroutine write_state_array
```

267b ⟨*Declaration of 52-bit* `tao_random_numbers` 267b⟩≡
```
private :: write_state_array
```

267c ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡
```
subroutine read_state_array (a, unit)
  real(kind=tao_r64), dimension(:), intent(inout) :: a
  integer, intent(in) :: unit
  real(kind=tao_r64) :: x
  integer :: i, idum
  do i = 1, size (a)
     read (unit = unit, fmt = *) idum, x
     a(i) = 2.0_tao_r64**(-52) * x
  end do
end subroutine read_state_array
```

267d ⟨*Declaration of 52-bit* `tao_random_numbers` 267b⟩+≡
```
private :: read_state_array
```

267e ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡
```
subroutine find_free_unit (u, iostat)
  integer, intent(out) :: u
  integer, intent(out), optional :: iostat
  logical :: exists, is_open
  integer :: i, status
  do i = MIN_UNIT, MAX_UNIT
     inquire (unit = i, exist = exists, opened = is_open, &
              iostat = 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
```

268a ⟨*Variables in* tao_random_numbers 268a⟩≡

```
integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99
```

268b ⟨*Declaration of* tao_random_numbers 253b⟩+≡

```
private :: find_free_unit
```

268c ⟨*Implementation of* tao_random_numbers 253f⟩+≡

```
subroutine write_state_name (s, name)
  type(tao_random_state), intent(in) :: s
  character(len=*), intent(in) :: name
  integer :: unit
  call find_free_unit (unit)
  open (unit = unit, action = "write", status = "replace", file = name)
  call write_state_unit (s, unit)
  close (unit = unit)
end subroutine write_state_name
```

268d ⟨*Implementation of* tao_random_numbers 253f⟩+≡

```
subroutine write_raw_state_name (s, name)
  type(tao_random_raw_state), intent(in) :: s
  character(len=*), intent(in) :: name
  integer :: unit
  call find_free_unit (unit)
  open (unit = unit, action = "write", status = "replace", file = name)
  call write_raw_state_unit (s, unit)
  close (unit = unit)
end subroutine write_raw_state_name
```

268e ⟨*Implementation of* tao_random_numbers 253f⟩+≡

```
subroutine read_state_name (s, name)
  type(tao_random_state), intent(inout) :: s
  character(len=*), intent(in) :: name
  integer :: unit
  call find_free_unit (unit)
  open (unit = unit, action = "read", status = "old", file = name)
```

```
    call read_state_unit (s, unit)
    close (unit = unit)
  end subroutine read_state_name
```

269a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  subroutine read_raw_state_name (s, name)
    type(tao_random_raw_state), intent(inout) :: s
    character(len=*), intent(in) :: name
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "read", status = "old", file = name)
    call read_raw_state_unit (s, unit)
    close (unit = unit)
  end subroutine read_raw_state_name
```

C.3.6 Marshaling and Unmarshaling

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

269b ⟨*Interfaces of* `tao_random_numbers` 257d⟩+≡

```
  interface tao_random_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
```

269c ⟨*Declaration of* `tao_random_numbers` 253b⟩+≡

```
  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
```

269d ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine marshal_state (s, ibuf, dbuf)
    type(tao_random_state), intent(in) :: s
    integer, dimension(:), intent(inout) :: ibuf
    real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
```

```
    integer :: buf_size
    buf_size = size (s%buffer)
    ibuf(1) = s%buffer_end
    ibuf(2) = s%last
    ibuf(3) = buf_size
    ibuf(4:3+buf_size) = s%buffer
    call marshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
  end subroutine marshal_state
```

270a ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine marshal_state_size (s, iwords, dwords)
    type(tao_random_state), intent(in) :: s
    integer, intent(out) :: iwords, dwords
    call marshal_raw_state_size (s%state, iwords, dwords)
    iwords = iwords + 3 + size (s%buffer)
  end subroutine marshal_state_size
```

270b ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine unmarshal_state (s, ibuf, dbuf)
    type(tao_random_state), intent(inout) :: s
    integer, dimension(:), intent(in) :: ibuf
    real(kind=tao_r64), dimension(:), intent(in) :: dbuf
    integer :: buf_size
    s%buffer_end = ibuf(1)
    s%last = ibuf(2)
    buf_size = ibuf(3)
    s%buffer = ibuf(4:3+buf_size)
    call unmarshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
  end subroutine unmarshal_state
```

270c ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine marshal_raw_state (s, ibuf, dbuf)
    type(tao_random_raw_state), intent(in) :: s
    integer, dimension(:), intent(inout) :: ibuf
    real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
    ibuf(1) = size (s%x)
    ibuf(2:1+size(s%x)) = s%x
  end subroutine marshal_raw_state
```

270d ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine marshal_raw_state_size (s, iwords, dwords)
    type(tao_random_raw_state), intent(in) :: s
    integer, intent(out) :: iwords, dwords
    iwords = 1 + size (s%x)
    dwords = 0
  end subroutine marshal_raw_state_size
```

271a ⟨*Implementation of 30-bit* tao_random_numbers 253a⟩+≡
```
pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  buf_size = ibuf(1)
  s%x = ibuf(2:1+buf_size)
end subroutine unmarshal_raw_state
```

271b ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡
```
pure subroutine marshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  integer :: buf_size
  buf_size = size (s%buffer)
  ibuf(1) = s%buffer_end
  ibuf(2) = s%last
  ibuf(3) = buf_size
  dbuf(1:buf_size) = s%buffer
  call marshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine marshal_state
```

271c ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡
```
pure subroutine marshal_state_size (s, iwords, dwords)
  type(tao_random_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  call marshal_raw_state_size (s%state, iwords, dwords)
  iwords = iwords + 3
  dwords = dwords + size(s%buffer)
end subroutine marshal_state_size
```

271d ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡
```
pure subroutine unmarshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  s%buffer_end = ibuf(1)
  s%last = ibuf(2)
  buf_size = ibuf(3)
  s%buffer = dbuf(1:buf_size)
  call unmarshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine unmarshal_state
```

272a ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡

```
pure subroutine marshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  ibuf(1) = size (s%x)
  dbuf(1:size(s%x)) = s%x
end subroutine marshal_raw_state
```

272b ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡

```
pure subroutine marshal_raw_state_size (s, iwords, dwords)
  type(tao_random_raw_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  iwords = 1
  dwords = size (s%x)
end subroutine marshal_raw_state_size
```

272c ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡

```
pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  buf_size = ibuf(1)
  s%x = dbuf(1:buf_size)
end subroutine unmarshal_raw_state
```

C.4 High Level Routines

272d ⟨tao_random_numbers.f90 272d⟩≡

```
! tao_random_numbers.f90 --
⟨Copyleft notice 1⟩
module tao_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
  ⟨Declaration of tao_random_numbers 253b⟩
  ⟨Declaration of 30-bit tao_random_numbers 266d⟩
  ⟨Interfaces of tao_random_numbers 257d⟩
  ⟨Interfaces of 30-bit tao_random_numbers 279f⟩
  ⟨Parameters in tao_random_numbers 252a⟩
  ⟨Variables in tao_random_numbers 268a⟩
```

```
  ⟨Variables in 30-bit tao_random_numbers 252c⟩
  ⟨Declaration of 30-bit tao_random_numbers types 260b⟩
  character(len=*), public, parameter :: TAO_RANDOM_NUMBERS_RCS_ID = &
       "$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of tao_random_numbers 253f⟩
  ⟨Implementation of 30-bit tao_random_numbers 253a⟩
end module tao_random_numbers
```

273a ⟨tao52_random_numbers.f90 273a⟩≡

```
! tao52_random_numbers.f90 --
⟨Copyleft notice 1⟩
module tao52_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
  ⟨Declaration of tao_random_numbers 253b⟩
  ⟨Declaration of 52-bit tao_random_numbers 267b⟩
  ⟨Interfaces of tao_random_numbers 257d⟩
  ⟨Interfaces of 52-bit tao_random_numbers 280d⟩
  ⟨Parameters in tao_random_numbers 252a⟩
  ⟨Variables in tao_random_numbers 268a⟩
  ⟨Variables in 52-bit tao_random_numbers 257g⟩
  ⟨Declaration of 52-bit tao_random_numbers types 260d⟩
  character(len=*), public, parameter :: TAO52_RANDOM_NUMBERS_RCS_ID = &
       "$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of tao_random_numbers 253f⟩
  ⟨Implementation of 52-bit tao_random_numbers 258b⟩
end module tao52_random_numbers
```

Ten functions are exported

273b ⟨Declaration of tao_random_numbers 253b⟩+≡

```
public :: tao_random_number
public :: tao_random_seed
public :: tao_random_create
public :: tao_random_destroy
public :: tao_random_copy
public :: tao_random_read
public :: tao_random_write
public :: tao_random_flush
! public :: tao_random_luxury
public :: tao_random_test
```

C.4.1 Single Random Numbers

A random integer r with $0 \leq r < 2^{30} = 1073741824$:

274a ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡
```
pure subroutine integer_stateless &
     (state, buffer, buffer_end, last, r)
  integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
  integer, intent(in) :: buffer_end
  integer, intent(inout) :: last
  integer, intent(out) :: r
  integer, parameter :: NORM = 1
  ⟨Body of tao_random_* 274b⟩
end subroutine integer_stateless
```

274b ⟨*Body of* `tao_random_*` 274b⟩≡
```
⟨Step last and reload buffer iff necessary 274d⟩
r = NORM * buffer(last)
```

The low level routine `generate` will fill an array $a_1, \ldots, a_n$, which will be consumed and refilled like an input buffer. We need at least $n \geq K$ for the call to `generate`.

274c ⟨*Variables in 30-bit* `tao_random_numbers` 252c⟩+≡
```
integer(kind=tao_i32), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
integer, save, private :: s_buffer_end = size (s_buffer)
integer, save, private :: s_last = size (s_buffer)
```

Increment the index `last` and reload the array `buffer`, iff this buffer is exhausted. Throughout these routines, `last` will point to random number that has just been consumed. For the array filling routines below, this is simpler than pointing to the next waiting number.

274d ⟨*Step* `last` *and reload* `buffer` *iff necessary* 274d⟩≡
```
last = last + 1
if (last > buffer_end) then
   call generate (buffer, state)
   last = 1
end if
```

A random real $r \in [0, 1)$. This is almost identical to `tao_random_integer`, but we duplicate the code to avoid the function call overhead for speed.

274e ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡
```
pure subroutine real_stateless (state, buffer, buffer_end, last, r)
  integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
  integer, intent(in) :: buffer_end
  integer, intent(inout) :: last
  real(kind=default), intent(out) :: r
```

```
    real(kind=default), parameter :: NORM = 1.0_default / M
    ⟨Body of tao_random_* 274b⟩
  end subroutine real_stateless
```

A random real $r \in [0, 1)$.

275a ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
  pure subroutine real_stateless (state, buffer, buffer_end, last, r)
    real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    real(kind=default), intent(out) :: r
    integer, parameter :: NORM = 1
    ⟨Body of tao_random_* 274b⟩
  end subroutine real_stateless
```

The low level routine `generate` will fill an array $a_1, \ldots, a_N$, which will be consumed and refilled like an input buffer.

275b ⟨*Variables in 52-bit* `tao_random_numbers` 257g⟩+≡

```
  real(kind=tao_r64), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
  integer, save, private :: s_buffer_end = size (s_buffer)
  integer, save, private :: s_last = size (s_buffer)
```

C.4.2 Arrays of Random Numbers

Fill the array $j_1, \ldots, j_\nu$ 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.

275c ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  pure subroutine integer_array_stateless &
       (state, buffer, buffer_end, last, v, num)
    integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    integer, dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    integer, parameter :: NORM = 1
    ⟨Body of tao_random_*_array 275d⟩
  end subroutine integer_array_stateless
```

275d ⟨*Body of* `tao_random_*_array` 275d⟩≡

```
  integer :: nu, done, todo, chunk
  ⟨Set nu to num or size(v) 276a⟩
  ⟨Prepare array buffer and done, todo, chunk 276b⟩
```

```
v(1:chunk) = NORM * buffer(last+1:last+chunk)
do
   ⟨Update last, done and todo and set new chunk 276c⟩
   ⟨Reload buffer or exit 276d⟩
   v(done+1:done+chunk) = NORM * buffer(1:chunk)
end do
```

276a ⟨*Set* `nu` *to* `num` *or* `size(v)` 276a⟩≡

```
if (present (num)) then
   nu = num
else
   nu = size (v)
end if
```

`last` is used as an offset into the buffer `buffer`, as usual. `done` is an offset into the target. We still have to process all `nu` numbers. The first chunk can only use what's left in the buffer.

276b ⟨*Prepare array* `buffer` *and* `done`, `todo`, `chunk` 276b⟩≡

```
if (last >= buffer_end) then
   call generate (buffer, state)
   last = 0
end if
done = 0
todo = nu
chunk = min (todo, buffer_end - last)
```

This logic is a bit weird, but after the first chunk, `todo` will either vanish (in which case we're done) or we have consumed all of the buffer and must reload. In any case we can pretend that the next chunk can use the whole buffer.

276c ⟨*Update* `last`, `done` *and* `todo` *and set new* `chunk` 276c⟩≡

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

276d ⟨*Reload* `buffer` *or exit* 276d⟩≡

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

276e ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
pure subroutine real_array_stateless &
     (state, buffer, buffer_end, last, v, num)
```

```
    integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    real(kind=default), parameter :: NORM = 1.0_default / M
    ⟨Body of tao_random_*_array 275d⟩
  end subroutine real_array_stateless
```

Fill the array $v_1, \ldots, v_\nu$ with uniform deviates $v_i \in [0, 1)$.

277a ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
  pure subroutine real_array_stateless &
       (state, buffer, buffer_end, last, v, num)
    real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    integer, parameter :: NORM = 1
    ⟨Body of tao_random_*_array 275d⟩
  end subroutine real_array_stateless
```

C.4.3 Procedures With Explicit `tao_random_state`

Unfortunately, this is very boring, but Fortran's lack of parametric polymorphism forces this duplication on us:

277b ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  elemental subroutine integer_state (s, r)
    type(tao_random_state), intent(inout) :: s
    integer, intent(out) :: r
    call integer_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
  end subroutine integer_state
```

277c ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
  elemental subroutine real_state (s, r)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(out) :: r
    call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
  end subroutine real_state
```

277d ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
  elemental subroutine real_state (s, r)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(out) :: r
```

```
    call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
  end subroutine real_state
```

278a ⟨*Implementation of 30-bit* tao_random_numbers 253a⟩+≡

```
  pure subroutine integer_array_state (s, v, num)
    type(tao_random_state), intent(inout) :: s
    integer, dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    call integer_array_stateless &
         (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
  end subroutine integer_array_state
```

278b ⟨*Implementation of 30-bit* tao_random_numbers 253a⟩+≡

```
  pure subroutine real_array_state (s, v, num)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    call real_array_stateless &
           (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
  end subroutine real_array_state
```

278c ⟨*Implementation of 52-bit* tao_random_numbers 258b⟩+≡

```
  pure subroutine real_array_state (s, v, num)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    call real_array_stateless &
         (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
  end subroutine real_array_state
```

C.4.4 Static Procedures

First make sure that `tao_random_seed` has been called to initialize the generator state:

278d ⟨*Initialize a virginal random number generator* 278d⟩≡

```
  if (s_virginal) then
     call tao_random_seed ()
  end if
```

278e ⟨*Implementation of 30-bit* tao_random_numbers 253a⟩+≡

```
  subroutine integer_static (r)
    integer, intent(out) :: r
    ⟨Initialize a virginal random number generator 278d⟩
    call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
  end subroutine integer_static
```

279a ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
subroutine real_static (r)
  real(kind=default), intent(out) :: r
  ⟨Initialize a virginal random number generator 278d⟩
  call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static
```

279b ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
subroutine real_static (r)
  real(kind=default), intent(out) :: r
  ⟨Initialize a virginal random number generator 278d⟩
  call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static
```

279c ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
subroutine integer_array_static (v, num)
  integer, dimension(:), intent(out) :: v
  integer, optional, intent(in) :: num
  ⟨Initialize a virginal random number generator 278d⟩
  call integer_array_stateless &
       (s_state, s_buffer, s_buffer_end, s_last, v, num)
end subroutine integer_array_static
```

279d ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡

```
subroutine real_array_static (v, num)
  real(kind=default), dimension(:), intent(out) :: v
  integer, optional, intent(in) :: num
  ⟨Initialize a virginal random number generator 278d⟩
  call real_array_stateless &
       (s_state, s_buffer, s_buffer_end, s_last, v, num)
end subroutine real_array_static
```

279e ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
subroutine real_array_static (v, num)
  real(kind=default), dimension(:), intent(out) :: v
  integer, optional, intent(in) :: num
  ⟨Initialize a virginal random number generator 278d⟩
  call real_array_stateless &
       (s_state, s_buffer, s_buffer_end, s_last, v, num)
end subroutine real_array_static
```

C.4.5 Generic Procedures

279f ⟨*Interfaces of 30-bit* `tao_random_numbers` 279f⟩≡

```
interface tao_random_number
```

```
    module procedure ⟨Specific procedures for 30-bit tao_random_number 280a⟩
  end interface
```

280a ⟨*Specific procedures for 30-bit* `tao_random_number` 280a⟩≡

```
  integer_static, integer_state, &
  integer_array_static, integer_array_state, &
  real_static, real_state, real_array_static, real_array_state
```

These are not exported

280b ⟨*Declaration of 30-bit* `tao_random_numbers` 266d⟩+≡

```
  private :: &
       integer_stateless, integer_array_stateless, &
       real_stateless, real_array_stateless
```

280c ⟨*Declaration of 30-bit* `tao_random_numbers` 266d⟩+≡

```
  private :: ⟨Specific procedures for 30-bit tao_random_number 280a⟩
```

280d ⟨*Interfaces of 52-bit* `tao_random_numbers` 280d⟩≡

```
  interface tao_random_number
    module procedure ⟨Specific procedures for 52-bit tao_random_number 280e⟩
  end interface
```

280e ⟨*Specific procedures for 52-bit* `tao_random_number` 280e⟩≡

```
  real_static, real_state, real_array_static, real_array_state
```

Thes are not exported

280f ⟨*Declaration of 52-bit* `tao_random_numbers` 267b⟩+≡

```
  private :: real_stateless, real_array_stateless
```

280g ⟨*Declaration of 52-bit* `tao_random_numbers` 267b⟩+≡

```
  private :: ⟨Specific procedures for 52-bit tao_random_number 280e⟩
```

C.4.6 Luxury

280h ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  pure subroutine luxury_stateless &
       (buffer_size, buffer_end, last, consumption)
    integer, intent(in) :: buffer_size
    integer, intent(inout) :: buffer_end
    integer, intent(inout) :: last
    integer, intent(in) :: consumption
    if (consumption >= 1 .and. consumption <= buffer_size) then
       buffer_end = consumption
       last = min (last, buffer_end)
    else
       !!! print *, "tao_random_luxury: ", "invalid consumption ", &
       !!!      consumption, ", not in [ 1,", buffer_size, "]."
```

```
      buffer_end = buffer_size
    end if
  end subroutine luxury_stateless
```

281a ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  elemental subroutine luxury_state (s)
    type(tao_random_state), intent(inout) :: s
    call luxury_state_integer (s, size (s%buffer))
  end subroutine luxury_state
```

281b ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  elemental subroutine luxury_state_integer (s, consumption)
    type(tao_random_state), intent(inout) :: s
    integer, intent(in) :: consumption
    call luxury_stateless (size (s%buffer), s%buffer_end, s%last, consumption)
  end subroutine luxury_state_integer
```

281c ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  elemental subroutine luxury_state_real (s, consumption)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(in) :: consumption
    call luxury_state_integer (s, int (consumption * size (s%buffer)))
  end subroutine luxury_state_real
```

281d ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  subroutine luxury_static ()
    ⟨Initialize a virginal random number generator 278d⟩
    call luxury_static_integer (size (s_buffer))
  end subroutine luxury_static
```

281e ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  subroutine luxury_static_integer (consumption)
    integer, intent(in) :: consumption
    ⟨Initialize a virginal random number generator 278d⟩
    call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
  end subroutine luxury_static_integer
```

281f ⟨*Implementation of* `tao_random_numbers` 253f⟩+≡

```
  subroutine luxury_static_real (consumption)
    real(kind=default), intent(in) :: consumption
    ⟨Initialize a virginal random number generator 278d⟩
    call luxury_static_integer (int (consumption * size (s_buffer)))
  end subroutine luxury_static_real
```

281g ⟨*Interfaces of* `tao_random_numbers` *(unused luxury)* 281g⟩≡

```
  interface tao_random_luxury
     module procedure ⟨Specific procedures for tao_random_luxury 282c⟩
  end interface
```

282a ⟨*Declaration of* `tao_random_numbers` *(unused luxury)* 282a⟩≡
```
private :: luxury_stateless
```

282b ⟨*Declaration of* `tao_random_numbers` *(unused luxury)* 282a⟩+≡
```
private :: ⟨Specific procedures for tao_random_luxury 282c⟩
```

282c ⟨*Specific procedures for* `tao_random_luxury` 282c⟩≡
```
luxury_static, luxury_state, &
luxury_static_integer, luxury_state_integer, &
luxury_static_real, luxury_state_real
```

C.5 Testing

C.5.1 30-bit

282d ⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩+≡
```
subroutine tao_random_test (name)
  character(len=*), optional, intent(in) :: name
  character (len = *), parameter :: &
       OK = "(1x,i10,' is ok.')", &
       NOT_OK = "(1x,i10,' is not ok, (expected ',i10,')!')"
  ⟨Parameters in tao_random_test 282e⟩
  integer, parameter :: &
       A_2027082 = 461390032
  integer, dimension(N) :: a
  type(tao_random_state) :: s, t
  integer, dimension(:), allocatable :: ibuf
  real(kind=tao_r64), dimension(:), allocatable :: dbuf
  integer :: i, ibuf_size, dbuf_size
  print *, TAO_RANDOM_NUMBERS_RCS_ID
  print *, "testing the 30-bit tao_random_numbers ..."
  ⟨Perform simple tests of tao_random_numbers 283a⟩
  ⟨Perform more tests of tao_random_numbers 283d⟩
end subroutine tao_random_test
```

282e ⟨*Parameters in* `tao_random_test` 282e⟩≡
```
integer, parameter :: &
     SEED = 310952, &
     N = 2009, M = 1009, &
     N_SHORT = 1984
```

DEK's "official" test expects $a_{1009\cdot 2009+1} = a_{2027082} = 461390032$:

283a ⟨*Perform simple tests of* `tao_random_numbers` 283a⟩≡

```
! call tao_random_luxury ()
call tao_random_seed (SEED)
do i = 1, N+1
   call tao_random_number (a, M)
end do
```

⟨*Test* `a(1) = A_2027082` 283b⟩

283b ⟨*Test* `a(1) = A_2027082` 283b⟩≡

```
if (a(1) == A_2027082) then
   print OK, a(1)
else
   print NOT_OK, a(1), A_2027082
end if
```

Deja vu all over again, but 2027081 is factored the other way around this time

283c ⟨*Perform simple tests of* `tao_random_numbers` 283a⟩+≡

```
call tao_random_seed (SEED)
do i = 1, M+1
   call tao_random_number (a)
end do
```

⟨*Test* `a(1) = A_2027082` 283b⟩

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

283d ⟨*Perform more tests of* `tao_random_numbers` 283d⟩≡

```
print *, "testing the stateless stuff ..."
call tao_random_create (s, SEED)
do i = 1, N_SHORT
   call tao_random_number (s, a, M)
end do
call tao_random_create (t, s)
do i = 1, N+1 - N_SHORT
   call tao_random_number (s, a, M)
end do
```

⟨*Test* `a(1) = A_2027082` 283b⟩

and restart the saved generator

283e ⟨*Perform more tests of* `tao_random_numbers` 283d⟩+≡

```
do i = 1, N+1 - N_SHORT
   call tao_random_number (t, a, M)
end do
```

⟨*Test* `a(1) = A_2027082` 283b⟩

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

284a ⟨*Perform more tests of* `tao_random_numbers` 283d⟩+≡

```
if (present (name)) then
   print *, "testing I/O ..."
   call tao_random_seed (s, SEED)
   do i = 1, N_SHORT
      call tao_random_number (s, a, M)
   end do
   call tao_random_write (s, name)
   do i = 1, N+1 - N_SHORT
      call tao_random_number (s, a, M)
   end do
   ⟨Test a(1) = A_2027082 283b⟩
   call tao_random_read (s, name)
   do i = 1, N+1 - N_SHORT
      call tao_random_number (s, a, M)
   end do
   ⟨Test a(1) = A_2027082 283b⟩
end if
```

And finally using marshaling/unmarshaling:

284b ⟨*Perform more tests of* `tao_random_numbers` 283d⟩+≡

```
print *, "testing marshaling/unmarshaling ..."
call tao_random_seed (s, SEED)
do i = 1, N_SHORT
   call tao_random_number (s, a, M)
end do
call tao_random_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 283b⟩
call tao_random_unmarshal (s, ibuf, dbuf)
do i = 1, N+1 - N_SHORT
   call tao_random_number (s, a, M)
end do
⟨Test a(1) = A_2027082 283b⟩
```

C.5.2 52-bit

DEK's "official" test expects $x_{1009\cdot 2009+1} = x_{2027082} = 0.27452626307394156768$:

284c ⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩+≡

```
subroutine tao_random_test (name)
  character(len=*), optional, intent(in) :: name
  character(len=*), parameter :: &
       OK = "(1x,f22.20,' is ok.')", &
       NOT_OK = "(1x,f22.20,' is not ok, (A_2027082 ',f22.20,')!')"
  ⟨Parameters in tao_random_test 282e⟩
  real(kind=default), parameter :: &
       A_2027082 = 0.27452626307394156768_default
  real(kind=default), dimension(N) :: a
  type(tao_random_state) :: s, t
  integer, dimension(:), allocatable :: ibuf
  real(kind=tao_r64), dimension(:), allocatable :: dbuf
  integer :: i, ibuf_size, dbuf_size
  print *, TAO52_RANDOM_NUMBERS_RCS_ID
  print *, "testing the 52-bit tao_random_numbers ..."
  ⟨Perform simple tests of tao_random_numbers 283a⟩
  ⟨Perform more tests of tao_random_numbers 283d⟩
end subroutine tao_random_test
```

C.5.3 Test Program

285 ⟨`tao_test.f90` 285⟩≡

```
program tao_test
  use tao_random_numbers, only: test30 => tao_random_test
  use tao52_random_numbers, only: test52 => tao_random_test
  implicit none
  call test30 ("tmp.tao")
  call test52 ("tmp.tao")
end program tao_test
```

—D— Special Functions

286a ⟨specfun.f90 286a⟩≡

```
! specfun.f90 --
⟨Copyleft notice 1⟩
module specfun
  use kinds
! use constants
  implicit none
  private
  ⟨Declaration of specfun procedures 286b⟩
  character(len=*), public, parameter :: SPECFUN_RCS_ID = &
       "$Id: specfun.nw 314 2010-04-17 20:32:33Z ohl $"
  !WK:
  real(kind=default), public, parameter :: &
       PI = 3.1415926535897932384626433832795028841972_default
contains
  ⟨Implementation of specfun procedures 287c⟩
end module specfun
```

The algorithm is stolen from the FORTRAN version in routine C303 of the CERN library [24]. It has an accuracy which is approximately one digit less than machine precision.

286b ⟨Declaration of specfun procedures 286b⟩≡

```
public :: gamma
```

The so-called reflection formula is used for negative arguments:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \tag{D.1}$$

Here's the identity transformation that pulls the argument of Γ into $[3,4]$:

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

287a ⟨*Pull u into the intervall* $[3,4]$ 287a⟩≡

```
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:

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

287b ⟨*Clenshaw's recurrence formula* 287b⟩≡

```
alpha = 2*g
b1 = 0
b2 = 0
do i = 15, 0, -1
   b0 = c(i) + alpha * b1 - b2
   b2 = b1
   b1 = b0
end do
g = f * (b0 - g * b2)
```

Note that we're assuming that `c(0)` is in fact $c_0/2$. This is for compatibility with the CERN library routines.

287c ⟨*Implementation of* `specfun` *procedures* 287c⟩≡

```
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 = ⟨c0/2, c1, c2, ..., c15 for Γ(x) 288a⟩
  u = x
  if (u <= 0.0) then
```

```
      if (u == int (u)) then
         g = huge (g)
         return
      else
         u = 1 - u
      end if
   endif
```
⟨*Pull u into the intervall* $[3,4]$ 287a⟩

```
   g = 2*u - 7
```
⟨*Clenshaw's recurrence formula* 287b⟩

```
   if (x < 0) then
      g = PI / (sin (PI * x) * g)
   end if
end function gamma
```

288a ⟨$c_0/2, c_1, c_2, \ldots, c_{15}$ *for* $\Gamma(x)$ 288a⟩≡

```
(/ 3.65738772508338244_default, &
   1.95754345666126827_default, &
   0.33829711382616039_default, &
   0.04208951276557549_default, &
   0.00428765048212909_default, &
   0.00036521216929462_default, &
   0.00002740064222642_default, &
   0.00000181240233365_default, &
   0.00000010965775866_default, &
   0.00000000598718405_default, &
   0.00000000030769081_default, &
   0.00000000001431793_default, &
   0.00000000000065109_default, &
   0.00000000000002596_default, &
   0.00000000000000111_default, &
   0.00000000000000004_default /)
```

D.1 Test

288b ⟨stest.f90 288b⟩≡

```
! stest.f90 --
```
⟨*Copyleft notice* 1⟩

```
module stest_functions
  use kinds
  use constants
  use specfun
```

```
    private
    ⟨Declaration of stest_functions procedures 289a⟩
  contains
    ⟨Implementation of stest_functions procedures 289b⟩
  end module stest_functions
```

289a ⟨*Declaration of* `stest_functions` *procedures* 289a⟩≡

```
  public :: gauss_multiplication
```

Gauss' multiplication fomula can serve as a non-trivial test

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \tag{D.4}$$

289b ⟨*Implementation of* `stest_functions` *procedures* 289b⟩≡

```
  pure function gauss_multiplication (x, n) result (delta)
    real(kind=default), intent(in) :: x
    integer, intent(in) :: n
    real(kind=default) :: delta
    real(kind=default) :: gxn
    integer :: k
    gxn = (2*PI)**(0.5_double*(1-n)) * n**(n*x-0.5_double)
    do k = 0, n - 1
       gxn = gxn * gamma (x + real (k, kind=default) / n)
    end do
    delta = abs ((gamma (n*x) - gxn) / gamma (n*x))
  end function gauss_multiplication
```

289c ⟨`stest.f90` 288b⟩+≡

```
  program stest
    use kinds
    use specfun
    use stest_functions !NODEP!
    implicit none
    integer :: i, steps
    real(kind=default) :: x, g, xmin, xmax
    xmin = -4.5
    xmax =  4.5
    steps = 100 ! 9
    do i = 0, steps
       x = xmin + ((xmax - xmin) / real (steps)) * i
       print "(f6.3,4(1x,e9.2))", x, &
            gauss_multiplication (x, 2), &
            gauss_multiplication (x, 3), &
            gauss_multiplication (x, 4), &
```

```
          gauss_multiplication (x, 5)
  end do
end program stest
```

—E— Statistics

291a ⟨vamp_stat.f90 291a⟩≡
```
! vamp_stat.f90 --
⟨Copyleft notice 1⟩
module vamp_stat
  use kinds
  implicit none
  private
  ⟨Declaration of vamp_stat procedures 291b⟩
  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 291c⟩
end module vamp_stat
```

291b ⟨Declaration of vamp_stat procedures 291b⟩≡
```
public :: average, standard_deviation, value_spread
```

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

291c ⟨Implementation of vamp_stat procedures 291c⟩≡
```
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
```

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

292a ⟨*Implementation of* vamp_stat *procedures* 291c⟩+≡

```
pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
     s = huge (s)
  else
     s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
                    0.0_default))
  end if
end function standard_deviation
```

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

292b ⟨*Implementation of* vamp_stat *procedures* 291c⟩+≡

```
pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread
```

292c ⟨*Declaration of* vamp_stat *procedures* 291b⟩+≡

```
public :: standard_deviation_percent, value_spread_percent
```

292d ⟨*Implementation of* vamp_stat *procedures* 291c⟩+≡

```
pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
     s = huge (s)
  else
     s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent
```

292e ⟨*Implementation of* vamp_stat *procedures* 291c⟩+≡

```
pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
```

```
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
     s = huge (s)
  else
     s = 100.0 * value_spread (x) / abs_avg
  end if
end function value_spread_percent
```

—F— HISTOGRAMMING

Merged WK's improvements for WHIZARD. TODO *after* merging:

1. `bins3` is a bad undescriptive name
2. `bins3` should be added to `histogram2`
3. `write_histogram2_unit` for symmetry.

There's almost no sanity checking. If you call one of these functions on a histogram that has not been initialized, you loose. — *Big time.*

294a ⟨`histograms.f90` 294a⟩≡

```
! histograms.f90 --
⟨Copyleft notice 1⟩
module histograms
  use kinds
  use utils, only: find_free_unit
  implicit none
  private
  ⟨Declaration of histograms procedures 295b⟩
  ⟨Interfaces of histograms procedures 295c⟩
  ⟨Variables in histograms 295e⟩
  ⟨Declaration of histograms types 294b⟩
  character(len=*), public, parameter :: HISTOGRAMS_RCS_ID = &
       "$Id: histograms.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of histograms procedures 295f⟩
end module histograms
```

294b ⟨*Declaration of* `histograms` *types* 294b⟩≡

```
type, public :: histogram
   private
   integer :: n_bins
   real(kind=default) :: x_min, x_max
```

```
    real(kind=default), dimension(:), pointer :: bins => null ()
    real(kind=default), dimension(:), pointer :: bins2 => null ()
    real(kind=default), dimension(:), pointer :: bins3 => null ()
 end type histogram
```

295a ⟨*Declaration of* histograms *types* 294b⟩+≡

```
 type, public :: histogram2
    private
    integer, dimension(2) :: n_bins
    real(kind=default), dimension(2) :: x_min, x_max
    real(kind=default), dimension(:,:), pointer :: bins => null ()
    real(kind=default), dimension(:,:), pointer :: bins2 => null ()
 end type histogram2
```

295b ⟨*Declaration of* histograms *procedures* 295b⟩≡

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

295c ⟨*Interfaces of* histograms *procedures* 295c⟩≡

```
 interface create_histogram
    module procedure create_histogram1, create_histogram2
 end interface
 interface fill_histogram
    module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
 end interface
 interface delete_histogram
    module procedure delete_histogram1, delete_histogram2
 end interface
 interface write_histogram
    module procedure write_histogram1, write_histogram2
    module procedure write_histogram1_unit
 end interface
```

295d ⟨*Declaration of* histograms *procedures* 295b⟩+≡

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

295e ⟨*Variables in* histograms 295e⟩≡

```
 integer, parameter, private :: N_BINS_DEFAULT = 10
```

295f ⟨*Implementation of* histograms *procedures* 295f⟩≡

```
 elemental subroutine create_histogram1 (h, x_min, x_max, nb)
   type(histogram), intent(out) :: h
```

```
    real(kind=default), intent(in) :: x_min, x_max
    integer, intent(in), optional :: nb
    if (present (nb)) then
       h%n_bins = nb
    else
       h%n_bins = N_BINS_DEFAULT
    end if
    h%x_min = x_min
    h%x_max = x_max
    allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
    h%bins = 0
    h%bins2 = 0
    allocate (h%bins3(0:h%n_bins+1))
    h%bins3 = 0
  end subroutine create_histogram1
```

296a ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  pure subroutine create_histogram2 (h, x_min, x_max, nb)
    type(histogram2), intent(out) :: h
    real(kind=default), dimension(:), intent(in) :: x_min, x_max
    integer, intent(in), dimension(:), optional :: nb
    if (present (nb)) then
       h%n_bins = nb
    else
       h%n_bins = N_BINS_DEFAULT
    end if
    h%x_min = x_min
    h%x_max = x_max
    allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
              h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
    h%bins = 0
    h%bins2 = 0
  end subroutine create_histogram2
```

296b ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  elemental subroutine fill_histogram1 (h, x, weight, excess)
    type(histogram), intent(inout) :: h
    real(kind=default), intent(in) :: x
    real(kind=default), intent(in), optional :: weight
    real(kind=default), intent(in), optional :: excess
    integer :: i
    if (x < h%x_min) then
       i = 0
    else if (x > h%x_max) then
       i = h%n_bins + 1
```

```
    else
       i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
  !WK! i = min (max (i, 0), h%n_bins + 1)
    end if
    if (present (weight)) then
       h%bins(i) = h%bins(i) + weight
       h%bins2(i) = h%bins2(i) + weight*weight
    else
       h%bins(i) = h%bins(i) + 1
       h%bins2(i) = h%bins2(i) + 1
    end if
    if (present (excess)) h%bins3(i) = h%bins3(i) + excess
  end subroutine fill_histogram1
```

297a ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  elemental subroutine fill_histogram2s (h, x1, x2, weight)
    type(histogram2), intent(inout) :: h
    real(kind=default), intent(in) :: x1, x2
    real(kind=default), intent(in), optional :: weight
    call fill_histogram2v (h, (/ x1, x2 /), weight)
  end subroutine fill_histogram2s
```

297b ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  pure subroutine fill_histogram2v (h, x, weight)
    type(histogram2), intent(inout) :: h
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(in), optional :: weight
    integer, dimension(2) :: i
    i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
    i = min (max (i, 0), h%n_bins + 1)
    if (present (weight)) then
       h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight
       h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight*weight
    else
       h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1
       h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1
    end if
  end subroutine fill_histogram2v
```

297c ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  elemental subroutine delete_histogram1 (h)
    type(histogram), intent(inout) :: h
    deallocate (h%bins, h%bins2)
    deallocate (h%bins3)
  end subroutine delete_histogram1
```

298a ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
elemental subroutine delete_histogram2 (h)
  type(histogram2), intent(inout) :: h
  deallocate (h%bins, h%bins2)
end subroutine delete_histogram2
```

298b ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
subroutine write_histogram1 (h, name, over)
  type(histogram), intent(in) :: h
  character(len=*), intent(in), optional :: name
  logical, intent(in), optional :: over
  integer :: i, iounit
  if (present (name)) then
     call find_free_unit (iounit)
     if (iounit > 0) then
        open (unit = iounit, action = "write", status = "replace", &
              file = name)
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                "underflow", h%bins(0), sqrt (h%bins2(0))
           end if
        end if
        do i = 1, h%n_bins
           write (unit = iounit, fmt = *) &
                midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
        end do
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                "overflow", h%bins(h%n_bins+1), &
                sqrt (h%bins2(h%n_bins+1))
           end if
        end if
        close (unit = iounit)
     else
        print *, "write_histogram: Can't find a free unit!"
     end if
  else
     if (present (over)) then
        if (over) then
           print *, "underflow", h%bins(0), sqrt (h%bins2(0))
        end if
     end if
```

```
    do i = 1, h%n_bins
       print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
    end do
    if (present (over)) then
       if (over) then
          print *, "overflow", h%bins(h%n_bins+1), &
                   sqrt (h%bins2(h%n_bins+1))
       end if
    end if
  end if
end subroutine write_histogram1
```

299a ⟨*Declaration of* histograms *procedures* 295b⟩+≡

```
!WK! public :: write_histogram1_unit
```

I don't like the `format` statement with the line number. Use a character constant instead (after we have merged with WHIZARD's branch).

299b ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
subroutine write_histogram1_unit (h, iounit, over, show_excess)
  type(histogram), intent(in) :: h
  integer, intent(in) :: iounit
  logical, intent(in), optional :: over, show_excess
  integer :: i
  logical :: show_exc
  show_exc = .false.; if (present(show_excess)) show_exc = show_excess
  if (present (over)) then
     if (over) then
        if (show_exc) then
           write (unit = iounit, fmt = 1) &
                "underflow", h%bins(0), sqrt (h%bins2(0)), h%bins3(0)
        else
           write (unit = iounit, fmt = 1) &
                "underflow", h%bins(0), sqrt (h%bins2(0))
        end if
     end if
  end if
  do i = 1, h%n_bins
     if (show_exc) then
        write (unit = iounit, fmt = 1) &
             midpoint (h, i), h%bins(i), sqrt (h%bins2(i)), h%bins3(i)
     else
        write (unit = iounit, fmt = 1) &
             midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
```

```
      end if
    end do
    if (present (over)) then
      if (over) then
        if (show_exc) then
          write (unit = iounit, fmt = 1) &
               "overflow", h%bins(h%n_bins+1), &
               sqrt (h%bins2(h%n_bins+1)), &
               h%bins3(h%n_bins+1)
        else
          write (unit = iounit, fmt = 1) &
               "overflow", h%bins(h%n_bins+1), &
               sqrt (h%bins2(h%n_bins+1))
        end if
      end if
    end if
  1 format (1x,4(G16.9,2x))
  end subroutine write_histogram1_unit
```

300a ⟨*Declaration of* histograms *procedures* 295b⟩+≡

```
  private :: midpoint
```

300b ⟨*Interfaces of* histograms *procedures* 295c⟩+≡

```
  interface midpoint
     module procedure midpoint1, midpoint2
  end interface
```

300c ⟨*Declaration of* histograms *procedures* 295b⟩+≡

```
  private :: midpoint1, midpoint2
```

300d ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  elemental function midpoint1 (h, bin) result (x)
    type(histogram), intent(in) :: h
    integer, intent(in) :: bin
    real(kind=default) :: x
    x = h%x_min + (h%x_max - h%x_min) * (bin - 0.5) / h%n_bins
  end function midpoint1
```

300e ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
  elemental function midpoint2 (h, bin, d) result (x)
    type(histogram2), intent(in) :: h
    integer, intent(in) :: bin, d
    real(kind=default) :: x
    x = h%x_min(d) + (h%x_max(d) - h%x_min(d)) * (bin - 0.5) / h%n_bins(d)
  end function midpoint2
```

301 ⟨*Implementation of* histograms *procedures* 295f⟩+≡

```
subroutine write_histogram2 (h, name, over)
  type(histogram2), intent(in) :: h
  character(len=*), intent(in), optional :: name
  logical, intent(in), optional :: over
  integer :: i1, i2, iounit
  if (present (name)) then
     call find_free_unit (iounit)
     if (iounit > 0) then
        open (unit = iounit, action = "write", status = "replace", &
              file = name)
        if (present (over)) then
           if (over) then
              write (unit = iounit, fmt = *) &
                   "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
              do i2 = 1, h%n_bins(2)
                 write (unit = iounit, fmt = *) &
                      "x1 underflow", midpoint (h, i2, 2), &
                      h%bins(0,i2), sqrt (h%bins2(0,i2))
              end do
              do i1 = 1, h%n_bins(1)
                 write (unit = iounit, fmt = *) &
                      "x2 underflow", midpoint (h, i1, 1), &
                      h%bins(i1,0), sqrt (h%bins2(i1,0))
              end do
           end if
        end if
        do i1 = 1, h%n_bins(1)
           do i2 = 1, h%n_bins(2)
              write (unit = iounit, fmt = *) &
                   midpoint (h, i1, 1), midpoint (h, i2, 2), &
                   h%bins(i1,i2), sqrt (h%bins2(i1,i2))
           end do
        end do
        if (present (over)) then
           if (over) then
              do i2 = 1, h%n_bins(2)
                 write (unit = iounit, fmt = *) &
                      "x1 overflow", midpoint (h, i2, 2), &
                      h%bins(h%n_bins(1)+1,i2), &
                      sqrt (h%bins2(h%n_bins(1)+1,i2))
              end do
              do i1 = 1, h%n_bins(1)
```

```
                write (unit = iounit, fmt = *) &
                     "x2 overflow", midpoint (h, i1, 1), &
                     h%bins(i1,h%n_bins(2)+1), &
                     sqrt (h%bins2(i1,h%n_bins(2)+1))
             end do
             write (unit = iounit, fmt = *) "double overflow", &
                  h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
                  sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
          end if
       end if
       close (unit = iounit)
    else
       print *, "write_histogram: Can't find a free unit!"
    end if
 else
    if (present (over)) then
       if (over) then
          print *, "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
          do i2 = 1, h%n_bins(2)
             print *, "x1 underflow", midpoint (h, i2, 2), &
                  h%bins(0,i2), sqrt (h%bins2(0,i2))
          end do
          do i1 = 1, h%n_bins(1)
             print *, "x2 underflow", midpoint (h, i1, 1), &
                  h%bins(i1,0), sqrt (h%bins2(i1,0))
          end do
       end if
    end if
    do i1 = 1, h%n_bins(1)
       do i2 = 1, h%n_bins(2)
          print *, midpoint (h, i1, 1), midpoint (h, i2, 2), &
               h%bins(i1,i2), sqrt (h%bins2(i1,i2))
       end do
    end do
    if (present (over)) then
       if (over) then
          do i2 = 1, h%n_bins(2)
             print *, "x1 overflow", midpoint (h, i2, 2), &
                  h%bins(h%n_bins(1)+1,i2), &
                  sqrt (h%bins2(h%n_bins(1)+1,i2))
          end do
          do i1 = 1, h%n_bins(1)
             print *, "x2 overflow", midpoint (h, i1, 1), &
```

```
                   h%bins(i1,h%n_bins(2)+1), &
                   sqrt (h%bins2(i1,h%n_bins(2)+1))
           end do
           print *, "double overflow", &
                h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
                sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
        end if
     end if
  end if
end subroutine write_histogram2
```

—G— Miscellaneous Utilities

304a ⟨utils.f90 304a⟩≡

```
! utils.f90 --
⟨Copyleft notice 1⟩
module utils
  use kinds
  implicit none
  private
  ⟨Declaration of utils procedures 304b⟩
  ⟨Parameters in utils 311c⟩
  ⟨Variables in utils 312b⟩
  ⟨Interfaces of utils procedures 304c⟩
  character(len=*), public, parameter :: UTILS_RCS_ID = &
       "$Id: utils.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of utils procedures 305c⟩
end module utils
```

G.1 Memory Management

304b ⟨Declaration of utils procedures 304b⟩≡

```
public :: create_array_pointer
private :: create_integer_array_pointer
private :: create_real_array_pointer
private :: create_integer_array2_pointer
private :: create_real_array2_pointer
```

304c ⟨Interfaces of utils procedures 304c⟩≡

```
interface create_array_pointer
   module procedure &
        create_integer_array_pointer, &
```

```
         create_real_array_pointer, &
         create_integer_array2_pointer, &
         create_real_array2_pointer
end interface
```

305a ⟨*Body of* `create_*_array_pointer` 305a⟩≡

```
if (associated (lhs)) then
   if (size (lhs) /= n) then
      deallocate (lhs)
      if (present (lb)) then
         allocate (lhs(lb:n+lb-1))
      else
         allocate (lhs(n))
      end if
   end if
else
   if (present (lb)) then
      allocate (lhs(lb:n+lb-1))
   else
      allocate (lhs(n))
   end if
end if
lhs = 0
```

305b ⟨*Body of* `create_*_array2_pointer` 305b⟩≡

```
if (associated (lhs)) then
   if (any (ubound (lhs) /= n)) then
      deallocate (lhs)
      if (present (lb)) then
         allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
      else
         allocate (lhs(n(1),n(2)))
      end if
   end if
else
   if (present (lb)) then
      allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
   else
      allocate (lhs(n(1),n(2)))
   end if
end if
lhs = 0
```

305c ⟨*Implementation of* `utils` *procedures* 305c⟩≡

```
pure subroutine create_integer_array_pointer (lhs, n, lb)
```

```
    integer, dimension(:), pointer :: lhs
    integer, intent(in) :: n
    integer, intent(in), optional :: lb
    ⟨Body of create_*_array_pointer 305a⟩
  end subroutine create_integer_array_pointer
```

306a ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
  pure subroutine create_real_array_pointer (lhs, n, lb)
    real(kind=default), dimension(:), pointer :: lhs
    integer, intent(in) :: n
    integer, intent(in), optional :: lb
    ⟨Body of create_*_array_pointer 305a⟩
  end subroutine create_real_array_pointer
```

306b ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
  pure subroutine create_integer_array2_pointer (lhs, n, lb)
    integer, dimension(:,:), pointer :: lhs
    integer, dimension(:), intent(in) :: n
    integer, dimension(:), intent(in), optional :: lb
    ⟨Body of create_*_array2_pointer 305b⟩
  end subroutine create_integer_array2_pointer
```

306c ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
  pure subroutine create_real_array2_pointer (lhs, n, lb)
    real(kind=default), dimension(:,:), pointer :: lhs
    integer, dimension(:), intent(in) :: n
    integer, dimension(:), intent(in), optional :: lb
    ⟨Body of create_*_array2_pointer 305b⟩
  end subroutine create_real_array2_pointer
```

Copy an allocatable array component of a derived type, reshaping the target if necessary. The target can be `disassociated`, but its association *must not* be undefined.

306d ⟨*Declaration of* utils *procedures* 304b⟩+≡

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

306e ⟨*Interfaces of* utils *procedures* 304c⟩+≡

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

```
        copy_real_array2_pointer
end interface
```

307a ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
  integer, dimension(:), pointer :: lhs
  integer, dimension(:), intent(in) :: rhs
  integer, intent(in), optional :: lb
  call create_integer_array_pointer (lhs, size (rhs), lb)
  lhs = rhs
end subroutine copy_integer_array_pointer
```

307b ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
pure subroutine copy_real_array_pointer (lhs, rhs, lb)
  real(kind=default), dimension(:), pointer :: lhs
  real(kind=default), dimension(:), intent(in) :: rhs
  integer, intent(in), optional :: lb
  call create_real_array_pointer (lhs, size (rhs), lb)
  lhs = rhs
end subroutine copy_real_array_pointer
```

307c ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
  integer, dimension(:,:), pointer :: lhs
  integer, dimension(:,:), intent(in) :: rhs
  integer, dimension(:), intent(in), optional :: lb
  call create_integer_array2_pointer &
       (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
  lhs = rhs
end subroutine copy_integer_array2_pointer
```

307d ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
  real(kind=default), dimension(:,:), pointer :: lhs
  real(kind=default), dimension(:,:), intent(in) :: rhs
  integer, dimension(:), intent(in), optional :: lb
  call create_real_array2_pointer &
       (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
  lhs = rhs
end subroutine copy_real_array2_pointer
```

G.2 Sorting

307e ⟨*Declaration of* `utils` *procedures* 304b⟩+≡

```
public :: swap
```

```
private :: swap_integer, swap_real
```

308a ⟨*Interfaces of* `utils` *procedures* 304c⟩+≡

```
interface swap
   module procedure swap_integer, swap_real
end interface
```

308b ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
elemental subroutine swap_integer (a, b)
  integer, intent(inout) :: a, b
  integer :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_integer
```

308c ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
elemental subroutine swap_real (a, b)
  real(kind=default), intent(inout) :: a, b
  real(kind=default) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_real
```

Straight insertion:

308d ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
pure subroutine sort_real (key, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  ⟨Set rev to reverse or .false. 308e⟩
  do i = 1, size (key) - 1
     ⟨Set j to minloc(key) 309a⟩
     if (j /= i) then
        call swap (key(i), key(j))
     end if
  end do
end subroutine sort_real
```

308e ⟨*Set* `rev` *to* `reverse` *or* `.false.` 308e⟩≡

```
if (present (reverse)) then
   rev = reverse
else
   rev = .false.
end if
```

309a ⟨*Set* j *to* minloc(key) 309a⟩≡
```
if (rev) then
   j = sum (maxloc (key(i:))) + i - 1
else
   j = sum (minloc (key(i:))) + i - 1
end if
```

309b ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
pure subroutine sort_real_and_real_array (key, table, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  real(kind=default), dimension(:,:), intent(inout) :: table
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  ⟨Set rev to reverse or .false. 308e⟩
  do i = 1, size (key) - 1
     ⟨Set j to minloc(key) 309a⟩
     if (j /= i) then
        call swap (key(i), key(j))
        call swap (table(:,i), table(:,j))
     end if
  end do
end subroutine sort_real_and_real_array
```

309c ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
pure subroutine sort_real_and_integer (key, table, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  integer, dimension(:), intent(inout) :: table
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  ⟨Set rev to reverse or .false. 308e⟩
  do i = 1, size (key) - 1
     ⟨Set j to minloc(key) 309a⟩
     if (j /= i) then
        call swap (key(i), key(j))
        call swap (table(i), table(j))
     end if
  end do
end subroutine sort_real_and_integer
```

309d ⟨*Declaration of* utils *procedures* 304b⟩+≡
```
public :: sort
private :: sort_real, sort_real_and_real_array, sort_real_and_integer
```

310a ⟨*Interfaces of* utils *procedures* 304c⟩+≡
```
interface sort
   module procedure &
        sort_real, sort_real_and_real_array, &
        sort_real_and_integer
end interface
```

G.3 Mathematics

310b ⟨*Declaration of* utils *procedures* 304b⟩+≡
```
public :: outer_product
```

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

310c ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
pure function outer_product (x, y) result (xy)
  real(kind=default), dimension(:), intent(in) :: x, y
  real(kind=default), dimension(size(x),size(y)) :: xy
  xy = spread (x, dim=2, ncopies=size(y)) &
         * spread (y, dim=1, ncopies=size(x))
end function outer_product
```

Greatest common divisor and least common multiple

310d ⟨*Declaration of* utils *procedures* 304b⟩+≡
```
public :: factorize, gcd, lcm
private :: gcd_internal
```

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

310e ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
pure recursive function gcd_internal (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
  if (n <= 0) then
     gcd_m_n = m
  else
     gcd_m_n = gcd_internal (n, modulo (m, n))
  end if
end function gcd_internal
```

Wrap an elemental procedure around the recursive procedure:

310f ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
elemental function gcd (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
```

```
    gcd_m_n = gcd_internal (m, n)
  end function gcd
```

As long as `m*n` does not overflow, we can use $\gcd(m,n)\,\mathrm{lcm}(m,n) = mn$:

311a ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
  elemental function lcm (m, n) result (lcm_m_n)
    integer, intent(in) :: m, n
    integer :: lcm_m_n
    lcm_m_n = (m * n) / gcd (m, n)
  end function lcm
```

A very simple minded factorization procedure, that is not fool proof at all. It maintains `n == product (factors(1:i))`, however, and will work in all cases of practical relevance.

311b ⟨*Implementation of* `utils` *procedures* 305c⟩+≡

```
  pure subroutine factorize (n, factors, i)
    integer, intent(in) :: n
    integer, dimension(:), intent(out) :: factors
    integer, intent(out) :: i
    integer :: nn, p
    nn = n
    i = 0
    do p = 1, size (PRIMES)
       try: do
          if (modulo (nn, PRIMES(p)) == 0) then
             i = i + 1
             factors(i) = PRIMES(p)
             nn = nn / PRIMES(p)
             if (i >= size (factors)) then
                factors(i) = nn
                return
             end if
          else
             exit try
          end if
       end do try
       if (nn == 1) then
          return
       end if
    end do
  end subroutine factorize
```

311c ⟨*Parameters in* `utils` 311c⟩≡

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

G.4 I/O

312a ⟨*Declaration of* utils *procedures* 304b⟩+≡
```
public :: find_free_unit
```

312b ⟨*Variables in* utils 312b⟩≡
```
integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99
```

312c ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
subroutine find_free_unit (u, iostat)
  integer, intent(out) :: u
  integer, intent(out), optional :: iostat
  logical :: exists, is_open
  integer :: i, status
  do i = MIN_UNIT, MAX_UNIT
     inquire (unit = i, exist = exists, opened = is_open, &
              iostat = status)
     if (status == 0) then
        if (exists .and. .not. is_open) then
           u = i
           if (present (iostat)) then
              iostat = 0
           end if
           return
        end if
     end if
  end do
  if (present (iostat)) then
     iostat = -1
  end if
  u = -1
end subroutine find_free_unit
```

—H— Linear Algebra

313a ⟨linalg.f90 313a⟩≡
```
! linalg.f90 --
⟨Copyleft notice 1⟩
module linalg
  use kinds
  use utils
  implicit none
  private
  ⟨Declaration of linalg procedures 313b⟩
  character(len=*), public, parameter :: LINALG_RCS_ID = &
       "$Id: linalg.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of linalg procedures 314⟩
end module linalg
```

H.1 LU Decomposition

313b ⟨Declaration of linalg procedures 313b⟩≡
```
public :: lu_decompose
```

$$A = LU \tag{H.1a}$$

In more detail

$$\begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ l_{21} & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \ldots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \ldots & u_{1n} \\ 0 & u_{22} & \ldots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & u_{nn} \end{pmatrix} \tag{H.1b}$$

Rewriting (H.1) in block matrix notation

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

we can solve it easily

$$u_{11} = a_{11} \tag{H.3a}$$

$$u_{1\cdot} = a_{1\cdot} \tag{H.3b}$$

$$l_{\cdot 1} = \frac{a_{\cdot 1}}{a_{11}} \tag{H.3c}$$

$$LU = A - \frac{a_{\cdot 1} \otimes a_{1\cdot}}{a_{11}} \tag{H.3d}$$

and (H.3c) and (H.3d) define a simple iterative algorithm if we work from the outside in. It just remains to add pivoting.

314 ⟨*Implementation of* `linalg` *procedures* 314⟩≡

```
pure subroutine lu_decompose (a, pivots, eps, l, u)
  real(kind=default), dimension(:,:), intent(inout) :: a
  integer, dimension(:), intent(out), optional :: pivots
  real(kind=default), intent(out), optional :: eps
  real(kind=default), dimension(:,:), intent(out), optional :: l, u
  real(kind=default), dimension(size(a,dim=1)) :: vv
  integer, dimension(size(a,dim=1)) :: p
  integer :: j, pivot
  ⟨eps = 1 315a⟩
  vv = maxval (abs (a), dim=2)
  if (any (vv == 0.0)) then
     a = 0.0
     ⟨pivots = 0 and eps = 0 315c⟩
     return
  end if
  vv = 1.0 / vv
  do j = 1, size (a, dim=1)
     pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
     if (j /= pivot) then
        call swap (a(pivot,:), a(j,:))
        ⟨eps = - eps 315b⟩
        vv(pivot) = vv(j)
     end if
     p(j) = pivot
     if (a(j,j) == 0.0) then
        a(j,j) = tiny (a(j,j))
```

```
      end if
      a(j+1:,j) = a(j+1:,j) / a(j,j)
      a(j+1:,j+1:) &
           = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
   end do
   ⟨Return optional arguments in lu_decompose 315d⟩
 end subroutine lu_decompose
```

315a ⟨eps = 1 315a⟩≡

```
 if (present (eps)) then
    eps = 1.0
 end if
```

315b ⟨eps = - eps 315b⟩≡

```
 if (present (eps)) then
    eps = - eps
 end if
```

315c ⟨pivots = 0 *and* eps = 0 315c⟩≡

```
 if (present (pivots)) then
    pivots = 0
 end if
 if (present (eps)) then
    eps = 0
 end if
```

315d ⟨*Return optional arguments in* lu_decompose 315d⟩≡

```
 if (present (pivots)) then
    pivots = p
 end if
 if (present (l)) then
    do j = 1, size (a, dim=1)
       l(1:j-1,j) = 0.0
       l(j,j) = 1.0
       l(j+1:,j) = a(j+1:,j)
    end do
    do j = size (a, dim=1), 1, -1
       call swap (l(j,:), l(p(j),:))
    end do
 end if
 if (present (u)) then
    do j = 1, size (a, dim=1)
       u(1:j,j) = a(1:j,j)
       u(j+1:,j) = 0.0
    end do
 end if
```

H.2 Determinant

316a ⟨*Declaration of* `linalg` *procedures* 313b⟩+≡
```
public :: determinant
```

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

316b ⟨*Implementation of* `linalg` *procedures* 314⟩+≡
```
pure subroutine determinant (a, det)
  real(kind=default), dimension(:,:), intent(in) :: a
  real(kind=default), intent(out) :: det
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu
  integer :: i
  lu = a
  call lu_decompose (lu, eps = det)
  do i = 1, size (a, dim = 1)
     det = det * lu(i,i)
  end do
end subroutine determinant
```

H.3 Diagonalization

The code is an implementation of the algorithm presented in [16, 17], but independent from the code presented in [18] to avoid legal problems.

A Jacobi rotation around the angle ϕ in row p and column q

$$P(\phi;p,q) = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos\phi & \cdots & \sin\phi & & \\ & & \vdots & 1 & \vdots & & \\ & & -\sin\phi & \cdots & \cos\phi & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \tag{H.4}$$

results in

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

317a ⟨*Declaration of* `linalg` *procedures* 313b⟩+≡

```
public :: diagonalize_real_symmetric
```

317b ⟨*Implementation of* `linalg` *procedures* 314⟩+≡

```
pure subroutine diagonalize_real_symmetric (a, eval, evec, num_rot)
  real(kind=default), dimension(:,:), intent(in) :: a
  real(kind=default), dimension(:), intent(out) :: eval
  real(kind=default), dimension(:,:), intent(out) :: evec
  integer, intent(out), optional :: num_rot
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: aa
  real(kind=default) :: off_diagonal_norm, threshold, &
       c, g, h, s, t, tau, cot_2phi
  logical, dimension(size(eval),size(eval)) :: upper_triangle
  integer, dimension(size(eval)) :: one_to_ndim
  integer :: p, q, ndim, j, sweep
  integer, parameter :: MAX_SWEEPS = 50
  ndim = size (eval)
  one_to_ndim = (/ (j, j=1,ndim) /)
  upper_triangle = &
       spread (one_to_ndim, dim=1, ncopies=ndim) &
         > spread (one_to_ndim, dim=2, ncopies=ndim)
  aa = a
  call unit (evec)
  ⟨Initialize num_rot 320e⟩
  sweeps: do sweep = 1, MAX_SWEEPS
     off_diagonal_norm = sum (abs (aa), mask=upper_triangle)
     if (off_diagonal_norm == 0.0) then
        eval = diag (aa)
        return
     end if
     if (sweep < 4) then
        threshold = 0.2 * off_diagonal_norm / ndim**2
     else
```

```
          threshold = 0.0
       end if
       do p = 1, ndim - 1
          do q = p + 1, ndim
             ⟨Perform the Jacobi rotation resulting in A'_pq = 0 318⟩
          end do
       end do
    end do sweeps
    if (present (num_rot)) then
       num_rot = -1
    end if
  !!! print *, "linalg::diagonalize_real_symmetric: exceeded sweep count"
  end subroutine diagonalize_real_symmetric
```

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

```
  g = 100 * abs (aa (p,q))
  if ((sweep > 4) &
       .and. (g <= min (spacing (aa(p,p)), spacing (aa(q,q))))) then
     aa(p,q) = 0.0
  else if (abs (aa(p,q)) > threshold) then
     ⟨Determine φ for the Jacobi rotation P(φ;p,q) with A'_pq = 0 319a⟩
     ⟨A' = P^T(φ;p,q) · A · P(φ;p,q) 319c⟩
     ⟨V' = V · P(φ;p,q) 320d⟩
     ⟨Update num_rot 320f⟩
  end if
```

We want

$$A'_{pq} = (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) = 0 \tag{H.6}$$

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

$$t = \frac{1}{2\cot 2\phi} = \frac{A_{pq}}{A_{pp} - A_{qq}} \tag{H.11}$$

$$h = A_{qq} - A_{pp} \tag{H.12}$$

319a ⟨*Determine ϕ for the Jacobi rotation $P(\phi; p, q)$ with $A'_{pq} = 0$* 319a⟩≡

```
h = aa(q,q) - aa(p,p)
if (g <= spacing (h)) then
   t = aa(p,q) / h
else
   cot_2phi = 0.5 * h / aa(p,q)
   t = sign (1.0_default, cot_2phi) &
         / (abs (cot_2phi) + sqrt (1.0 + cot_2phi**2))
end if
```

Trivia

$$\cos^2\phi = \frac{\cos^2\phi}{\cos^2\phi + \sin^2\phi} = \frac{1}{1 + \tan^2\phi} \tag{H.13a}$$

$$\sin\phi = \tan\phi\cos\phi \tag{H.13b}$$

$$\tau\sin\phi = \frac{\sin^2}{1 + \cos\phi} = \frac{1 - \cos^2}{1 + \cos\phi} = 1 - \cos\phi \tag{H.13c}$$

319b ⟨*Determine ϕ for the Jacobi rotation $P(\phi; p, q)$ with $A'_{pq} = 0$* 319a⟩+≡

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

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

319c ⟨$A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$ 319c⟩≡

```
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:

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

320a ⟨$A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$ 319c⟩+≡

```
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:

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

320b ⟨*Implementation of* `linalg` *procedures* 314⟩+≡

```
pure subroutine jacobi_rotation (s, tau, vp, vq)
  real(kind=default), intent(in) :: s, tau
  real(kind=default), dimension(:), intent(inout) :: vp, vq
  real(kind=default), dimension(size(vp)) :: vp_tmp
  vp_tmp = vp
  vp = vp - s * (vq     + tau * vp)
  vq = vq + s * (vp_tmp - tau * vq)
end subroutine jacobi_rotation
```

320c ⟨*Declaration of* `linalg` *procedures* 313b⟩+≡

```
private :: jacobi_rotation
```

320d ⟨$V' = V \cdot P(\phi; p, q)$ 320d⟩≡

```
call jacobi_rotation (s, tau, evec(:,p), evec(:,q))
```

320e ⟨*Initialize* `num_rot` 320e⟩≡

```
if (present (num_rot)) then
   num_rot = 0
end if
```

320f ⟨*Update* `num_rot` 320f⟩≡

```
if (present (num_rot)) then
   num_rot = num_rot + 1
end if
```

321a ⟨*Implementation of* `linalg` *procedures* 314⟩+≡
```
pure subroutine unit (u)
  real(kind=default), dimension(:,:), intent(out) :: u
  integer :: i
  u = 0.0
  do i = 1, min (size (u, dim = 1), size (u, dim = 2))
     u(i,i) = 1.0
  end do
end subroutine unit
```

321b ⟨*Implementation of* `linalg` *procedures* 314⟩+≡
```
pure function diag (a) result (d)
  real(kind=default), dimension(:,:), intent(in) :: a
  real(kind=default), dimension(min(size(a,dim=1),size(a,dim=2))) :: d
  integer :: i
  do i = 1, min (size (a, dim = 1), size (a, dim = 2))
     d(i) = a(i,i)
  end do
end function diag
```

321c ⟨*Declaration of* `linalg` *procedures* 313b⟩+≡
```
public :: unit, diag
```

H.4 Test

321d ⟨`la_sample.f90` 321d⟩≡
```
! la_sample.f90 --
⟨Copyleft notice 1⟩
program la_sample
  use kinds
  use utils
  use tao_random_numbers
  use linalg
  implicit none
  integer, parameter :: N = 200
  real(kind=default), dimension(N,N) :: a, evec, a0, l, u, NAG_bug
  real(kind=default), dimension(N) :: b, eval
  real(kind=default) :: d
  integer :: i
  call system_clock (i)
  call tao_random_seed (i)
  print *, i
  do i = 1, N
```

```
     call tao_random_number (a(:,i))
  end do
  NAG_bug = (a + transpose (a)) / 2
  a = NAG_bug
  a0 = a
  call lu_decompose (a, l=l, u=u)
  a = matmul (l, u)
  print *, maxval (abs(a-a0))
  call determinant (a, d)
  print *, d
  call diagonalize_real_symmetric (a, eval, evec)
  print *, product (eval)
  stop
  call sort (eval, evec)
  do i = 1, N
     b = matmul (a, evec(:,i)) - eval(i) * evec(:,i)
     write (unit = *, fmt = "(A,I3, 2(A,E11.4))") &
          "eval #", i, " = ", eval(i), ", |(A-lambda)V|_infty = ", &
          maxval (abs(b)) / maxval (abs(evec(:,i)))
  end do
end program la_sample
```

—I—
Products

323 ⟨products.f90 323⟩≡

```
! products.f90 --
⟨Copyleft notice 1⟩
module products
  use kinds
  implicit none
  private
  public :: dot, sp, spc
  character(len=*), public, parameter :: PRODUCTS_RCS_ID = &
       "$Id: products.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  pure function dot (p, q) result (pq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    real(kind=default) :: pq
    pq = p(0)*q(0) - dot_product (p(1:), q(1:))
  end function dot
  pure function sp (p, q) result (sppq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: sppq
    sppq = cmplx (p(2), p(3)) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
         - cmplx (q(2), q(3)) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
  end function sp
  pure function spc (p, q) result (spcpq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: spcpq
    spcpq = conjg (sp (p, q))
  end function spc
end module products
```

—J—
Kinematics

324a ⟨kinematics.f90 324a⟩≡
```
! kinematics.f90 --
⟨Copyleft notice 1⟩
module kinematics
  use kinds
  use constants
  use products, only: dot
  use specfun, only: gamma
  implicit none
  private
  ⟨Declaration of kinematics procedures 324b⟩
  ⟨Interfaces of kinematics procedures 324c⟩
  ⟨Declaration of kinematics types 326g⟩
  character(len=*), public, parameter :: KINEMATICS_RCS_ID = &
       "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of kinematics procedures 325a⟩
end module kinematics
```

J.1 Lorentz Transformations

324b ⟨Declaration of kinematics procedures 324b⟩≡
```
public :: boost_velocity
private :: boost_one_velocity, boost_many_velocity
public :: boost_momentum
private :: boost_one_momentum, boost_many_momentum
```

324c ⟨Interfaces of kinematics procedures 324c⟩≡
```
interface boost_velocity
   module procedure boost_one_velocity, boost_many_velocity
```

```
  end interface
  interface boost_momentum
     module procedure boost_one_momentum, boost_many_momentum
  end interface
```

Boost a four vector p to the inertial frame moving with the velocity 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

$$p_0' = \gamma p_0 - \vec b\vec p \tag{J.2a}$$

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

325a ⟨*Implementation of* `kinematics` *procedures* 325a⟩≡

```
  pure function boost_one_velocity (p, beta) result (p_prime)
    real(kind=default), dimension(0:), intent(in) :: p
    real(kind=default), dimension(1:), intent(in) :: beta
    real(kind=default), dimension(0:3) :: p_prime
    real(kind=default), dimension(1:3) :: b
    real(kind=default) :: gamma, b_dot_p
    gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
    b = gamma * beta
    b_dot_p = dot_product (b, p(1:3))
    p_prime(0) = gamma * p(0) - b_dot_p
    p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
  end function boost_one_velocity
```

325b ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡

```
  pure function boost_many_velocity (p, beta) result (p_prime)
    real(kind=default), dimension(:,0:), intent(in) :: p
    real(kind=default), dimension(1:), intent(in) :: beta
    real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
    integer :: i
    do i = 1, size (p, dim=1)
       p_prime(i,:) = boost_one_velocity (p(i,:), beta)
    end do
  end function boost_many_velocity
```

Boost a four vector p to the rest frame of the four vector q. The velocity is $\vec{\beta} = \vec{q}/|q_0|$:

326a ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡
```
pure function boost_one_momentum (p, q) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p, q
  real(kind=default), dimension(0:3) :: p_prime
  p_prime = boost_velocity (p, q(1:3) / abs (q(0)))
end function boost_one_momentum
```

326b ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡
```
pure function boost_many_momentum (p, q) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(0:), intent(in) :: q
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  p_prime = boost_many_velocity (p, q(1:3) / abs (q(0)))
end function boost_many_momentum
```

J.2 Massive Phase Space

$$\lambda(a,b,c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca = (a-b-c)^2 - 4bc \tag{J.3}$$

and permutations

326c ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡
```
pure function lambda (a, b, c) result (lam)
  real(kind=default), intent(in) :: a, b, c
  real(kind=default) :: lam
  lam = a**2 + b**2 + c**2 - 2*(a*b + b*c + c*a)
end function lambda
```

326d ⟨*Declaration of* `kinematics` *procedures* 324b⟩+≡
```
public :: lambda
```

326e ⟨*Declaration of* `kinematics` *procedures* 324b⟩+≡
```
public :: two_to_three
private :: two_to_three_massive, two_to_three_massless
```

326f ⟨*Interfaces of* `kinematics` *procedures* 324c⟩+≡
```
interface two_to_three
   module procedure two_to_three_massive, two_to_three_massless
end interface
```

326g ⟨*Declaration of* `kinematics` *types* 326g⟩≡
```
type, public :: LIPS3
   real(kind=default), dimension(3,0:3) :: p
   real(kind=default) :: jacobian
end type LIPS3
```

$$\mathrm{dLIPS}_3 = \int \frac{\mathrm{d}^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{\mathrm{d}^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{\mathrm{d}^3\vec{p}_3}{(2\pi)^3 2E_3} (2\pi)^4 \delta^4(p_1+p_2+p_3-p_a-p_b) \quad \text{(J.4)}$$

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.

327a ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡

```
pure function two_to_three_massive &
     (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
       s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
       1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive
```

A specialized version for massless particles can be faster, because the kinematics is simpler:

327b ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡

```
pure function two_to_three_massless (s, t1, s2, phi, cos_theta3, phi3) &
     result (p)
  real(kind=default), intent(in) :: s, t1, s2, phi, cos_theta3, phi3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: pa_abs, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (s) / 2
  p1_abs = (s - s2) / (2 * sqrt (s))
```

```
    p3_abs = sqrt (s2) / 2
    p%jacobian = 1.0 / ((2*PI)**5 * 32 * s)
    cos_theta = 1 + t1 / (2*pa_abs*p1_abs)
    p%p(1,0) = p1_abs
    p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p23(1:3) = - p%p(1,1:3)
    p23(0) = on_shell (p23, sqrt (s2))
    p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3)
  end function two_to_three_massless
```

328a ⟨*Declaration of* kinematics *procedures* 324b⟩+≡

```
  public :: one_to_two
  private :: one_to_two_massive, one_to_two_massless
```

328b ⟨*Interfaces of* kinematics *procedures* 324c⟩+≡

```
  interface one_to_two
     module procedure one_to_two_massive, one_to_two_massless
  end interface
```

328c ⟨*Implementation of* kinematics *procedures* 325a⟩+≡

```
  pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
    real(kind=default), dimension(0:), intent(in) :: p12
    real(kind=default), intent(in) :: cos_theta, phi, m1, m2
    real(kind=default), dimension(2,0:3) :: p
    real(kind=default) :: s, p1_abs
    s = dot (p12, p12)
    p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
    p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p(2,1:3) = - p(1,1:3)
    p(1,0) = on_shell (p(1,:), m1)
    p(2,0) = on_shell (p(2,:), m2)
    p = boost_momentum (p, - p12)
  end function one_to_two_massive
```

328d ⟨*Implementation of* kinematics *procedures* 325a⟩+≡

```
  pure function one_to_two_massless (p12, cos_theta, phi) result (p)
    real(kind=default), dimension(0:), intent(in) :: p12
    real(kind=default), intent(in) :: cos_theta, phi
    real(kind=default), dimension(2,0:3) :: p
    real(kind=default) :: p1_abs
    p1_abs = sqrt (dot (p12, p12)) / 2
    p(1,0) = p1_abs
    p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p(2,0) = p1_abs
    p(2,1:3) = - p(1,1:3)
    p = boost_momentum (p, - p12)
```

```
end function one_to_two_massless
```

329a ⟨*Declaration of* kinematics *procedures* 324b⟩+≡

```
public :: polar_to_cartesian, on_shell
```

329b ⟨*Implementation of* kinematics *procedures* 325a⟩+≡

```
pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
  real(kind=default), intent(in) :: v_abs, cos_theta, phi
  real(kind=default), dimension(3) :: v
  real(kind=default) :: sin_phi, cos_phi, sin_theta
  sin_theta = sqrt (1.0 - cos_theta**2)
  cos_phi = cos (phi)
  sin_phi = sin (phi)
  v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
end function polar_to_cartesian
```

329c ⟨*Implementation of* kinematics *procedures* 325a⟩+≡

```
pure function on_shell (p, m) result (E)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), intent(in) :: m
  real(kind=default) :: E
  E = sqrt (m**2 + dot_product (p(1:3), p(1:3)))
end function on_shell
```

J.3 Massive 3-Particle Phase Space Revisited

$$\begin{CD} U_1 @>\xi_1>> P_1 @>\phi_1>> M \\ @V\pi_UVV @VV\pi_PV @| \\ U_2 @>\xi_2>> P_2 @>\phi_2>> M \end{CD} \tag{J.6}$$

$$\begin{CD} U_1 @>\xi>> P_1 @>\phi>> M \\ @V\pi_UVV @VV\pi_PV @VV\pi V \\ U_2 @>\xi>> P_2 @>\phi>> M \end{CD} \tag{J.7}$$

329d ⟨kinematics.f90 324a⟩+≡

```
module phase_space
  use kinds
  use constants
  use kinematics !NODEP!
  use tao_random_numbers
  implicit none
  private
```

```
  ⟨Declaration of phase_space procedures 331b⟩
  ⟨Interfaces of phase_space procedures 331c⟩
  ⟨Declaration of phase_space types 330a⟩
  character(len=*), public, parameter :: PHASE_SPACE_RCS_ID = &
       "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of phase_space procedures 331d⟩
end module phase_space
```

$$\texttt{LIPS3\_unit} : [0,1]^5 \tag{J.8}$$

330a ⟨*Declaration of* phase_space *types* 330a⟩≡

```
type, public :: LIPS3_unit
   real(kind=default), dimension(5) :: x
   real(kind=default) :: s
   real(kind=default), dimension(2) :: mass_in
   real(kind=default), dimension(3) :: mass_out
   real(kind=default) :: jacobian
end type LIPS3_unit
```

330b ⟨*Declaration of* phase_space *types* 330a⟩+≡

```
type, public :: LIPS3_unit_massless
   real(kind=default), dimension(5) :: x
   real(kind=default) :: s
   real(kind=default) :: jacobian
end type LIPS3_unit_massless
```

$$\texttt{LIPS3\_s2\_t1\_angles} : (s_2, t_1, \phi, \cos\theta_3, \phi_3) \tag{J.9}$$

330c ⟨*Declaration of* phase_space *types* 330a⟩+≡

```
type, public :: LIPS3_s2_t1_angles
   real(kind=default) :: s2, t1, phi, cos_theta3, phi3
   real(kind=default) :: s
   real(kind=default), dimension(2) :: mass_in
   real(kind=default), dimension(3) :: mass_out
   real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles
```

330d ⟨*Declaration of* phase_space *types* 330a⟩+≡

```
type, public :: LIPS3_s2_t1_angles_massless
   real(kind=default) :: s2, t1, phi, cos_theta3, phi3
   real(kind=default) :: s
   real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles_massless
```

$$\texttt{LIPS3\_momenta} : (p_1, p_2, p_3) \tag{J.10}$$

330e ⟨*Declaration of* phase_space *types* 330a⟩+≡

```
  type, public :: LIPS3_momenta
     real(kind=default), dimension(0:3,3) :: p
     real(kind=default) :: s
     real(kind=default), dimension(2) :: mass_in
     real(kind=default), dimension(3) :: mass_out
     real(kind=default) :: jacobian
  end type LIPS3_momenta
```

331a ⟨*Declaration of* phase_space *types* 330a⟩+≡

```
  type, public :: LIPS3_momenta_massless
     real(kind=default), dimension(0:3,3) :: p
     real(kind=default) :: s
     real(kind=default) :: jacobian
  end type LIPS3_momenta_massless
```

331b ⟨*Declaration of* phase_space *procedures* 331b⟩≡

```
  public :: random_LIPS3
  private :: random_LIPS3_unit, random_LIPS3_unit_massless
```

331c ⟨*Interfaces of* phase_space *procedures* 331c⟩≡

```
  interface random_LIPS3
     module procedure random_LIPS3_unit, random_LIPS3_unit_massless
  end interface
```

331d ⟨*Implementation of* phase_space *procedures* 331d⟩≡

```
  pure subroutine random_LIPS3_unit (rng, lips)
    type(tao_random_state), intent(inout) :: rng
    type(LIPS3_unit), intent(inout) :: lips
    call tao_random_number (rng, lips%x)
    lips%jacobian = 1
  end subroutine random_LIPS3_unit
```

331e ⟨*Implementation of* phase_space *procedures* 331d⟩+≡

```
  pure subroutine random_LIPS3_unit_massless (rng, lips)
    type(tao_random_state), intent(inout) :: rng
    type(LIPS3_unit_massless), intent(inout) :: lips
    call tao_random_number (rng, lips%x)
    lips%jacobian = 1
  end subroutine random_LIPS3_unit_massless
```

331f ⟨*Declaration of* phase_space *procedures* 331b⟩+≡

```
  private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
```

331g ⟨*(Unused) Interfaces of* phase_space *procedures* 331g⟩≡

```
  interface assignment(=)
     module procedure &
          LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
  end interface
```

332a ⟨*Implementation of* phase_space *procedures* 331d⟩+≡
```
pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
  type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
  type(LIPS3_unit), intent(in) :: unit
end subroutine  LIPS3_unit_to_s2_t1_angles
```

332b ⟨*Implementation of* phase_space *procedures* 331d⟩+≡
```
pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
  type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
  type(LIPS3_unit_massless), intent(in) :: unit
end subroutine  LIPS3_unit_to_s2_t1_angles_m0
```

J.4 Massless n-Particle Phase Space: RAMBO

332c ⟨*Declaration of* kinematics *procedures* 324b⟩+≡
```
public :: massless_isotropic_decay
```

The massless RAMBO algorithm [25]:

332d ⟨*Implementation of* kinematics *procedures* 325a⟩+≡
```
pure function massless_isotropic_decay (roots, ran) result (p)
  real (kind=default), intent(in) :: roots
  real (kind=default), dimension(:,:), intent(in) :: ran
  real (kind=default), dimension(size(ran,dim=1),0:3) :: p
  real (kind=default), dimension(size(ran,dim=1),0:3) :: q
  real (kind=default), dimension(0:3) :: qsum
  real (kind=default) :: cos_theta, sin_theta, phi, qabs, x, r, z
  integer :: k
  ⟨Generate isotropic null vectors 332e⟩
  ⟨Boost and rescale the vectors 333a⟩
end function massless_isotropic_decay
```

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

332e ⟨*Generate isotropic null vectors* 332e⟩≡
```
do k = 1, size (p, dim = 1)
   q(k,0) = - log (ran(k,1) * ran(k,2))
   cos_theta = 2 * ran(k,3) - 1
   sin_theta = sqrt (1 - cos_theta**2)
   phi = 2 * PI * ran(k,4)
   q(k,1) = q(k,0) * sin_theta * cos (phi)
   q(k,2) = q(k,0) * sin_theta * sin (phi)
   q(k,3) = q(k,0) * cos_theta
enddo
```

The proof that the Jacobian of the transformation vanishes can be found in [25]. The transformation is really a Lorentz boost (as can be seen easily).

333a ⟨*Boost and rescale the vectors* 333a⟩≡
```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
   r = dot (q(k,:), qsum) / qabs
   z = (q(k,0) + r) / (qsum(0) + qabs)
   p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
   p(k,0) = x * r
enddo
```

333b ⟨*Declaration of* `kinematics` *procedures* 324b⟩+≡
```
public :: phase_space_volume
```

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

333c ⟨*Implementation of* `kinematics` *procedures* 325a⟩+≡
```
pure function phase_space_volume (n, roots) result (volume)
  integer, intent(in) :: n
  real (kind=default), intent(in) :: roots
  real (kind=default) :: volume
  real (kind=default) :: nd
  nd = n
  volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

J.5 Tests

333d ⟨`ktest.f90` 333d⟩≡
```
program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default) :: &
       ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: t1_min, t1_max
  real(kind=default), dimension(5) :: r
  type(LIPS3) :: p
```

```
  integer :: i
  character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
  ma = 1.0
  mb = 1.0
  m1 = 10.0
  m2 = 20.0
  m3 = 30.0
  s = 100.0 ** 2
  do i = 1, 10
     call tao_random_number (r)
     s2 = (r(1) * (sqrt (s) - m1) + (1 - r(1)) * (m2 + m3)) ** 2
     t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
          + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
     t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
          - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
     t1 = r(2) * t1_max + (1 - r(2)) * t1_min
     phi = 2*PI * r(3)
     cos_theta3 = 2 * r(4) - 1
     phi3 = 2*PI * r(5)
     p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
     print fmt, "p1       = ", p%p(1,:)
     print fmt, "p2       = ", p%p(2,:)
     print fmt, "p3       = ", p%p(3,:)
     print fmt, "p1,2,3^2 = ", dot (p%p(1,:), p%p(1,:)), &
          dot (p%p(2,:), p%p(2,:)), dot (p%p(3,:), p%p(3,:))
     print fmt, "sum(p)   = ", p%p(1,:) + p%p(2,:) + p%p(3,:)
     print fmt, "|J|      = ", p%jacobian
  end do
end program ktest
```

Trivial check for typos, should be removed from the finalized program!

334 ⟨*Trivial* ktest.f90 334⟩≡

```
program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default), dimension(0:3) :: p, q, p_prime, p0
  real(kind=default) :: m
  character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
  integer :: i
```

```
  do i = 1, 5
     if (i == 1) then
        p = (/ 1.0_double, 0.0_double, 0.0_double, 0.0_double /)
        m = 1.0
     else
        call tao_random_number (p)
        m = sqrt (PI)
     end if
     call tao_random_number (q(1:3))
     q(0) = sqrt (m**2 + dot_product (q(1:3), q(1:3)))
     p_prime = boost_momentum (p, q)
     print fmt, "p    = ", p
     print fmt, "q    = ", q
     print fmt, "p'   = ", p_prime
     print fmt, "p^2  = ", dot (p, p)
     print fmt, "p'^2 = ", dot (p_prime, p_prime)
     if (dot (p, p) > 0.0) then
        p0 = boost_momentum (p, p)
        print fmt, "p0   = ", p0
        print fmt, "p0^2 = ", dot (p0, p0)
     end if
  end do
end program ktest
```

—K—
Coordinates

336 ⟨coordinates.f90 336⟩≡
```
! coordinates.f90 --
⟨Copyleft notice 1⟩
module coordinates
  use kinds
  use constants, only: PI
  use specfun, only: gamma
  implicit none
  private
  ⟨Declaration of coordinates procedures 337a⟩
contains
  ⟨Implementation of coordinates procedures 337b⟩
end module coordinates
```

K.1 Angular Spherical Coordinates

$$\begin{aligned} x_n &= r\cos\theta_{n-2} \\ x_{n-1} &= r\sin\theta_{n-2}\cos\theta_{n-3} \\ &\cdots \\ x_3 &= r\sin\theta_{n-2}\sin\theta_{n-3}\cdots\cos\theta_1 \\ x_2 &= r\sin\theta_{n-2}\sin\theta_{n-3}\cdots\sin\theta_1\cos\phi \\ x_1 &= r\sin\theta_{n-2}\sin\theta_{n-3}\cdots\sin\theta_1\sin\phi \end{aligned} \tag{K.1}$$

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

$$\begin{aligned}
x_n &= r\cos\theta_{n-2} \\
x_{n-1} &= rP_{n-2}\cos\theta_{n-3} \\
&\cdots \\
x_3 &= rP_2\cos\theta_1 \\
x_2 &= rP_1\cos\phi \\
x_1 &= rP_1\sin\phi
\end{aligned} \tag{K.4}$$

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.

337a ⟨*Declaration of* `coordinates` *procedures* 337a⟩≡

```
public :: spherical_to_cartesian_2, &
     spherical_to_cartesian, spherical_to_cartesian_j
```

337b ⟨*Implementation of* `coordinates` *procedures* 337b⟩≡

```
pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: theta
  real(kind=default), dimension(:), intent(out), optional :: x
  real(kind=default), intent(out), optional :: jacobian
  real(kind=default), dimension(size(theta)) :: cos_theta
  real(kind=default), dimension(size(theta)+1) :: product_sin_theta
  integer :: n, i
  n = size (theta) + 2
  cos_theta = cos (theta)
  product_sin_theta(n-1) = 1.0_default
  do i = n - 2, 1, -1
     product_sin_theta(i) = &
          product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
  end do
```

```
    if (present (x)) then
       x(1) = r * product_sin_theta(1) * sin (phi)
       x(2) = r * product_sin_theta(1) * cos (phi)
       x(3:) = r * product_sin_theta(2:n-1) * cos_theta
    end if
    if (present (jacobian)) then
       jacobian = r**(n-1) * product (product_sin_theta)
    end if
  end subroutine spherical_to_cartesian_2
```

Note that `call` inside of a function breaks `F`-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where `theta` could not be assumed shape ...

338a ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
  pure function spherical_to_cartesian (r, phi, theta) result (x)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: theta
    real(kind=default), dimension(size(theta)+2) :: x
    call spherical_to_cartesian_2 (r, phi, theta, x = x)
  end function spherical_to_cartesian
```

338b ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
  pure function spherical_to_cartesian_j (r, phi, theta) &
       result (jacobian)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: theta
    real(kind=default) :: jacobian
    call spherical_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
  end function spherical_to_cartesian_j
```

338c ⟨*Declaration of* `coordinates` *procedures* 337a⟩+≡

```
  public :: cartesian_to_spherical_2, &
       cartesian_to_spherical, cartesian_to_spherical_j
```

338d ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
  pure subroutine cartesian_to_spherical_2 (x, r, phi, theta, jacobian)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(out), optional :: r, phi
    real(kind=default), dimension(:), intent(out), optional :: theta
    real(kind=default), intent(out), optional :: jacobian
    real(kind=default) :: local_r
    real(kind=default), dimension(size(x)-2) :: cos_theta
    real(kind=default), dimension(size(x)-1) :: product_sin_theta
```

```
    integer :: n, i
    n = size (x)
    local_r = sqrt (dot_product (x, x))
    product_sin_theta(n-1) = 1
    do i = n, 3, -1
       cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
       product_sin_theta(i-2) = &
            product_sin_theta(i-1) * sqrt (1 - cos_theta(i-2)**2)
    end do
    if (present (r)) then
       r = local_r
    end if
    if (present (phi)) then
       phi = atan2 (x(1), x(2))
    end if
    if (present (theta)) then
       theta = acos (cos_theta)
    end if
    if (present (jacobian)) then
       jacobian = local_r**(1-n) / product (product_sin_theta)
    end if
  end subroutine cartesian_to_spherical_2
```

339a ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
  pure subroutine cartesian_to_spherical (x, r, phi, theta)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(out) :: r, phi
    real(kind=default), dimension(:), intent(out) :: theta
    call cartesian_to_spherical_2 (x, r, phi, theta)
  end subroutine cartesian_to_spherical
```

339b ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
  pure function cartesian_to_spherical_j (x) result (jacobian)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default) :: jacobian
    call cartesian_to_spherical_2 (x, jacobian = jacobian)
  end function cartesian_to_spherical_j
```

K.2 Trigonometric Spherical Coordinates

339c ⟨*Declaration of* `coordinates` *procedures* 337a⟩+≡

```
  public :: spherical_cos_to_cartesian_2, &
       spherical_cos_to_cartesian, spherical_cos_to_cartesian_j
```

Using the cosine, we have to drop P_1 from the Jacobian

340a ⟨*Implementation of* coordinates *procedures* 337b⟩+≡
```
pure subroutine spherical_cos_to_cartesian_2 (r, phi, cos_theta, x, jacobian)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: cos_theta
  real(kind=default), dimension(:), intent(out), optional :: x
  real(kind=default), intent(out), optional :: jacobian
  real(kind=default), dimension(size(cos_theta)+1) :: product_sin_theta
  integer :: n, i
  n = size (cos_theta) + 2
  product_sin_theta(n-1) = 1.0_default
  do i = n - 2, 1, -1
     product_sin_theta(i) = &
          product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
  end do
  if (present (x)) then
     x(1) = r * product_sin_theta(1) * sin (phi)
     x(2) = r * product_sin_theta(1) * cos (phi)
     x(3:) = r * product_sin_theta(2:n-1) * cos_theta
  end if
  if (present (jacobian)) then
     jacobian = r**(n-1) * product (product_sin_theta(2:))
  end if
end subroutine spherical_cos_to_cartesian_2
```

340b ⟨*Implementation of* coordinates *procedures* 337b⟩+≡
```
pure function spherical_cos_to_cartesian (r, phi, theta) result (x)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: theta
  real(kind=default), dimension(size(theta)+2) :: x
  call spherical_cos_to_cartesian_2 (r, phi, theta, x = x)
end function spherical_cos_to_cartesian
```

340c ⟨*Implementation of* coordinates *procedures* 337b⟩+≡
```
pure function spherical_cos_to_cartesian_j (r, phi, theta) &
     result (jacobian)
  real(kind=default), intent(in) :: r, phi
  real(kind=default), dimension(:), intent(in) :: theta
  real(kind=default) :: jacobian
  call spherical_cos_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
end function spherical_cos_to_cartesian_j
```

340d ⟨*Declaration of* coordinates *procedures* 337a⟩+≡
```
public :: cartesian_to_spherical_cos_2, &
     cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
```

341a ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
pure subroutine cartesian_to_spherical_cos_2 (x, r, phi, cos_theta, jacobian)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(out), optional :: r, phi
  real(kind=default), dimension(:), intent(out), optional :: cos_theta
  real(kind=default), intent(out), optional :: jacobian
  real(kind=default) :: local_r
  real(kind=default), dimension(size(x)-2) :: local_cos_theta
  real(kind=default), dimension(size(x)-1) :: product_sin_theta
  integer :: n, i
  n = size (x)
  local_r = sqrt (dot_product (x, x))
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
     local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
     product_sin_theta(i-2) = &
          product_sin_theta(i-1) * sqrt (1 - local_cos_theta(i-2)**2)
  end do
  if (present (r)) then
     r = local_r
  end if
  if (present (phi)) then
     phi = atan2 (x(1), x(2))
  end if
  if (present (cos_theta)) then
     cos_theta = local_cos_theta
  end if
  if (present (jacobian)) then
     jacobian = local_r**(1-n) / product (product_sin_theta(2:))
  end if
end subroutine cartesian_to_spherical_cos_2
```

341b ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
pure subroutine cartesian_to_spherical_cos (x, r, phi, cos_theta)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(out) :: r, phi
  real(kind=default), dimension(:), intent(out), optional :: cos_theta
  call cartesian_to_spherical_cos_2 (x, r, phi, cos_theta)
end subroutine cartesian_to_spherical_cos
```

341c ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
pure function cartesian_to_spherical_cos_j (x) result (jacobian)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: jacobian
  call cartesian_to_spherical_cos_2 (x, jacobian = jacobian)
```

```
end function cartesian_to_spherical_cos_j
```

K.3 Surface of a Sphere

342a ⟨*Declaration of* `coordinates` *procedures* 337a⟩+≡

```
public :: surface
```

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

342b ⟨*Implementation of* `coordinates` *procedures* 337b⟩+≡

```
pure function surface (n) result (vol)
  integer, intent(in) :: n
  real(kind=default) :: vol
  real(kind=default) :: n_by_2
  n_by_2 = 0.5_default * n
  vol = 2 * PI**n_by_2 / gamma (n_by_2)
end function surface
```

—L— Idiomatic Fortran90 Interface for MPI

343a ⟨mpi90.f90 343a⟩≡
```
! mpi90.f90 --
⟨Copyleft notice 1⟩
module mpi90
  use kinds
  use mpi
  implicit none
  private
  ⟨Declaration of mpi90 procedures 343b⟩
  ⟨Interfaces of mpi90 procedures 346c⟩
  ⟨Parameters in mpi90 (never defined)⟩
  ⟨Variables in mpi90 (never defined)⟩
  ⟨Declaration of mpi90 types 348b⟩
  character(len=*), public, parameter :: MPI90_RCS_ID = &
       "$Id: mpi90.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  ⟨Implementation of mpi90 procedures 344a⟩
end module mpi90
```

L.1 Basics

343b ⟨Declaration of mpi90 procedures 343b⟩≡
```
public :: mpi90_init
public :: mpi90_finalize
public :: mpi90_abort
public :: mpi90_print_error
public :: mpi90_size
public :: mpi90_rank
```

344a ⟨*Implementation of* mpi90 *procedures* 344a⟩≡

```
subroutine mpi90_init (error)
  integer, intent(out), optional :: error
  integer :: local_error
  character(len=*), parameter :: FN = "mpi90_init"
  external mpi_init
  call mpi_init (local_error)
  ⟨Handle local_error (no mpi90_abort) 344b⟩
end subroutine mpi90_init
```

344b ⟨*Handle* local_error *(no* mpi90_abort*)* 344b⟩≡

```
if (present (error)) then
   error = local_error
else
   if (local_error /= MPI_SUCCESS) then
      call mpi90_print_error (local_error, FN)
      stop
   end if
end if
```

344c ⟨*Handle* local_error 344c⟩≡

```
if (present (error)) then
   error = local_error
else
   if (local_error /= MPI_SUCCESS) then
      call mpi90_print_error (local_error, FN)
      call mpi90_abort (local_error)
      stop
   end if
end if
```

344d ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
subroutine mpi90_finalize (error)
  integer, intent(out), optional :: error
  integer :: local_error
  character(len=*), parameter :: FN = "mpi90_finalize"
  external mpi_finalize
  call mpi_finalize (local_error)
  ⟨Handle local_error 344c⟩
end subroutine mpi90_finalize
```

344e ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
subroutine mpi90_abort (code, domain, error)
  integer, intent(in), optional :: code, domain
  integer, intent(out), optional :: error
  character(len=*), parameter :: FN = "mpi90_abort"
```

```
    integer :: local_domain, local_code, local_error
    external mpi_abort
    if (present (code)) then
       local_code = code
    else
       local_code = MPI_ERR_UNKNOWN
    end if
    ⟨Set default for domain 345b⟩
    call mpi_abort (local_domain, local_code, local_error)
    ⟨Handle local_error (no mpi90_abort) 344b⟩
  end subroutine mpi90_abort
```

345a ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_print_error (error, msg)
    integer, intent(in) :: error
    character(len=*), optional :: msg
    character(len=*), parameter :: FN = "mpi90_print_error"
    integer :: msg_len, local_error
    external mpi_error_string
    call mpi_error_string (error, msg, msg_len, local_error)
    if (local_error /= MPI_SUCCESS) then
       print *, "PANIC: even MPI_ERROR_STRING() failed!!!"
       call mpi90_abort (local_error)
    else if (present (msg)) then
       print *, trim (msg), ": ", trim (msg(msg_len+1:))
    else
       print *, "mpi90: ", trim (msg(msg_len+1:))
    end if
  end subroutine mpi90_print_error
```

345b ⟨*Set default for* domain 345b⟩≡

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

345c ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_size (sz, domain, error)
    integer, intent(out) :: sz
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_size"
    integer :: local_domain, local_error
    external mpi_comm_size
```

```
    ⟨Set default for domain 345b⟩
    call mpi_comm_size (local_domain, sz, local_error)
    ⟨Handle local_error 344c⟩
  end subroutine mpi90_size
```

346a ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_rank (rank, domain, error)
    integer, intent(out) :: rank
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_rank"
    integer :: local_domain, local_error
    external mpi_comm_rank
    ⟨Set default for domain 345b⟩
    call mpi_comm_rank (local_domain, rank, local_error)
    ⟨Handle local_error 344c⟩
  end subroutine mpi90_rank
```

L.2 Point to Point

346b ⟨*Declaration of* mpi90 *procedures* 343b⟩+≡

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

346c ⟨*Interfaces of* mpi90 *procedures* 346c⟩≡

```
  interface mpi90_send
     module procedure &
          mpi90_send_integer, mpi90_send_double, &
          mpi90_send_integer_array, mpi90_send_double_array, &
          mpi90_send_integer_array2, mpi90_send_double_array2
  end interface
```

346d ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_send_integer (value, target, tag, domain, error)
    integer, intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    call mpi90_send_integer_array ((/ value /), target, tag, domain, error)
  end subroutine mpi90_send_integer
```

346e ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_send_double (value, target, tag, domain, error)
```

```
    real(kind=default), intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    call mpi90_send_double_array ((/ value /), target, tag, domain, error)
  end subroutine mpi90_send_double
```

347a ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_send_integer_array (buffer, target, tag, domain, error)
    integer, dimension(:), intent(in) :: buffer
    integer, intent(in) ::  target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_send_integer_array"
    integer, parameter :: datatype = MPI_INTEGER
    ⟨Body of mpi90_send_*_array 347b⟩
  end subroutine mpi90_send_integer_array
```

347b ⟨*Body of* `mpi90_send_*_array` 347b⟩≡

```
  integer :: local_domain, local_error
  external mpi_send
  ⟨Set default for domain 345b⟩
  call mpi_send (buffer, size (buffer), datatype, target, tag, &
                 local_domain, local_error)
  ⟨Handle local_error 344c⟩
```

347c ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_send_double_array (buffer, target, tag, domain, error)
    real(kind=default), dimension(:), intent(in) :: buffer
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_send_double_array"
    integer, parameter :: datatype = MPI_DOUBLE_PRECISION
    ⟨Body of mpi90_send_*_array 347b⟩
  end subroutine mpi90_send_double_array
```

347d ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_send_integer_array2 (value, target, tag, domain, error)
    integer, dimension(:,:), intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    integer, dimension(size(value)) :: buffer
    buffer = reshape (value, shape(buffer))
    call mpi90_send_integer_array (buffer, target, tag, domain, error)
```

```
  end subroutine mpi90_send_integer_array2
```

348a ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_send_double_array2 (value, target, tag, domain, error)
    real(kind=default), dimension(:,:), intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    real(kind=default), dimension(size(value)) :: buffer
    buffer = reshape (value, shape(buffer))
    call mpi90_send_double_array (buffer, target, tag, domain, error)
  end subroutine mpi90_send_double_array2
```

348b ⟨*Declaration of* `mpi90` *types* 348b⟩≡

```
  type, public :: mpi90_status
     integer :: count, source, tag, error
  end type mpi90_status
```

348c ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_receive_integer (value, source, tag, domain, status, error)
    integer, intent(out) :: value
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    integer, dimension(1)  :: buffer
    call mpi90_receive_integer_array (buffer, source, tag, domain, status, error)
    value = buffer(1)
  end subroutine mpi90_receive_integer
```

348d ⟨*Interfaces of* `mpi90` *procedures* 346c⟩+≡

```
  interface mpi90_receive
     module procedure &
          mpi90_receive_integer, mpi90_receive_double, &
          mpi90_receive_integer_array, mpi90_receive_double_array, &
          mpi90_receive_integer_array2, mpi90_receive_double_array2
  end interface
```

348e ⟨*Set defaults for* `source`, `tag` *and* `domain` 348e⟩≡

```
  if (present (source)) then
     local_source = source
  else
     local_source = MPI_ANY_SOURCE
  end if
  if (present (tag)) then
     local_tag = tag
  else
```

```
    local_tag = MPI_ANY_TAG
end if
⟨Set default for domain 345b⟩
```

349a ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
subroutine mpi90_receive_double (value, source, tag, domain, status, error)
  real(kind=default), intent(out) :: value
  integer, intent(in), optional :: source, tag, domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  real(kind=default), dimension(1) :: buffer
  call mpi90_receive_double_array (buffer, source, tag, domain, status, error)
  value = buffer(1)
end subroutine mpi90_receive_double
```

349b ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
subroutine mpi90_receive_integer_array &
     (buffer, source, tag, domain, status, error)
  integer, dimension(:), intent(out) :: buffer
  integer, intent(in), optional :: source, tag, domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  character(len=*), parameter :: FN = "mpi90_receive_integer_array"
  integer, parameter :: datatype = MPI_INTEGER
  ⟨Body of mpi90_receive_*_array 349c⟩
end subroutine mpi90_receive_integer_array
```

349c ⟨*Body of* `mpi90_receive_*_array` 349c⟩≡

```
integer :: local_source, local_tag, local_domain, local_error
integer, dimension(MPI_STATUS_SIZE) :: local_status
external mpi_receive, mpi_get_count
⟨Set defaults for source, tag and domain 348e⟩
call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
               local_domain, local_status, local_error)
⟨Handle local_error 344c⟩
if (present (status)) then
   call decode_status (status, local_status, datatype)
end if
```

349d ⟨*Declaration of* `mpi90` *procedures* 343b⟩+≡

```
private :: decode_status
```

Can we ignore `ierror`???

349e ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
subroutine decode_status (status, mpi_status, datatype)
```

```
    type(mpi90_status), intent(out) :: status
    integer, dimension(:), intent(in) :: mpi_status
    integer, intent(in), optional :: datatype
    integer :: ierror
    if (present (datatype)) then
       call mpi_get_count (mpi_status, datatype, status%count, ierror)
    else
       status%count = 0
    end if
    status%source = mpi_status(MPI_SOURCE)
    status%tag = mpi_status(MPI_TAG)
    status%error = mpi_status(MPI_ERROR)
  end subroutine decode_status
```

350a ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_receive_double_array &
       (buffer, source, tag, domain, status, error)
    real(kind=default), dimension(:), intent(out) :: buffer
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_receive_double_array"
    integer, parameter :: datatype = MPI_DOUBLE_PRECISION
    ⟨Body of mpi90_receive_*_array 349c⟩
  end subroutine mpi90_receive_double_array
```

350b ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_receive_integer_array2 &
       (value, source, tag, domain, status, error)
    integer, dimension(:,:), intent(out) :: value
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    integer, dimension(size(value)) :: buffer
    call mpi90_receive_integer_array &
         (buffer, source, tag, domain, status, error)
    value = reshape (buffer, shape(value))
  end subroutine mpi90_receive_integer_array2
```

350c ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_receive_double_array2 &
       (value, source, tag, domain, status, error)
    real(kind=default), dimension(:,:), intent(out) :: value
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
```

```
    integer, intent(out), optional :: error
    real(kind=default), dimension(size(value)) :: buffer
    call mpi90_receive_double_array &
          (buffer, source, tag, domain, status, error)
    value = reshape (buffer, shape(value))
  end subroutine mpi90_receive_double_array2
```

351a ⟨*Interfaces of* `mpi90` *procedures* 346c⟩+≡

```
  interface mpi90_receive_pointer
     module procedure &
          mpi90_receive_integer_pointer, mpi90_receive_double_pointer
  end interface
```

351b ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_receive_integer_pointer &
       (buffer, source, tag, domain, status, error)
    integer, dimension(:), pointer :: buffer
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_receive_integer_pointer"
    integer, parameter :: datatype = MPI_INTEGER
    ⟨Body of mpi90_receive_*_pointer 351c⟩
  end subroutine mpi90_receive_integer_pointer
```

351c ⟨*Body of* `mpi90_receive_*_pointer` 351c⟩≡

```
  integer :: local_source, local_tag, local_domain, local_error, buffer_size
  integer, dimension(MPI_STATUS_SIZE) :: local_status
  integer :: ierror
  external mpi_receive, mpi_get_count
  ⟨Set defaults for source, tag and domain 348e⟩
```

351d ⟨*Body of* `mpi90_receive_*_pointer` 351c⟩+≡

```
  call mpi_probe (local_source, local_tag, local_domain, &
                  local_status, local_error)
  ⟨Handle local_error 344c⟩
```

Can we ignore `ierror`???

351e ⟨*Body of* `mpi90_receive_*_pointer` 351c⟩+≡

```
  call mpi_get_count (local_status, datatype, buffer_size, ierror)
  if (associated (buffer)) then
     if (size (buffer) /= buffer_size) then
        deallocate (buffer)
        allocate (buffer(buffer_size))
     end if
```

```
else
   allocate (buffer(buffer_size))
end if
```

352a ⟨*Body of* `mpi90_receive_*_pointer` 351c⟩+≡

```
call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
               local_domain, local_status, local_error)
```

352b ⟨*Body of* `mpi90_receive_*_pointer` 351c⟩+≡

```
⟨Handle local_error 344c⟩
if (present (status)) then
   call decode_status (status, local_status, datatype)
end if
```

352c ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
subroutine mpi90_receive_double_pointer &
     (buffer, source, tag, domain, status, error)
  real(kind=default), dimension(:), pointer :: buffer
  integer, intent(in), optional :: source, tag, domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  character(len=*), parameter :: FN = "mpi90_receive_double_pointer"
  integer, parameter :: datatype = MPI_DOUBLE_PRECISION
  ⟨Body of mpi90_receive_*_pointer 351c⟩
end subroutine mpi90_receive_double_pointer
```

L.3 Collective Communication

352d ⟨*Declaration of* `mpi90` *procedures* 343b⟩+≡

```
public :: mpi90_broadcast
```

352e ⟨*Interfaces of* `mpi90` *procedures* 346c⟩+≡

```
interface mpi90_broadcast
   module procedure &
        mpi90_broadcast_integer, mpi90_broadcast_integer_array, &
        mpi90_broadcast_integer_array2, mpi90_broadcast_integer_array3, &
        mpi90_broadcast_double, mpi90_broadcast_double_array, &
        mpi90_broadcast_double_array2, mpi90_broadcast_double_array3, &
        mpi90_broadcast_logical, mpi90_broadcast_logical_array, &
        mpi90_broadcast_logical_array2, mpi90_broadcast_logical_array3
end interface
```

352f ⟨*Set default for* `domain` 345b⟩+≡

```
if (present (domain)) then
   local_domain = domain
```

```
  else
     local_domain = MPI_COMM_WORLD
  end if
```

353a ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_integer (value, root, domain, error)
    integer, intent(inout) :: value
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    integer, dimension(1) :: buffer
    buffer(1) = value
    call mpi90_broadcast_integer_array (buffer, root, domain, error)
    value = buffer(1)
  end subroutine mpi90_broadcast_integer
```

353b ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_double (value, root, domain, error)
    real(kind=default), intent(inout) :: value
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    real(kind=default), dimension(1) :: buffer
    buffer(1) = value
    call mpi90_broadcast_double_array (buffer, root, domain, error)
    value = buffer(1)
  end subroutine mpi90_broadcast_double
```

353c ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_logical (value, root, domain, error)
    logical, intent(inout) :: value
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    logical, dimension(1) :: buffer
    buffer(1) = value
    call mpi90_broadcast_logical_array (buffer, root, domain, error)
    value = buffer(1)
  end subroutine mpi90_broadcast_logical
```

353d ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_integer_array (buffer, root, domain, error)
    integer, dimension(:), intent(inout) :: buffer
    integer, intent(in) ::  root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
```

```
    character(len=*), parameter :: FN = "mpi90_broadcast_integer_array"
    integer, parameter :: datatype = MPI_INTEGER
    ⟨Body of mpi90_broadcast_*_array 354a⟩
  end subroutine mpi90_broadcast_integer_array
```

354a ⟨*Body of* `mpi90_broadcast_*_array` 354a⟩≡

```
  integer :: local_domain, local_error
  external mpi_bcast
  ⟨Set default for domain 345b⟩
  call mpi_bcast (buffer, size (buffer), datatype, root, &
                  local_domain, local_error)
  ⟨Handle local_error 344c⟩
```

354b ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_double_array (buffer, root, domain, error)
    real(kind=default), dimension(:), intent(inout) :: buffer
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    integer, parameter :: datatype = MPI_DOUBLE_PRECISION
    character(len=*), parameter :: FN = "mpi90_broadcast_double_array"
    ⟨Body of mpi90_broadcast_*_array 354a⟩
  end subroutine mpi90_broadcast_double_array
```

354c ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_logical_array (buffer, root, domain, error)
    logical, dimension(:), intent(inout) :: buffer
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    integer, parameter :: datatype = MPI_LOGICAL
    character(len=*), parameter :: FN = "mpi90_broadcast_logical_array"
    ⟨Body of mpi90_broadcast_*_array 354a⟩
  end subroutine mpi90_broadcast_logical_array
```

354d ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_integer_array2 (value, root, domain, error)
    integer, dimension(:,:), intent(inout) :: value
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    integer, dimension(size(value)) :: buffer
    buffer = reshape (value, shape(buffer))
    call mpi90_broadcast_integer_array (buffer, root, domain, error)
    value = reshape (buffer, shape(value))
  end subroutine mpi90_broadcast_integer_array2
```

355a ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡
```
subroutine mpi90_broadcast_double_array2 (value, root, domain, error)
  real(kind=default), dimension(:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  real(kind=default), dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_double_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_double_array2
```

355b ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡
```
subroutine mpi90_broadcast_logical_array2 (value, root, domain, error)
  logical, dimension(:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  logical, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_logical_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_logical_array2
```

355c ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡
```
subroutine mpi90_broadcast_integer_array3 (value, root, domain, error)
  integer, dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_integer_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_integer_array3
```

355d ⟨*Implementation of* mpi90 *procedures* 344a⟩+≡
```
subroutine mpi90_broadcast_double_array3 (value, root, domain, error)
  real(kind=default), dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  real(kind=default), dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_double_array (buffer, root, domain, error)
```

```
    value = reshape (buffer, shape(value))
  end subroutine mpi90_broadcast_double_array3
```

356 ⟨*Implementation of* `mpi90` *procedures* 344a⟩+≡

```
  subroutine mpi90_broadcast_logical_array3 (value, root, domain, error)
    logical, dimension(:,:,:), intent(inout) :: value
    integer, intent(in) :: root
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    logical, dimension(size(value)) :: buffer
    buffer = reshape (value, shape(buffer))
    call mpi90_broadcast_logical_array (buffer, root, domain, error)
    value = reshape (buffer, shape(value))
  end subroutine mpi90_broadcast_logical_array3
```

—M—
Poor Man's Elemental Procedures

On one hand, I want to take advantage of Fortran95's improvements, but on the other hand, I want to continue to use `F` as a style guide and also allow people with Fortran90 compilers to use the library.

M.1 *m4* Macros

357a ⟨f95.m4 357a⟩≡
```
dnl f95.m4 --
divert(-1)dnl
⟨Kill m4(1) builtins 357b⟩
define(`_specific_sv',`dnl')
define(`_interface_sv',`dnl')
define(`_specific_sva',`dnl')
define(`_interface_sva',`dnl')
define(`_begin_f90',`divert(-1)dnl')
define(`_end_f90',`divert`'dnl')
divert`'dnl
```

357b ⟨Kill m4(1) builtins 357b⟩≡
```
undefine(`eval')
```

357c ⟨f90.m4 357c⟩≡
```
dnl f90.m4 --
divert(-1)dnl
⟨Kill m4(1) builtins 357b⟩
define(`pure',`')
define(`elemental',`')
define(`_specific_sv',`private :: $1_s, $1_v')
define(`_interface_sv',`interface $1
     module procedure $1_s, $1_v
  end interface`'define($1,$1_s)')
define(`_specific_sva',`private :: $1_s, $1_v, $1_a')
```

```
define(`_interface_sva',`interface $1
     module procedure $1_s, $1_v, $1_a
  end interface''define($1,$1_s)')
define(`_begin_f90',`dnl')
define(`_end_f90',`dnl')
divert`'dnl
```

M.2 Miscellaneous Utilities

358a ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
_begin_f90
```

358b ⟨*Declaration of* utils *procedures* 304b⟩+≡

```
_begin_f90
private :: swap_integer_array, swap_real_array
_end_f90
```

358c ⟨*Interfaces of* utils *procedures* 304c⟩+≡

```
_begin_f90
interface swap
   module procedure swap_integer_array, swap_real_array
end interface
_end_f90
```

358d ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure subroutine swap_integer_array (a, b)
  integer, dimension(:), intent(inout) :: a, b
  integer, dimension(max(size(a),size(b))) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_integer_array
```

358e ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure subroutine swap_real_array (a, b)
  real(kind=default), dimension(:), intent(inout) :: a, b
  real(kind=default), dimension(max(size(a),size(b))) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_real_array
```

358f ⟨*Declaration of* utils *procedures* 304b⟩+≡

```
_specific_sva(gcd)
_specific_sva(lcm)
```

359a ⟨*Interfaces of* utils *procedures* 304c⟩+≡

```
_interface_sva(gcd)
_interface_sva(lcm)
```

359b ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure function gcd_v (m, n) result (gcd_m_n)
  integer, dimension(:), intent(in) :: m, n
  integer, dimension(size(m)) :: gcd_m_n
  integer :: i
  do i = 1, size (m)
     gcd_m_n(i) = gcd (m(i), n(i))
  end do
end function gcd_v
```

359c ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure function lcm_v (m, n) result (lcm_m_n)
  integer, dimension(:), intent(in) :: m, n
  integer, dimension(size(m)) :: lcm_m_n
  integer :: i
  do i = 1, size (m)
     lcm_m_n(i) = lcm (m(i), n(i))
  end do
end function lcm_v
```

This abuses the _a suffix, which is used elsewhere for two-dimensional arrays:

359d ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure function gcd_a (m, n) result (gcd_m_n)
  integer, dimension(:), intent(in) :: m
  integer, intent(in) :: n
  integer, dimension(size(m)) :: gcd_m_n
  integer :: i
  do i = 1, size (m)
     gcd_m_n(i) = gcd (m(i), n)
  end do
end function gcd_a
```

359e ⟨*Implementation of* utils *procedures* 305c⟩+≡

```
pure function lcm_a (m, n) result (lcm_m_n)
  integer, dimension(:), intent(in) :: m
  integer, intent(in) :: n
  integer, dimension(size(m)) :: lcm_m_n
  integer :: i
  do i = 1, size (m)
     lcm_m_n(i) = lcm (m(i), n)
  end do
end function lcm_a
```

360a ⟨*Implementation of* utils *procedures* 305c⟩+≡
```
_end_f90
```

M.3 Errors and Exceptions

360b ⟨*Implementation of* exceptions *procedures* 246c⟩+≡
```
_begin_f90
```

360c ⟨*Declaration of* exceptions *procedures* 246b⟩+≡
```
_specific_sv(raise_exception)
_specific_sv(clear_exception)
```

360d ⟨*Interfaces of* exceptions *procedures* 360d⟩≡
```
_interface_sv(raise_exception)
_interface_sv(clear_exception)
```

360e ⟨*Implementation of* exceptions *procedures* 246c⟩+≡
```
pure subroutine raise_exception_v (exc, level, message, origin)
  type(exception), dimension(:), intent(inout) :: exc
  integer, dimension(:), intent(in) :: level
  character(len=*), dimension(:), intent(in), optional :: message, origin
  integer :: i
  do i = 1, size (exc)
     call raise_exception (exc(i), level(i), message(i), origin(i))
  end do
end subroutine raise_exception_v
```

360f ⟨*Implementation of* exceptions *procedures* 246c⟩+≡
```
pure subroutine clear_exception_v (exc)
  type(exception), dimension(:), intent(inout) :: exc
  integer :: i
  do i = 1, size (exc)
     call clear_exception (exc(i))
  end do
end subroutine clear_exception_v
```

360g ⟨*Implementation of* exceptions *procedures* 246c⟩+≡
```
_end_f90
```

M.4 The Abstract Datatype division

360h ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
_begin_f90
```

361a ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
_specific_sv(create_division)
_specific_sv(create_empty_division)
_specific_sva(copy_division)
_specific_sv(set_rigid_division)
_specific_sv(reshape_division)
_specific_sv(delete_division)
```
361b ⟨*Interfaces of* divisions *procedures* 61b⟩+≡
```
_interface_sv(create_division)
_interface_sv(create_empty_division)
_interface_sva(copy_division)
_interface_sv(set_rigid_division)
_interface_sv(reshape_division)
_interface_sv(delete_division)
```
361c ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine create_division_v (d, x_min, x_max, x_min_true, x_max_true)
  type(division_t), dimension(:), intent(out) :: d
  real(kind=default), dimension(:), intent(in) :: x_min, x_max
  real(kind=default), dimension(:), intent(in), optional :: &
       x_min_true, x_max_true
  integer :: j
  do j = 1, size (d)
     if (present (x_min_true) .and. present (x_max_true)) then
        call create_division &
             (d(j), x_min(j), x_max(j), x_min_true(j), x_max_true(j))
     else
        call create_division (d(j), x_min(j), x_max(j))
     end if
  end do
end subroutine create_division_v
```
361d ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine create_empty_division_v (d)
  type(division_t), dimension(:), intent(out) :: d
  integer :: j
  do j = 1, size (d)
     call create_empty_division (d(j))
  end do
end subroutine create_empty_division_v
```
361e ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine copy_division_v (lhs, rhs)
  type(division_t), dimension(:), intent(inout) :: lhs
  type(division_t), dimension(:), intent(in) :: rhs
```

```
    integer :: j
    do j = 1, size(lhs)
       call copy_division (lhs(j), rhs(j))
    end do
  end subroutine copy_division_v
```

This abuses the _a suffix, which is used elsewhere for two-dimensional arrays:

362a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine copy_division_a (lhs, rhs)
    type(division_t), dimension(:), intent(inout) :: lhs
    type(division_t), intent(in) :: rhs
    integer :: j
    do j = 1, size(lhs)
       call copy_division (lhs(j), rhs)
    end do
  end subroutine copy_division_a
```

362b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine set_rigid_division_v (d, ng)
    type(division_t), dimension(:), intent(inout) :: d
    integer, dimension(:), intent(in) :: ng
    integer :: j
    do j = 1, size(d)
       call set_rigid_division (d(j), ng(j))
    end do
  end subroutine set_rigid_division_v
```

362c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine reshape_division_v (d, max_num_div, ng, use_variance)
    type(division_t), dimension(:), intent(inout) :: d
    integer, dimension(:), intent(in) :: max_num_div
    integer, dimension(:), intent(in), optional :: ng
    logical, intent(in), optional :: use_variance
    integer :: j
    do j = 1, size(d)
       call reshape_division (d(j), max_num_div(j), ng(j), use_variance)
    end do
  end subroutine reshape_division_v
```

362d ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine delete_division_v (d)
    type(division_t), dimension(:), intent(inout) :: d
    integer :: j
    do j = 1, size(d)
       call delete_division (d(j))
    end do
```

```
  end subroutine delete_division_v
```

363a ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
  _specific_sv(inject_division)
  _specific_sv(inject_division_short)
```

363b ⟨*Interfaces of* divisions *procedures* 61b⟩+≡
```
  _interface_sv(inject_division)
  _interface_sv(inject_division_short)
```

363c ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
  pure subroutine inject_division_v (d, r, cell, x, x_mid, idx, wgt)
    type(division_t), dimension(:), intent(in) :: d
    real(kind=default), dimension(:), intent(in) :: r
    integer, dimension(:), intent(in) :: cell
    real(kind=default), dimension(:), intent(out) :: x, x_mid
    integer, dimension(:), intent(out) :: idx
    real(kind=default), dimension(:), intent(out) :: wgt
    integer :: j
    do j = 1, size (d)
       call inject_division (d(j), r(j), cell(j), x(j), &
                            x_mid(j), idx(j), wgt(j))
    end do
  end subroutine inject_division_v
```

363d ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
  pure subroutine inject_division_short_v (d, r, x, idx, wgt)
    type(division_t), dimension(:), intent(in) :: d
    real(kind=default), dimension(:), intent(in) :: r
    real(kind=default), dimension(:), intent(out) :: x
    integer, dimension(:), intent(out) :: idx
    real(kind=default), dimension(:), intent(out) :: wgt
    integer :: j
    do j = 1, size (d)
       call inject_division_short (d(j), r(j), x(j), idx(j), wgt(j))
    end do
  end subroutine inject_division_short_v
```

363e ⟨*Declaration of* divisions *procedures* 38a⟩+≡
```
  _specific_sv(record_integral)
  _specific_sv(record_variance)
  _specific_sv(clear_integral_and_variance)
```

363f ⟨*Declaration of* divisions *procedures (removed from WHIZARD)* 60c⟩+≡
```
  _specific_sv(record_efficiency)
```

364a ⟨*Interfaces of* divisions *procedures* 61b⟩+≡
```
_interface_sv(record_integral)
_interface_sv(record_variance)
_interface_sv(clear_integral_and_variance)
```

364b ⟨*Interfaces of* divisions *procedures (removed from WHIZARD)* 364b⟩≡
```
_interface_sv(record_efficiency)
```

364c ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine record_integral_v (d, i, f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: f
  integer :: j
  do j = 1, size (d)
     call record_integral (d(j), i(j), f)
  end do
end subroutine record_integral_v
```

364d ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine record_variance_v (d, i, var_f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: var_f
  integer :: j
  do j = 1, size (d)
     call record_variance (d(j), i(j), var_f)
  end do
end subroutine record_variance_v
```

364e ⟨*Implementation of* divisions *procedures (removed from WHIZARD)* 45b⟩+≡
```
pure subroutine record_efficiency_v (d, i, eff_f)
  type(division_t), dimension(:), intent(inout) :: d
  integer, dimension(:), intent(in) :: i
  real(kind=default), intent(in) :: eff_f
  integer :: j
  do j = 1, size (d)
     call record_efficiency (d(j), i(j), eff_f)
  end do
end subroutine record_efficiency_v
```

364f ⟨*Implementation of* divisions *procedures* 38b⟩+≡
```
pure subroutine clear_integral_and_variance_v (d)
  type(division_t), dimension(:), intent(inout) :: d
  integer :: j
  do j = 1, size (d)
```

```
      call clear_integral_and_variance (d(j))
    end do
  end subroutine clear_integral_and_variance_v
```

365a ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  _specific_sv(refine_division)
```

365b ⟨*Interfaces of* divisions *procedures* 61b⟩+≡

```
  _interface_sv(refine_division)
```

365c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine refine_division_v (d)
    type(division_t), dimension(:), intent(inout) :: d
    integer :: j
    do j = 1, size (d)
       call refine_division (d(j))
    end do
  end subroutine refine_division_v
```

365d ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  _specific_sv(probability)
  _specific_sv(inside_division)
  _specific_sv(stratified_division)
  _specific_sv(volume_division)
  _specific_sv(rigid_division)
  _specific_sv(adaptive_division)
  _specific_sv(quadrupole_division)
```

365e ⟨*Interfaces of* divisions *procedures* 61b⟩+≡

```
  _interface_sv(probability)
  _interface_sv(inside_division)
  _interface_sv(stratified_division)
  _interface_sv(volume_division)
  _interface_sv(rigid_division)
  _interface_sv(adaptive_division)
  _interface_sv(quadrupole_division)
```

365f ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure function probability_v (d, xi) result (p)
    type(division_t), dimension(:), intent(in) :: d
    real(kind=default), dimension(:), intent(in) :: xi
    real(kind=default), dimension(size(d)) :: p
    integer :: j
    do j = 1, size (d)
       p(j) = probability (d(j), xi(j))
    end do
  end function probability_v
```

366a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
pure function inside_division_v (d, x) result (theta)
  type(division_t), dimension(:), intent(in) :: d
  real(kind=default), dimension(:), intent(in) :: x
  logical, dimension(size(d)) :: theta
  integer :: j
  do j = 1, size (d)
     theta(j) = inside_division (d(j), x(j))
  end do
end function inside_division_v
```

366b ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
pure function stratified_division_v (d) result (yorn)
  type(division_t), dimension(:), intent(in) :: d
  logical, dimension(size(d)) :: yorn
  integer :: j
  do j = 1, size (d)
     yorn(j) = stratified_division (d(j))
  end do
end function stratified_division_v
```

366c ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
pure function volume_division_v (d) result (vol)
  type(division_t), dimension(:), intent(in) :: d
  real(kind=default), dimension(size(d)) :: vol
  integer :: j
  do j = 1, size(d)
     vol(j) = volume_division (d(j))
  end do
end function volume_division_v
```

366d ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
pure function rigid_division_v (d) result (n)
  type(division_t), dimension(:), intent(in) :: d
  integer, dimension(size(d)) :: n
  integer :: j
  do j = 1, size(d)
     n(j) = rigid_division (d(j))
  end do
end function rigid_division_v
```

366e ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
pure function adaptive_division_v (d) result (n)
  type(division_t), dimension(:), intent(in) :: d
  integer, dimension(size(d)) :: n
  integer :: j
```

```
    do j = 1, size(d)
       n(j) = adaptive_division (d(j))
    end do
  end function adaptive_division_v
```

367a ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure function quadrupole_division_v (d) result (q)
    type(division_t), dimension(:), intent(in) :: d
    real(kind=default), dimension(size(d)) :: q
    integer :: j
    do j = 1, size (d)
       q(j) = quadrupole_division (d(j))
    end do
  end function quadrupole_division_v
```

367b ⟨*Declaration of* divisions *procedures* 38a⟩+≡

```
  _specific_sv(copy_history)
  _specific_sv(summarize_division)
```

367c ⟨*Interfaces of* divisions *procedures* 61b⟩+≡

```
  _interface_sv(copy_history)
  _interface_sv(summarize_division)
```

367d ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure subroutine copy_history_v (lhs, rhs)
    type(div_history), dimension(:), intent(inout) :: lhs
    type(div_history), dimension(:), intent(in) :: rhs
    integer :: j
    do j = 1, size (rhs)
       call copy_history (lhs(j), rhs(j))
    end do
  end subroutine copy_history_v
```

367e ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  pure function summarize_division_v (d) result (s)
    type(division_t), dimension(:), intent(in) :: d
    type(div_history), dimension(size(d))  :: s
    integer :: j
    do j = 1, size (d)
       s(j) = summarize_division (d(j))
    end do
  end function summarize_division_v
```

367f ⟨*Implementation of* divisions *procedures* 38b⟩+≡

```
  _end_f90
```

M.5 The Abstract Datatype `vamp_grid`

368a ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡
```
_begin_f90
```

368b ⟨*Declaration of* `vamp` *procedures* 77a⟩+≡
```
_specific_sv(vamp_create_empty_grid)
_specific_sv(vamp_nullify_covariance)
_specific_sv(vamp_get_variance)
_specific_sv(vamp_nullify_variance)
```

368c ⟨*Interfaces of* `vamp` *procedures* 94c⟩+≡
```
_interface_sv(vamp_create_empty_grid)
_interface_sv(vamp_nullify_covariance)
_interface_sv(vamp_get_variance)
_interface_sv(vamp_nullify_variance)
```

368d ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡
```
pure subroutine vamp_create_empty_grid_v (g)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer :: i
  do i = 1, size (g)
     call vamp_create_empty_grid (g(i))
  end do
end subroutine vamp_create_empty_grid_v
```

368e ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡
```
pure subroutine vamp_nullify_covariance_v (g)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer :: i
  do i = 1, size (g)
     call vamp_nullify_covariance (g(i))
  end do
end subroutine vamp_nullify_covariance_v
```

368f ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡
```
pure function vamp_get_variance_v (g) result (v)
  type(vamp_grid), dimension(:), intent(in) :: g
  real(kind=default), dimension(size(g)) :: v
  integer :: i
  do i = 1, size (g)
     v(i) = vamp_get_variance (g(i))
  end do
end function vamp_get_variance_v
```

369a ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine vamp_nullify_variance_v (g)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer :: i
  do i = 1, size (g)
     call vamp_nullify_variance (g(i))
  end do
end subroutine vamp_nullify_variance_v
```

369b ⟨*Declaration of* vamp *procedures* 77a⟩+≡
```
_specific_sv(vamp_copy_grid)
_specific_sv(vamp_delete_grid)
```

369c ⟨*Interfaces of* vamp *procedures* 94c⟩+≡
```
_interface_sv(vamp_copy_grid)
_interface_sv(vamp_delete_grid)
```

369d ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine vamp_copy_grid_v (lhs, rhs)
  type(vamp_grid), dimension(:), intent(inout) :: lhs
  type(vamp_grid), dimension(:), intent(in) :: rhs
  integer :: i
  do i = 1, size (lhs)
     call vamp_copy_grid (lhs(i), rhs(i))
  end do
end subroutine vamp_copy_grid_v
```

369e ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine vamp_delete_grid_v (g)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer :: i
  do i = 1, size (g)
     call vamp_delete_grid (g(i))
  end do
end subroutine vamp_delete_grid_v
```

369f ⟨*Declaration of* vamp *procedures* 77a⟩+≡
```
_specific_sv(vamp_copy_grids)
_specific_sv(vamp_delete_grids)
```

369g ⟨*Interfaces of* vamp *procedures* 94c⟩+≡
```
_interface_sv(vamp_copy_grids)
_interface_sv(vamp_delete_grids)
```

369h ⟨*Implementation of* vamp *procedures* 77c⟩+≡
```
pure subroutine vamp_copy_grids_v (lhs, rhs)
  type(vamp_grids), dimension(:), intent(inout) :: lhs
```

```
    type(vamp_grids), dimension(:), intent(in) :: rhs
    integer :: i
    do i = 1, size (lhs)
       call vamp_copy_grids (lhs(i), rhs(i))
    end do
  end subroutine vamp_copy_grids_v
```

370a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_delete_grids_v (g)
    type(vamp_grids), dimension(:), intent(inout) :: g
    integer :: i
    do i = 1, size (g)
       call vamp_delete_grids (g(i))
    end do
  end subroutine vamp_delete_grids_v
```

370b ⟨*Declaration of* vamp *procedures* 77a⟩+≡

```
  _specific_sva(vamp_create_history)
  _specific_sv(vamp_terminate_history)
  _specific_sva(vamp_copy_history)
  _specific_sva(vamp_delete_history)
```

370c ⟨*Interfaces of* vamp *procedures* 94c⟩+≡

```
  _interface_sva(vamp_create_history)
  _interface_sv(vamp_terminate_history)
  _interface_sva(vamp_copy_history)
  _interface_sva(vamp_delete_history)
```

370d ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_create_history_v (h, ndim, verbose)
    type(vamp_history), dimension(:), intent(inout) :: h
    integer, intent(in), optional :: ndim
    logical, intent(in), optional :: verbose
    integer :: i
    do i = 1, size (h)
       call vamp_create_history (h(i), ndim, verbose)
    end do
  end subroutine vamp_create_history_v
```

370e ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
  pure subroutine vamp_create_history_a (h, ndim, verbose)
    type(vamp_history), dimension(:,:), intent(inout) :: h
    integer, intent(in), optional :: ndim
    logical, intent(in), optional :: verbose
    integer :: i
    do i = 1, size (h, dim=2)
```

```
      call vamp_create_history_v (h(:,i), ndim, verbose)
   end do
 end subroutine vamp_create_history_a
```

371a ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 pure subroutine vamp_terminate_history_v (h)
   type(vamp_history), dimension(:), intent(inout) :: h
   integer :: i
   do i = 1, size (h)
      call vamp_terminate_history (h(i))
   end do
 end subroutine vamp_terminate_history_v
```

371b ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 pure subroutine vamp_copy_history_v (lhs, rhs)
   type(vamp_history), dimension(:), intent(out) :: lhs
   type(vamp_history), dimension(:), intent(in) :: rhs
   integer :: i
   do i = 1, size (rhs)
      call vamp_copy_history (lhs(i), rhs(i))
   end do
 end subroutine vamp_copy_history_v
```

371c ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 pure subroutine vamp_copy_history_a (lhs, rhs)
   type(vamp_history), dimension(:,:), intent(out) :: lhs
   type(vamp_history), dimension(:,:), intent(in) :: rhs
   integer :: i
   do i = 1, size (rhs, dim=2)
      call vamp_copy_history_v (lhs(:,i), rhs(:,i))
   end do
 end subroutine vamp_copy_history_a
```

371d ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 pure subroutine vamp_delete_history_v (h)
   type(vamp_history), dimension(:), intent(inout) :: h
   integer :: i
   do i = 1, size (h)
      call vamp_delete_history (h(i))
   end do
 end subroutine vamp_delete_history_v
```

371e ⟨*Implementation of* vamp *procedures* 77c⟩+≡

```
 pure subroutine vamp_delete_history_a (h)
   type(vamp_history), dimension(:,:), intent(inout) :: h
   integer :: i
```

```
    do i = 1, size (h, dim=2)
       call vamp_delete_history_v (h(:,i))
    end do
  end subroutine vamp_delete_history_a
```

372 ⟨*Implementation of* `vamp` *procedures* 77c⟩+≡

```
  _end_f90
```

—N—
Ideas

N.1 Toolbox for Interactive Optimization

Idea: Provide a OpenGL interface to visualize the grid optimization.

Motivation: Would help multi channel developers.

Implementation: Coding is straightforward, but interface design is hard.

N.2 Partially Non-Factorized Importance Sampling

Idea: Allow non-factorized grid optimization in two- or three-dimensional subspaces.

Motivation: Handle nastiest subspaces. Non-factorized approaches are impossible in higher than three dimensions (and probably only realistic in two dimensions), but there are cases that are best handled by including non-factorized optimization in two dimensions.

Implementation: The problem is that the present `vamp_sample_grid0` can't accomodate this, because other auxiliary information has to be collected, but a generalization is straightforward. Work has to start from an extended `divisions` module.

N.3 Correlated Importance Sampling (?)

Idea: Is it possible to include *some* correlations in a mainly factorized context?

Motivation: Would be nice ...

Implementation: First, I have to think about the maths ...

N.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region)

Idea: Solve `vegas`' nastiest problem by finding the direction(s) along which singularities are aligned.

Motivation: Automatically choose proper coordinate system in generator generators and separate wild and smooth directions.

Implementation: Diagonalize the covariance matrix $\mathrm{cov}(x_i x_j)$ to find better axes. Caveats:

- damp rotations (rotate only if eigenvalues are spread out sufficiently).
- be careful about blow up of the integration volume, which is $V' = V d^{d/2}$ in the worst case for hypercubes and can be even worse for stretched cubes. (An adaptive grid can help, since we will have more smooth directions!)

Maybe try non-linear transformations as well.

N.5 Automagic Multi Channel

Idea: Find and extract one singularity after the other.

Motivation: Obvious.

Implementation: Either use multiple of `vegas`' $p(x)$ for importance sampling. Or find hot region(s) and split the integration region (á la signal/background).

—O— Cross References

O.1 Identifiers

BUFFER_SIZE: 59b, 60a, 107b, 108a, 108b, 109, 265c
DEFAULT_BUFFER_SIZE: 252d, 261d, 261f, 274c, 275b
DEFAULT_SEED: 255a, 255c
EXC_DEFAULT: 246a, 246e
EXC_ERROR: 89b, 245c, 246a, 246c
EXC_FATAL: 50a, 50b, 51a, 90a, 96b, 245c, 246c
EXC_INFO: 95b, 168, 178a, 245c, 246c
EXC_NONE: 245b, 245c, 246c
EXC_WARN: 89b, 98a, 105b, 120, 123b, 134c, 136d, 137a, 168, 175d, 176a, 179b, 245c, 246c
K: 252a, 252b, 252a, 253c, 253d, 252a, 253e, 254a, 254d, 255d, 256a, 256b, 256c, 256d, 256e, 256f, 257a, 257c, 258a, 258c, 259c, 259e, 259g, 252a, 259h, 260a, 260b, 260d, 261d, 261f
L: 252a, 252b, 253d, 253e, 256b, 256c, 256d, 256e, 256f, 257a, 257c, 258c, 259h, 260a
LIPS3: 224b, 226b, 226f, 227a, 229b, 230a, 230c, 232c, 233b, 233c, 234a, 234b, 234c, 235a, 235b, 235c, 236b, 326g, 327a, 327b, 333d
LIPS3_m5i2a3: 226c, 226f, 227a, 227b, 228, 232c, 232d, 233b, 233c, 234a, 234b, 234c, 235a, 235b, 235c
LIPS3_momenta: 330e
LIPS3_momenta_massless: 331a
LIPS3_s2_t1_angles: 330c, 332a
LIPS3_s2_t1_angles_massless: 330d, 332b
LIPS3_unit: 330a, 331d, 332a
LIPS3_unit_massless: 330b, 331e, 332b
LIPS3_unit_to_s2_t1_angles: 331f, 331g, 332a
LIPS3_unit_to_s2_t1_angles_m0: 331f, 331g, 332b

M: 240b, 252c, 253d, 253e, 255d, 256f, 257a, 257g, 258c, 259h, 260a, 274e, 276e, 282e, 283a, 283c, 283d, 283e, 284a, 284b
MAX_SEED: 255b, 255c
MAX_UNIT: 267e, 268a, 312b, 312c
MIN_NUM_DIV: 46a
MIN_UNIT: 267e, 268a, 312b, 312c
NAME_LENGTH: 245b, 246a
NUM_DIV_DEFAULT: 77c, 78a, 78a
PI: 190b, 192, 193a, 193b, 223b, 223c, 224a, 225c, 226f, 227b, 228, 243b, 286a, 287c, 289b, 327a, 327b, 332e, 333c, 333d, 334, 336, 342b
PRIMES: 311b, 311c
QUAD_POWER: 92a, 92c
TAG_GRID: 176b, 176c, 177a, 177d
TAG_HISTORY: 176c, 177a, 177d
TAG_INTEGRAL: 176c, 177a, 177d
TAG_NEXT_FREE: 177d
TAG_STD_DEFS: 177d
TT: 255b, 255f
ULP: 259b, 259d, 259e, 259f, 259h, 260a
VAMP_MAX_WASTE: 173d, 175a, 175a
VAMP_ROOT: 166d, 167a, 167b, 167c, 168, 170a, 170e, 171a, 172a, 172b, 173a, 173b, 173d, 175c, 176a, 176b, 176c, 177e, 178a, 178c, 179b, 180d, 181a, 182d, 182e, 183a, 183b, 183f, 184a, 184b, 184c
abs_evec: 127a, 127b, 127c, 127f, 128c, 129a
accuracy: 93, 93, 93, 93, 93, 93, 93, 93, 95b, 102b, 119b, 139b, 139c, 140c, 168, 173d, 178a
adaptive_division: 57a, 57f, 365d, 365e, 366e
average: 107b, 109, 132c, 291b, 291c, 292a, 292d, 292e
avg_chi2: 93, 93, 93, 93, 93, 93, 93, 93, 93, 93, 94a, 95a, 102b, 105a, 106b, 107b, 109, 119b, 122b, 123e, 139b, 139c, 140c, 159b, 161, 164b, 168, 173d, 177e
_begin_f90: 357a, 357c, 358a, 358b, 358c, 360b, 360h, 368a
boost_many_momentum: 324b, 324c, 326b
boost_many_velocity: 324b, 324c, 325b, 326b
boost_momentum: 226f, 324b, 324c, 328c, 328d, 334
boost_one_momentum: 324b, 324c, 326a
boost_one_velocity: 324b, 324c, 325a, 325b
boost_velocity: 324b, 324c, 326a
buffer_end: 260c, 260e, 261d, 261f, 263g, 265c, 265d, 269d, 270b, 271b, 271d, 274a, 274d, 274e, 275a, 275b, 275c, 276b, 276c, 276e, 277a, 277b, 277c, 277d, 278a, 278b, 278c, 280h, 281b

calls: 83a, 83a, 83a, 83a, 83a, 24d, 83a, 83a, 83a, 83a, 76b, 83a, 83b, 88a, 97c, 99c, 105a, 105e, 106a, 106b, 107b, 109, 123e, 134a, 139b, 139c, 140c, 143b, 144b, 150, 151b, 156b, 158, 159b, 161, 162, 164b, 237, 240a, 240b, 241, 242
calls_per_cell: 76b, 83a, 83b, 87b, 88d, 96b, 97c, 97d, 143b, 144b, 150, 151b, 156b, 158, 162
cartesian_to_spherical: 338c, 339a
cartesian_to_spherical_2: 338c, 338d, 339a, 339b
cartesian_to_spherical_cos: 193a, 340d, 341b
cartesian_to_spherical_cos_2: 195b, 340d, 341a, 341b, 341c
cartesian_to_spherical_cos_j: 193b, 340d, 341c
cartesian_to_spherical_j: 338c, 339b
cell: 86a, 43b, 86a, 86a, 86b, 87a, 87c, 363c
check_inverses: 194c, 195a, 198c
check_inverses3: 194c, 195b, 198c
check_jacobians: 194c, 194d, 198c, 209c, 209d, 216e
check_kinematics: 232b, 232c, 237
cl: 131a, 131b, 131c, 131d
clear_exception: 24a, 24b, 24c, 24d, 102b, 119b, 212b, 213, 240a, 240b, 241, 242, 246d, 247a, 248, 360c, 360d, 360f
clear_integral_and_variance: 44c, 45c, 83a, 86b, 363e, 364a, 364f
cl_num: 131a, 131b, 131c, 131d
cl_pos: 131a, 131b, 131c, 131d
collect: 54b, 54c, 55c
constants: 190b, 220a, 243b, 286a, 288b, 324a, 329d, 333d, 334, 336
coordinates: 190b, 194b, 198c, 200b, 200c, 336
copy_array_pointer: 52b, 54a, 60d, 60e, 60f, 60g, 69, 96c, 158, 162, 163b, 306d, 306e
copy_division: 38a, 51a, 69, 69, 98b, 162, 361a, 361b, 361e, 362a
copy_history: 58b, 70b, 106b, 107b, 109, 164b, 367b, 367c, 367d
copy_integer_array2_pointer: 306d, 306e, 307c
copy_integer_array_pointer: 306d, 306e, 307a
copy_raw_state: 262c, 263f, 263g, 264a, 264b, 264c
copy_raw_state_to_state: 263f, 264b
copy_real_array2_pointer: 306d, 306e, 307d
copy_real_array_pointer: 306d, 306e, 307b
copy_state: 263f, 263g
copy_state_to_raw_state: 262b, 263f, 264c
cos_theta: 127d, 127e, 127f, 195b, 327a, 327b, 328c, 328d, 329b, 332d, 332e, 337b, 338d, 340a, 341a, 341b
create_array_pointer: 96c, 144b, 151b, 304b, 304c

create_division: 38a, 38b, 77c, 361a, 361b, 361c
create_empty_division: 38a, 39a, 98c, 146a, 361a, 361b, 361d
create_histogram: 212b, 213, 295b, 295c
create_histogram1: 295c, 295d, 295f
create_histogram2: 295c, 295d, 296a
create_integer_array2_pointer: 304b, 304c, 306b, 307c
create_integer_array_pointer: 304b, 304c, 305c, 307a
create_raw_state_from_raw_st: 261c, 261e, 261f, 262c
create_raw_state_from_seed: 261c, 261d, 262a
create_raw_state_from_state: 261c, 262b
create_real_array2_pointer: 304b, 304c, 306c, 307d
create_real_array_pointer: 304b, 304c, 306a, 307b
create_sample: 203, 205c, 217e
create_state_from_raw_state: 261c, 261f
create_state_from_seed: 261c, 261d
create_state_from_state: 261c, 261e
ctest: 132c
debug_division: 56a, 56b
decode_status: 349c, 349d, 349e, 352b
delete_division: 38a, 70a, 146a, 162, 163a, 361a, 361b, 362d
delete_histogram: 212b, 213, 295b, 295c
delete_histogram1: 295c, 295d, 297c
delete_histogram2: 295c, 295d, 298a
delete_sample: 203, 205b, 217f
delta: 47c, 47c, 47c, 48b, 48c, 114, 194d, 289b
descr_fmt: 61c, 62a, 62b, 143b, 144a, 144b, 147d, 148
destroy_raw_state: 262d, 262e, 263b
destroy_state: 262d, 262e, 263a
determinant: 113b, 115b, 316a, 316b, 321d
diag: 317b, 321b, 321c
diagonalize_real_symmetric: 317b, 127f, 128b, 128c, 129e, 140c, 317a, 317b, 321d
distribute: 15, 16, 54a, 54c, 55b, 102b
div_history: 58a, 58c, 59a, 59b, 68b, 68c, 68d, 70b, 105a, 107b, 109, 367d, 367e
division_efficiency: 60c, 60g
division_integral: 60c, 60e
division_t: 37b, 38b, 39a, 39b, 39c, 43b, 44b, 44d, 45a, 45b, 45c, 45e, 48e, 49b, 50a, 50b, 55d, 56b, 56c, 57b, 57c, 57d, 57e, 57f, 58c, 60d, 60e, 60f, 60g, 61c, 62b, 63b, 64a, 64b, 65b, 66a, 66b, 66d, 67a, 67b, 69, 70a, 76b, 96a, 98d, 361c, 361d, 361e, 362a, 362b, 362c, 362d, 363c, 363d, 364c,

364d, 364e, 364f, 365c, 365f, 366a, 366b, 366c, 366d, 366e, 367a, 367e
division_variance: 60c, 60f
division_x: 60c, 60d
domain: 77c, 77c, 23c, 24a, 24d, 77c, 77c, 77c, 77c, 77c, 116a, 166d, 172a, 185a, 185b, 186a, 186b, 187b, 187c, 188a, 188c, 189, 344e, 345b, 345c, 346a, 346d, 346e, 347a, 347c, 347d, 348a, 348c, 349a, 349b, 350a, 350b, 350c, 351b, 352c, 352f, 353a, 353b, 353c, 353d, 354b, 354c, 354d, 355a, 355b, 355c, 355d, 356
double_array2_fmt: 143b, 144a, 144b
double_array_fmt: 61c, 62a, 62b, 143b, 144a, 144b, 147d, 148
double_fmt: 61c, 62a, 62b, 143b, 144a, 144b, 147d, 148
dump_division: 56a, 56c, 213
dv2g: 76b, 83b, 83b, 89a, 97c, 143b, 144b, 150, 151b, 156b, 158, 162
dx: 37b, 38b, 43b, 44a, 48e, 52b, 54a, 57d, 61c, 62b, 64b, 65b, 66d, 67b, 69, 77c, 113b, 115b, 195a, 195b
_end_f90: 357a, 357c, 358b, 358c, 360a, 360g, 367f, 372
exception: 23c, 245b, 245b, 50a, 50b, 77c, 79d, 81, 82b, 85c, 92a, 93, 96a, 98d, 100b, 101c, 102b, 116a, 117b, 117d, 118b, 119b, 133d, 135, 137c, 138a, 139b, 139c, 140c, 166d, 167b, 167c, 168, 172a, 172b, 173a, 173d, 180d, 181a, 181b, 181c, 212b, 213, 237, 245b, 246c, 246e, 247a, 247b, 360e, 360f
exceptions: 245a, 23b, 245a, 37a, 75, 165c, 194b, 200b, 209b, 237, 245a
f: 22, 44d, 59b, 87d, 87d, 88a, 88b, 88c, 124b, 133d, 134a, 134b, 134c, 190b, 191a, 191b, 191c, 194a, 196b, 203, 205a, 208b, 210b, 212b, 213, 287a, 287b, 287c, 364c
f0: 203, 204a, 205a
f2: 88b, 88c
factorize: 103b, 310d, 311b
fill_histogram: 212b, 213, 295b, 295c
fill_histogram1: 295c, 295d, 296b
fill_histogram2s: 295c, 295d, 297a
fill_histogram2v: 295c, 295d, 297a, 297b
find_free_unit: 63b, 64a, 66a, 66b, 147b, 147c, 149a, 149b, 153a, 153b, 155a, 155b, 267e, 268b, 268c, 268d, 268e, 269a, 294a, 298b, 301, 312a, 312c
f_max: 76b, 84a, 88a, 88b, 97c, 99c, 105a, 106b, 107b, 109, 123e, 134a, 134c, 136a, 136d, 137a, 84a, 143b, 144b, 150, 151b, 156b, 158, 159b, 161, 162, 164b
f_min: 76b, 84a, 88a, 97c, 99c, 105a, 106b, 123e, 84a, 143b, 144b, 150, 151b, 156b, 158, 159b, 161, 162, 164b
f_norm: 203, 204a, 204b

fork_division: 49c, 50a, 50a, 97d
func: 14, 15, 16, 17, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 22, 85c, 22, 22, 22, 22, 22, 87d, 93, 102b, 112a, 112b, 114, 119b, 120, 124b, 133d, 135, 137c, 138a, 139b, 139c, 140c, 168, 173d, 175d, 179b, 180d, 181a, 181b, 181c
g: 14, 208a, 15, 16, 17, 208a, 29, 30, 208a, 77c, 79b, 79d, 80b, 81, 82b, 83a, 83b, 84a, 84c, 84d, 84e, 84f, 85a, 85c, 86a, 86b, 87a, 87b, 87c, 87d, 88a, 88b, 88c, 88d, 89a, 89b, 90c, 91, 92a, 92b, 93, 94a, 96a, 96b, 96c, 97b, 97c, 97d, 208a, 98b, 98c, 98d, 99a, 99b, 99c, 100a, 100b, 101c, 102b, 105b, 106b, 106c, 116a, 116b, 117b, 117d, 118b, 208a, 208a, 208a, 119b, 120, 121b, 122b, 123a, 123b, 123e, 124b, 133d, 134a, 134c, 208a, 208a, 135, 136a, 136b, 136c, 136d, 137a, 208a, 208a, 208a, 208a, 208a, 208a, 137c, 138a, 139b, 139c, 140c, 143b, 144b, 146a, 146b, 147a, 147b, 147c, 147d, 148, 149a, 149b, 150, 151b, 153a, 153b, 153c, 154b, 155a, 155b, 156b, 157, 158, 163a, 164a, 166d, 167b, 167c, 168, 170a, 172a, 172b, 173a, 173b, 173c, 173d, 175b, 175c, 175d, 176a, 176b, 176c, 177a, 179b, 180d, 181a, 181b, 181c, 182d, 182e, 183a, 183b, 183f, 184a, 184b, 184c, 185a, 185b, 186a, 186b, 187b, 187c, 188a, 188c, 189, 203, 204a, 208a, 208b, 209d, 234c, 235a, 235b, 235c, 287b, 287c, 289c, 317b, 318, 319a, 368d, 368e, 368f, 369a, 369e, 370a
g0: 171b, 172a, 172b, 173a, 173b, 173c, 173d, 175b, 175c, 175d, 176a, 176b, 176c, 177a, 179b, 181a, 181c, 183f, 184a, 184b, 184c, 203, 207a, 208a
g1: 233a, 235b, 236b
g12: 233a, 234c, 237
g2: 233a, 235c, 236b
g21: 233a, 235a, 237
gamma: 203, 205a, 205b, 205c, 206, 207a, 207c, 208a, 217e, 218b, 286b, 287c, 289b, 324a, 325a, 333c, 336, 342b
gap: 131b, 131c, 131d
gather_exceptions: 103a, 119b, 246d, 247b, 247b, 248
gauss_multiplication: 289a, 289b, 289c
gcd: 53, 310d, 310f, 311a, 358f, 359a, 359b, 359d
generate: 253a, 253a, 253a, 253a, 253b, 253a, 258b, 253a, 253a, 274d,

253a, 253a, 276b, 276d
grid: 23c, 24a, 24b, 24c, 77c, 196b, 210b, 240a, 240b
handle_exception: 24a, 24b, 24c, 24d, 120, 212b, 213, 240a, 240b, 241, 242, 246b, 246c
histogram: 212b, 213, 294b, 295f, 296b, 297c, 298b, 299b, 300d
histogram2: 295a, 295a, 296a, 297a, 297b, 298a, 300e, 301
histograms: 194b, 200b, 209b, 294a
i: 15, 16, 17, 127a, 127a, 127a, 43b, 44a, 44b, 44d, 45a, 45b, 47c, 48c, 50a, 50b, 52b, 52c, 54a, 54b, 55a, 55b, 55c, 55d, 56b, 56c, 59b, 61c, 62b, 64b, 65b, 72e, 73c, 73f, 74b, 74d, 91, 96a, 96c, 97c, 97d, 127a, 98b, 98c, 98d, 99a, 99b, 99c, 100b, 101b, 101c, 102b, 103b, 104b, 107b, 108b, 109, 112a, 112b, 114, 127a, 127b, 127c, 127d, 127e, 127f, 128c, 129a, 129e, 131a, 131d, 132b, 132c, 143b, 144b, 147d, 148, 150, 151b, 153c, 154b, 156b, 157, 158, 160, 168, 187c, 191c, 195a, 195b, 204a, 205a, 212b, 213, 217d, 217e, 237, 241, 247b, 266c, 266e, 267a, 267c, 267e, 282d, 283a, 283c, 283d, 283e, 284a, 284b, 284c, 287a, 287b, 287c, 289c, 296b, 297b, 298b, 299b, 308d, 309a, 309b, 309c, 127a, 311b, 312c, 316b, 321a, 321b, 321d, 325b, 333d, 334, 337b, 338d, 340a, 341a, 359b, 359c, 359d, 359e, 360e, 360f, 364c, 364d, 364e, 368d, 368e, 368f, 369a, 369d, 369e, 369h, 370a, 370d, 370e, 371a, 371b, 371c, 371d, 371e
ia: 87c, 88b, 88c, 88d, 133d, 134a
ihp: 31b, 31b, 112a, 190b, 193a, 194a, 195a
inject_division: 43a, 43b, 87c, 363a, 363b, 363c
inject_division_short: 43a, 44b, 134a, 363a, 363b, 363d
inside_division: 57a, 57b, 87d, 365d, 365e, 366a
integer_array_fmt: 143b, 144a, 144b, 147d, 148
integer_array_state: 278a, 280a
integer_array_stateless: 275c, 278a, 279c, 280b
integer_array_static: 279c, 280a
integer_fmt: 61c, 62a, 62b, 143b, 144a, 144b, 147d, 148
integer_state: 277b, 280a
integer_stateless: 274a, 277b, 278e, 280b
integer_static: 278e, 280a
integral: 93, 93, 93, 93, 23c, 24c, 24d, 93, 93, 93, 93, 93, 93, 93, 37b, 38b, 39a, 40b, 44d, 45c, 52b, 93, 52c, 54a, 54b, 55d, 56b, 56c, 58c, 60e, 93, 61c, 62b, 63a, 64b, 65b, 66d, 67b, 69, 70a, 89b, 93, 94a, 95a, 102b, 105a, 106b, 107b, 109, 119b, 122b, 123e, 139b, 139c, 140c, 159b, 161, 164b, 168, 173d, 177e, 196b, 197a, 197b, 198b, 210b, 211b, 212b, 213, 237, 240a, 240b, 241, 242
_interface_sv: 357a, 357c, 360d, 361b, 363b, 364a, 364b, 365b, 365e, 367c, 368c, 369c, 369g, 370c

_interface_sva: 357a, 357c, 359a, 361b, 370c
invariants_from_p: 226e, 226f, 232c, 233b, 233c, 234c, 235a
invariants_from_x: 226e, 227b, 232c, 233b, 233c, 234a, 234b, 234c, 235a, 235b, 235c
invariants_to_p: 226e, 227a, 232c, 233b, 233c, 234a, 234b, 234c, 235a, 235b, 235c
invariants_to_x: 226e, 228, 232c, 233b, 233c, 234c, 235a
iteration: 14, 15, 17, 93, 93, 93, 94a, 102b, 105b, 119b, 120, 122b, 123b, 168, 173d, 175d, 176a, 176c, 177a, 179b
iterations: 14, 15, 17, 93, 93, 93, 93, 93, 93, 93, 93, 93, 59b, 93, 102b, 107b, 109, 119b, 137c, 138a, 168, 173d, 181b, 181c, 196b, 197a, 197b, 198c, 200c, 210b, 211a, 211b, 212b, 213, 216a, 216b, 216c, 216d, 217d, 217e, 237, 240a, 240b, 241, 242
iv: 125b, 127a, 127b, 127c, 127d, 127f, 128c, 129a
j: 31c, 50a, 50b, 52a, 53, 79a, 86a, 87a, 96a, 97d, 87a, 87a, 98b, 98d, 99a, 99b, 103b, 104a, 104b, 107b, 109, 113b, 115b, 129e, 143b, 144b, 150, 151b, 159b, 161, 190b, 193b, 194a, 194d, 195b, 204a, 205a, 207b, 207c, 208a, 213, 217d, 217e, 253a, 253d, 253e, 254d, 255d, 256c, 256e, 256f, 258b, 258c, 259c, 259e, 259h, 308d, 309a, 309b, 309c, 314, 315d, 317b, 361c, 361d, 361e, 362a, 362b, 362c, 362d, 363c, 363d, 364c, 364d, 364e, 364f, 365c, 365f, 366a, 366b, 366c, 366d, 366e, 367a, 367d, 367e
jacobi: 76b, 83b, 83b, 87c, 97c, 99c, 134a, 143b, 144b, 150, 151b, 156b, 158, 162
jacobian: 31c, 31c, 31c, 112a, 112b, 113b, 115b, 224a, 225b, 225c, 226c, 226d, 226f, 227a, 227b, 228, 229b, 230a, 230c, 232c, 232d, 234c, 235a, 235b, 235c, 326g, 327a, 327b, 330a, 330b, 330c, 330d, 330e, 331a, 331d, 331e, 333d, 337b, 338b, 338d, 339b, 340a, 340c, 341a, 341c
jacobi_rotation: 320a, 320b, 320c, 320d
join_division: 49c, 50b, 99a
k: 47c, 48b, 48c, 87a, 87b, 229b, 230a, 230c, 231, 236b, 289b, 332d, 47c, 332e, 333a
kinematics: 220a, 237, 324a, 329d, 333d, 334
lambda: 223b, 225c, 226f, 227b, 228, 321d, 326c, 326d, 327a, 328c, 333d
last: 254c, 260c, 260e, 263g, 264d, 265c, 265d, 269d, 270b, 271b, 271d, 274a, 274b, 275b, 275b, 274d, 274e, 275a, 275b, 275c, 275d, 275b, 276b, 276c, 276d, 276e, 277a, 277b, 277c, 277d, 278a, 278b, 278c, 280h, 281b
lcm: 53, 310d, 311a, 358f, 359a, 359c, 359e
linalg: 75, 237, 313a, 317b, 321d
local_avg_chi2: 93, 95a, 102b, 105b, 119b, 120, 123b, 168, 173d, 175d, 176a, 177e, 179b
local_integral: 93, 95a, 95b, 102b, 105b, 119b, 123b, 168, 173d, 176a,

177e, 178a, 179b
local_std_dev: 93, 95a, 95b, 102b, 105b, 119b, 123b, 168, 173d, 176a, 177e, 178a, 179b
logical_fmt: 61c, 62a, 62b, 143b, 144a, 144b
lorentzian: 190b, 191b, 191c
lorentzian_normalized: 190b, 191a, 191b
lu_decompose: 313b, 314, 316b, 321d
luxury_state: 281a, 282c
luxury_state_integer: 281a, 281b, 281c, 282c
luxury_stateless: 280h, 281b, 281e, 282a
luxury_state_real: 281c, 282c
luxury_static: 281d, 282c
luxury_static_integer: 281d, 281e, 281f, 282c
luxury_static_real: 281f, 282c
m: 39c, 40a, 46b, 47b, 40a, 47c, 48b, 48c, 58c, 59b, 310e, 310f, 40a, 311a, 329c, 334, 359b, 359c, 359d, 359e
map_domain: 77c, 78b, 79a
marshal_div_history: 68a, 68b, 159b
marshal_div_history_size: 68a, 68c, 159b, 160
marshal_division: 66c, 66d, 156b
marshal_division_size: 66c, 67a, 156b, 157
marshal_raw_state: 269b, 269c, 269d, 270c, 271a, 271b, 272a
marshal_raw_state_size: 269b, 269c, 270a, 270d, 271c, 272b
marshal_state: 269b, 269c, 269d, 270b, 271b
marshal_state_size: 269b, 269c, 270a, 271c
massless_isotropic_decay: 231, 332c, 332d
midpoint: 298b, 299b, 300a, 300b, 301
midpoint1: 300b, 300c, 300d
midpoint2: 300b, 300c, 300e
more_pancake_than_cigar: 125b, 126a, 126b
mpi90: 165c, 200c, 218a, 218b, 237, 343a, 345a
mpi90_abort: 343b, 344c, 344e, 345a
mpi90_broadcast: 17, 168, 173d, 177e, 178a, 187b, 188a, 200c, 218b, 237, 241, 352d, 352e
mpi90_broadcast_double: 352e, 353b
mpi90_broadcast_double_array: 352e, 353b, 354b, 355a, 355d
mpi90_broadcast_double_array2: 352e, 355a
mpi90_broadcast_double_array3: 352e, 355d
mpi90_broadcast_integer: 352e, 353a
mpi90_broadcast_integer_array: 352e, 353a, 353d, 354d, 355c
mpi90_broadcast_integer_array2: 352e, 354d

mpi90_broadcast_integer_array3: 352e, 355c
mpi90_broadcast_logical: 352e, 353c
mpi90_broadcast_logical_array: 352e, 353c, 354c, 355b, 356
mpi90_broadcast_logical_array2: 352e, 355b
mpi90_broadcast_logical_array3: 352e, 356
mpi90_finalize: 200c, 218b, 237, 343b, 344d
mpi90_init: 200c, 218b, 237, 343b, 344a
mpi90_print_error: 343b, 344b, 344c, 345a
mpi90_rank: 17, 166d, 167b, 167c, 168, 170a, 170e, 171a, 172a, 172b, 173a, 173b, 173d, 180d, 181a, 182d, 182e, 183a, 183b, 183f, 184a, 184b, 184c, 187b, 188a, 200c, 218b, 237, 343b, 346a
mpi90_receive: 177a, 185b, 189, 346b, 348d
mpi90_receive_double: 348d, 349a
mpi90_receive_double_array: 348d, 349a, 350a, 350c
mpi90_receive_double_array2: 348d, 350c
mpi90_receive_double_pointer: 351a, 352c
mpi90_receive_integer: 348c, 348d
mpi90_receive_integer_array: 348c, 348d, 349b, 350b
mpi90_receive_integer_array2: 348d, 350b
mpi90_receive_integer_pointer: 351a, 351b
mpi90_receive_pointer: 351a, 351a, 351a, 186b, 346b, 351a
mpi90_send: 176c, 185a, 186a, 188c, 346b, 346c
mpi90_send_double: 346c, 346e
mpi90_send_double_array: 346c, 346e, 347c, 348a
mpi90_send_double_array2: 346c, 348a
mpi90_send_integer: 346c, 346d
mpi90_send_integer_array: 346c, 346d, 347a, 347d
mpi90_send_integer_array2: 346c, 347d
mpi90_size: 17, 168, 173d, 200c, 218b, 237, 343b, 345c
mpi90_status: 185b, 186b, 189, 348b, 348c, 349a, 349b, 349e, 350a, 350b, 350c, 351b, 352c
multi_channel: 196a, 197a, 198c, 210a, 211a, 216c
multi_channel_generator: 212a, 213, 216d
ndim: 77c, 79a, 81, 83a, 85c, 86a, 92a, 93, 96a, 96c, 105e, 128c, 129a, 144b, 146a, 151b, 156b, 157, 158, 159b, 160, 161, 162, 317b, 77c, 77c, 320a, 370d, 370e
ng: 37b, 38b, 39b, 39c, 42, 50a, 50b, 42, 51a, 42, 52b, 53, 54a, 57e, 58a, 58c, 59b, 61c, 62b, 64b, 65b, 66d, 67b, 68b, 68d, 69, 70b, 81, 42, 83a, 84c, 103b, 104b, 362b, 362c
norm: 127d, 127f, 204a, 204b
num_calls: 80b, 80b, 80b, 80b, 80b, 80b, 24a, 24c, 80b, 80b, 80b, 80b,

80b, 80b, 80b, 80b, 80b, 80b, 80b, 80b, 50a, 51a, 52b, 54a, 76b, 77c, 79d, 80b, 81, 82b, 83a, 97c, 111a, 116a, 116b, 117b, 117d, 118b, 80b, 80b, 119b, 121b, 138a, 143b, 144b, 147d, 148, 150, 151b, 153c, 154b, 156b, 158, 162, 163b, 164a, 166d, 167b, 167c, 172a, 172b, 173a, 173d, 181c, 188a
num_cells: 81, 83a, 83b, 96a, 97c
num_div: 42, 42, 42, 39c, 40b, 42, 42, 42, 42, 47c, 42, 50a, 50b, 52a, 52b, 53, 58a, 58c, 58e, 59b, 62b, 63a, 65b, 66d, 67b, 68b, 68d, 70b, 76b, 77c, 79b, 79d, 80b, 81, 82b, 83a, 92a, 42, 96a, 96c, 98c, 116a, 117b, 117d, 118b, 139b, 139c, 140c, 143b, 144b, 150, 151b, 156b, 158, 162, 163a, 166d, 167b, 167c, 172a, 172b, 173a
numeric_jacobian: 115a, 115b
object: 176b, 176c, 177a, 177b, 177c
one_to_two_massive: 328a, 328b, 328c
one_to_two_massless: 328a, 328b, 328d
on_shell: 327a, 327b, 328c, 329a, 329c
outer_product: 84d, 88b, 88d, 310b, 310c, 314
phase_space: 224b, 226a, 229b, 230c, 232c, 329d
phase_space_volume: 222b, 231, 237, 333b, 333c
phi: 31a, 31a, 31a, 112a, 112b, 113b, 114, 115b, 135, 181a, 190b, 192, 193a, 194a, 194d, 195a, 195b, 203, 207c, 208b, 209d, 213, 223b, 223c, 224b, 226b, 226c, 226f, 227a, 227b, 228, 232d, 327a, 327b, 328c, 328d, 329b, 330c, 330d, 332d, 332e, 333d, 337b, 338a, 338b, 338d, 339a, 340a, 340b, 340c, 341a, 341b
phi1: 233a, 234a, 236b
phi12: 233a, 233b, 236b, 237
phi2: 232d, 233a, 234b, 236b
phi21: 233a, 233c, 236b, 237
print_LIPS3_m5i2a3: 232b, 232d
print_history: 59a, 59b, 60b, 107b
print_history,: 60b
print_results: 198a, 198b, 198c
probabilities: 58c, 58d, 58e
probability: 48d, 48e, 90c, 365d, 365e, 365f
psi: 203, 206, 207c
quadrupole: 80b, 80b, 80b, 80b, 80b, 76b, 77c, 79d, 80b, 81, 82b, 92a, 97b, 116a, 117b, 117d, 118b, 139b, 139c, 140c, 143b, 144b, 150, 151b, 156b, 158, 162, 166d, 167b, 167c, 172a, 172b, 173a
quadrupole_division: 49a, 49b, 92a, 365d, 365e, 367a
r: 43b, 44b, 87c, 88c, 114, 127e, 127f, 128b, 128c, 133d, 134a, 135, 136b, 136d, 137a, 191b, 192, 193a, 195b, 249, 251f, 274a, 274b, 274e, 275a, 277b, 277c, 277d, 278e, 279a, 279b, 332d, 333a, 333d, 337b, 338a, 338b, 338d,

339a, 340a, 340b, 340c, 341a, 341b, 363c, 363d
raise_exception: 50a, 50b, 51a, 89b, 90a, 95b, 96b, 105b, 120, 123b, 134c, 136d, 137a, 168, 175d, 176a, 178a, 179b, 246d, 246e, 247b, 360c, 360d, 360e
random_LIPS3: 331b, 331c
random_LIPS3_unit: 331b, 331c, 331d
random_LIPS3_unit_massless: 331b, 331c, 331e
read_division: 61a, 61b, 144b
read_division_name: 61a, 61b, 64a
read_division_raw: 61a, 61b, 151b
read_division_raw_name: 61a, 61b, 66b
read_division_raw_unit: 61a, 61b, 65b
read_division_unit: 61a, 61b, 62b, 64a, 66b
read_grid_name: 142a, 142c, 147c, 182a, 182c, 183b
read_grid_raw_name: 142b, 143a, 153b
read_grid_raw_unit: 142b, 143a, 151b, 153b, 154b
read_grids_name: 142a, 142c, 149b, 183c, 183e, 184c
read_grids_raw_name: 142b, 143a, 155b
read_grids_raw_unit: 142b, 143a, 154b, 155b
read_grids_unit: 142a, 142c, 148, 149b, 183c, 183e, 184a
read_grid_unit: 142a, 142c, 144b, 147c, 148, 182a, 182c, 182e
read_raw_state_name: 265a, 265b, 269a
read_raw_state_unit: 265a, 265b, 265d, 266b, 269a
read_state_array: 265d, 266b, 266e, 266f, 267c, 267d
read_state_name: 265a, 265b, 268e
read_state_unit: 265a, 265b, 265d, 268e
real_array_state: 278b, 278c, 280a, 280e
real_array_stateless: 276e, 277a, 278b, 278c, 279d, 279e, 280b, 280f
real_array_static: 279d, 279e, 280a, 280e
real_state: 277c, 277d, 280a, 280e
real_stateless: 274e, 275a, 277c, 277d, 279a, 279b, 280b, 280f
real_static: 279a, 279b, 280a, 280e
rebin: 39c, 45e, 47c, 48a
rebinning_weights: 40a, 45e, 46b, 47a, 49b, 58c
record_efficiency: 44c, 45b, 88b, 134a, 363f, 364b, 364e
record_integral: 44c, 44d, 88b, 363e, 364a, 364c
record_variance: 44c, 45a, 88d, 363e, 364a, 364d
refine_division: 45d, 45e, 92a, 92b, 365a, 365b, 365c
reshape_division: 38a, 39c, 83a, 361a, 361b, 362c
rigid_division: 57a, 57e, 83a, 84c, 86a, 97c, 365d, 365e, 366d
s_buffer: 253f, 274c, 275b, 278e, 279a, 279b, 279c, 279d, 279e, 281d,

281e, 281f
s_buffer_end: 274c, 275b, 278e, 279a, 279b, 279c, 279d, 279e, 281e
schedule: 173d, 178b, 178c
seed_raw_state: 254b, 254c, 257f, 262a
seed_state: 254c, 257f
seed_stateless: 253f, 254b, 254d, 258d, 259a
seed_static: 253f, 257f
seed_value: 254d, 255c, 255d, 255f, 259c, 259e
select_rotation_axis: 125a, 127f, 140c
select_rotation_subspace: 125a, 129b
select_subspace_explicit: 128b, 128c, 129b, 129c
select_subspace_guess: 128c, 129b, 129c
set_grid_options: 79d, 80a, 80b, 81
set_rigid_division: 38a, 39b, 361a, 361b, 362b
sigma_raw: 229a, 229c, 230c, 236b
single_channel: 196a, 196b, 198c, 210a, 210b, 216a
single_channel_generator: 212a, 212b, 216b
sin_theta: 127d, 127e, 127f, 329b, 332d, 332e
s_last: 253f, 274c, 275b, 278e, 279a, 279b, 279c, 279d, 279e, 281e
sort: 126a, 129e, 132c, 140c, 178c, 309d, 310a, 321d
sort_real: 308d, 309d, 310a
sort_real_and_integer: 309c, 309d, 310a
sort_real_and_real_array: 309b, 309d, 310a
specfun: 286a, 288b, 289c, 324a, 336
_specific_sv: 357a, 357c, 360c, 361a, 363a, 363e, 363f, 365a, 365d, 367b, 368b, 369b, 369f, 370b
_specific_sva: 357a, 357c, 358f, 361a, 370b
spherical_cos_to_cartesian: 192, 339c, 340b
spherical_cos_to_cartesian_2: 195b, 339c, 340a, 340b, 340c
spherical_cos_to_cartesian_j: 339c, 340c
spherical_to_cartesian: 337a, 338a
spherical_to_cartesian_2: 337a, 337b, 338a, 338b
spherical_to_cartesian_j: 337a, 338b
s_state: 253f, 254a, 258a, 278e, 279a, 279b, 279c, 279d, 279e
standard_deviation: 132b, 132c, 291b, 292a, 292d
standard_deviation_percent: 49b, 58c, 292c, 292d
std_dev: 93, 93, 93, 93, 93, 93, 93, 93, 93, 93, 93, 93, 94a, 95a, 102b, 105a, 106b, 107b, 109, 119b, 122b, 123e, 139b, 139c, 140c, 159b, 161, 164b, 168, 173d, 177e, 198b
stest: 288b, 289c
stest_functions: 288b, 289c

stratified: 80b, 80b, 80b, 80b, 80b, 80b, 80b, 80b, 80b, 37b, 38b, 39b, 39c, 80b, 42, 44d, 45a, 51a, 80b, 52b, 54a, 57c, 58a, 58c, 59b, 61c, 62b, 64b, 65b, 66d, 67b, 68b, 68d, 69, 70b, 76b, 77c, 79d, 80b, 81, 82b, 80b, 83a, 97b, 105a, 106b, 107b, 109, 116a, 117b, 117d, 118b, 123e, 139b, 139c, 140c, 143b, 144b, 150, 151b, 156b, 158, 159b, 161, 162, 164b, 166d, 167b, 167c, 172a, 172b, 173a
stratified_division: 57a, 57c, 81, 96b, 365d, 365e, 366b
subdivide: 54a, 54c, 55a
subroutine: 14, 15, 17, 331d, 38b, 39a, 39b, 39c, 43b, 44b, 44d, 45a, 45b, 45c, 45e, 50a, 50b, 55a, 55b, 55c, 55d, 56b, 56c, 59a, 59b, 60d, 60e, 60f, 60g, 61c, 62b, 63b, 64a, 64b, 65b, 66a, 66b, 66d, 67a, 67b, 68b, 68c, 68d, 69, 70a, 70b, 72c, 72e, 73a, 73c, 73d, 73f, 74b, 74d, 77c, 79a, 79b, 79d, 80b, 81, 82b, 84e, 85a, 85c, 91, 92a, 92b, 93, 94a, 96a, 98d, 100b, 101c, 102b, 103b, 105e, 106a, 106b, 107b, 108b, 109, 113b, 114, 115b, 116a, 116b, 117b, 117d, 118b, 119b, 121b, 122b, 123a, 123e, 126a, 127f, 128b, 128c, 129e, 131d, 133d, 135, 137c, 138a, 139b, 139c, 140c, 143b, 144b, 147b, 147c, 147d, 148, 149a, 149b, 150, 151b, 153a, 153b, 153c, 154b, 155a, 155b, 156b, 157, 158, 159b, 160, 161, 162, 163a, 163b, 164a, 164b, 165a, 166d, 167b, 167c, 168, 170a, 170e, 171a, 172a, 172b, 173a, 173b, 173c, 173d, 178c, 180d, 181a, 181b, 181c, 182d, 182e, 183a, 183b, 183f, 184a, 184b, 184c, 185a, 185b, 186a, 186b, 187b, 187c, 188a, 188c, 189, 194d, 195a, 195b, 196b, 197a, 198b, 205b, 205c, 209d, 210b, 211a, 212b, 213, 232c, 232d, 246c, 246e, 247a, 247b, 251e, 253a, 253f, 254b, 254c, 254d, 258b, 258d, 261d, 261e, 261f, 262a, 262b, 262c, 263a, 263b, 263g, 264a, 264b, 264c, 264d, 265c, 265d, 266a, 266b, 266c, 266e, 267a, 267c, 267e, 268c, 268d, 268e, 269a, 269d, 270a, 270b, 270c, 270d, 271a, 271b, 271c, 271d, 272a, 272b, 272c, 274a, 274e, 275a, 275c, 276e, 277a, 277b, 277c, 277d, 278a, 278b, 278c, 278e, 279a, 279b, 279c, 279d, 279e, 280h, 281a, 281b, 281c, 281d, 281e, 281f, 282d, 284c, 295f, 296a, 296b, 297a, 297b, 297c, 298a, 298b, 299b, 301, 305c, 306a, 306b, 306c, 307a, 307b, 307c, 307d, 308b, 308c, 308d, 309b, 309c, 311b, 312c, 314, 316b, 317b, 320b, 321a, 331d, 331e, 332a, 332b, 337b, 338d, 339a, 340a, 341a, 341b, 344a, 344d, 344e, 345a, 345c, 346a, 346d, 346e, 347a, 347c, 347d, 348a, 348c, 349a, 349b, 349e, 350a, 350b, 350c, 351b, 352c, 353a, 353b, 353c, 353d, 354b, 354c, 354d, 355a, 355b, 355c, 355d, 356, 358d, 358e, 360e, 360f, 361c, 361d, 361e, 362a, 362b, 362c, 362d, 363c, 363d, 364c, 364d, 364e, 364f,

365c, 367d, 368d, 368e, 369a, 369d, 369e, 369h, 370a, 370d, 370e, 371a, 371b, 371c, 371d, 371e
sum_chi2: 76b, 79d, 89b, 94a, 97a, 99c, 111a, 116a, 117b, 121b, 122b, 143b, 144b, 147d, 148, 150, 151b, 153c, 154b, 156b, 158, 162, 163b, 188a
sum_division: 49c, 51b, 55d, 99b
sum_f: 87b, 88b, 88c, 88d
sum_f2: 87b, 88b, 88c, 88d
sum_integral: 76b, 79d, 89b, 94a, 97a, 99c, 111a, 116a, 117b, 121b, 122b, 143b, 144b, 147d, 148, 150, 151b, 153c, 154b, 156b, 158, 162, 163b, 188a
summarize_division: 58b, 58c, 106b, 367b, 367c, 367e
sum_weights: 76b, 79d, 84d, 84f, 89b, 94a, 97a, 99c, 111a, 116a, 117b, 121b, 122b, 143b, 144b, 147d, 148, 150, 151b, 153c, 154b, 156b, 158, 162, 163b, 188a
sum_x: 88d
sum_xx: 88d
surface: 191b, 342a, 342b
s_virginal: 253f, 254a, 258a, 278d
swap: 225a, 307e, 308a, 308d, 309b, 309c, 314, 315d, 358c
swap_integer: 307e, 308a, 308b
swap_integer_array: 358b, 358c, 358d
swap_real: 307e, 308a, 308c
swap_real_array: 358b, 358c, 358e
tao_random_copy: 251a, 261e, 263c, 273b
tao_random_create: 16, 24a, 198c, 200c, 215, 218b, 237, 261a, 250g, 250h, 251e, 251f, 261a, 273b, 283d
tao_random_destroy: 250i, 262d, 273b
tao_random_flush: 251b, 261d, 261f, 264b, 264d, 273b
tao_random_luxury: 250d, 250e, 250f, 281g, 273b, 280h, 281g, 283a
tao_random_marshal: 269b, 269c, 284b
tao_random_marshal_size: 269b, 269c, 284b
tao_random_number: 279f, 87c, 114, 132c, 134a, 134c, 136b, 136d, 137a, 195a, 195b, 217e, 232c, 237, 249, 250b, 251e, 251f, 273b, 279f, 280d, 283a, 283c, 283d, 283e, 284a, 284b, 321d, 331d, 331e, 333d, 334
tao52_random_numbers: 273a, 285
tao_random_numbers: 272d, 23b, 75, 272d, 272d, 132c, 165c, 194b, 198c, 200b, 200c, 209b, 217c, 220a, 237, 272d, 273a, 282d, 284c, 285, 321d, 329d, 333d, 334
tao_random_raw_state: 250a, 260b, 260b, 260b, 251e, 251f, 260b, 254b, 260b, 260c, 260d, 260e, 261f, 262a, 262b, 262c, 263b, 264a, 264b, 264c, 266a, 266b, 268d, 269a, 270c, 270d, 271a, 272a, 272b, 272c
tao_random_read: 251c, 265a, 273b, 284a

tao_random_seed: 198c, 200c, 215, 218b, 237, 257d, 250c, 255c, 257d, 273b, 257d, 278d, 283a, 283c, 284a, 284b, 321d
tao_random_state: 14, 15, 16, 17, 260c, 23c, 260c, 260c, 85c, 260c, 93, 102b, 114, 119b, 133d, 135, 137c, 138a, 139b, 139c, 140c, 168, 173d, 180d, 181a, 181b, 181c, 194d, 195a, 195b, 196b, 197a, 198c, 200c, 209d, 210b, 211a, 212b, 213, 217d, 232c, 237, 260c, 260c, 250a, 260c, 260c, 260c, 251e, 251f, 254c, 260c, 260e, 260c, 261d, 261e, 261f, 262b, 263a, 263g, 264b, 264c, 264d, 265c, 265d, 268c, 268e, 269d, 270a, 270b, 271b, 271c, 271d, 277b, 277c, 277d, 278a, 278b, 278c, 281a, 281b, 281c, 282d, 284c, 331d, 331e
tao_random_test: 251d, 273b, 282d, 284c, 285
tao_random_unmarshal: 269b, 269c, 284b
tao_random_write: 251c, 264e, 273b, 284a
tao_test: 285
two_to_three_massless: 326e, 326f, 327b
unit: 61c, 62b, 63b, 64a, 64b, 65b, 66a, 66b, 73d, 73f, 107b, 108b, 109, 127e, 128b, 143b, 144b, 147b, 147c, 147d, 148, 149a, 149b, 150, 151b, 153a, 153b, 153c, 154b, 155a, 155b, 182d, 182e, 183f, 184a, 251c, 265c, 265d, 266a, 266b, 266c, 266e, 267a, 267c, 267e, 268c, 268d, 268e, 269a, 298b, 299b, 301, 312c, 317b, 321a, 321c, 321d, 332a, 332b
unmarshal_div_history: 68a, 68d, 161
unmarshal_division: 66c, 67b, 158
unmarshal_raw_state: 269b, 269c, 270b, 271a, 271d, 272c
unmarshal_state: 269b, 269c, 270b, 271d
utils: 37a, 75, 132c, 165c, 220a, 237, 294a, 304a, 313a, 321d
value_spread: 291b, 292b, 292e
value_spread_percent: 49b, 58c, 292c, 292e
vamp: 2, 76a, 76a, 76a, 23b, 76a, 59b, 70c, 71b, 75, 76a, 89b, 107b, 109, 132c, 76a, 76a, 165b, 76a, 76a, 76a, 190b, 194b, 198c, 200c, 203, 209a, 217c, 220a, 246e
vamp_apply_equivalences: 91, 91, 119b
vamp_average_iterations: 94b, 93, 94b, 94c, 102b, 119b, 120, 122d, 168, 175d, 176a, 179b
vamp_average_iterations_grid: 94a, 94b, 94c
vamp_average_iterations_grids: 122b, 122c, 122d
vamp_broadcast_grids: 184d, 188a
vamp_broadcast_many_grids: 187a, 187c
vamp_broadcast_one_grid: 187a, 187b, 187c
vamp_check_jacobian: 114, 113a, 114, 194d, 209d
vamp_copy_grid: 162, 77a, 162, 163b, 369b, 369c, 369d
vamp_copy_grids: 163b, 115c, 163b, 369f, 369g, 369h

vamp_copy_history: 164b, 105c, 164b, 370b, 370c, 371b
vamp_create_empty_grid: 15, 17, 77b, 77b, 79b, 100b, 102b, 148, 154b, 163b, 166d, 168, 172a, 188a, 368b, 368c, 368d
vamp_create_grid: 77b, 24a, 77b, 77b, 77b, 77c, 77b, 116a, 139c, 140c, 166b, 166c, 166d, 196b, 210b, 212b, 240a, 240b, 242
vamp_create_grids: 172a, 115c, 116a, 171d, 171e, 172a, 172a, 197b, 211b, 213, 241
vamp_create_history: 105e, 105c, 105e, 196b, 197b, 210b, 211b, 213, 237, 370b, 370c, 370d
vamp_delete_grid: 15, 17, 163a, 163a, 163a, 77a, 163a, 101c, 102b, 139c, 140c, 148, 154b, 163a, 164a, 166b, 166c, 170a, 196b, 210b, 212b, 240a, 240b, 242, 369b, 369c, 369e
vamp_delete_grids: 164a, 115c, 164a, 171d, 171e, 173c, 197b, 211b, 213, 241, 369f, 369g, 370a
vamp_delete_history: 165a, 105c, 165a, 196b, 197b, 210b, 211b, 212b, 213, 370b, 370c, 371d
vamp_discard_integral: 79d, 24c, 79d, 77c, 79c, 79d, 117b, 119b, 139b, 166b, 166c, 167b, 179b, 196b, 210b, 212b, 240a, 240b, 242
vamp_discard_integrals: 117b, 117a, 117b, 117d, 171d, 171e, 172b, 197b, 211b, 213, 241
vamp_equivalence_final: 73a, 73c
vamp_equivalence_init: 72c, 72e
vamp_equivalences: 71b, 71b, 75, 76a
vamp_equivalences_complete: 74c, 74d
vamp_equivalence_set: 74a, 74b
vamp_equivalences_final: 73b, 73c
vamp_equivalences_init: 72d, 72e
vamp_equivalences_write: 73e, 73f
vamp_equivalence_write: 73d, 73f, 74d
vamp_fork_grid: 95c, 15, 17, 95c, 95c, 95d, 95c, 100a, 102b, 168
vamp_fork_grid_joints: 15, 17, 101b, 100a, 100b, 101a, 101b, 101c, 102b, 168
vamp_fork_grid_multi: 95c, 95d, 100b
vamp_fork_grid_single: 95c, 95d, 96a, 100b
vamp_get_covariance: 84d, 84b, 84d, 139c, 140c
vamp_get_history_multi: 123c, 123d, 123e
vamp_get_history_single: 106b, 105c, 105d, 106b
vamp_get_variance: 84f, 84b, 84f, 123a, 368b, 368c, 368f
vamp_grid: 14, 15, 17, 76b, 22, 23c, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 76b, 77c,

79b, 79d, 80b, 81, 82b, 84c, 84d, 84e, 84f, 85a, 85c, 90c, 92a, 93, 94a, 96a, 98d, 100a, 100b, 101c, 102b, 106b, 111a, 112a, 124b, 133d, 137c, 139b, 139c, 140c, 143b, 144b, 147b, 147c, 150, 151b, 153a, 153b, 156b, 157, 158, 162, 163a, 166d, 167b, 167c, 168, 170a, 180d, 181b, 182d, 182e, 183a, 183b, 185a, 185b, 186a, 186b, 187b, 187c, 190b, 191c, 194a, 196b, 203, 205a, 208b, 210b, 212b, 220a, 229b, 230a, 230c, 231, 236b, 237, 368d, 368e, 368f, 369a, 369d, 369e
vamp_grids: 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 111a, 91, 92b, 111a, 111a, 116a, 116b, 117b, 117d, 118b, 119b, 121b, 122b, 123a, 123e, 135, 138a, 147d, 148, 149a, 149b, 153c, 154b, 155a, 155b, 163b, 164a, 171b, 171c, 172a, 172b, 173a, 173b, 173c, 173d, 181a, 181c, 183f, 184a, 184b, 184c, 197a, 211a, 213, 237, 369h, 370a
vamp_grid_type: 22, 31c, 71a, 71b, 75, 76a, 124b
vamp_history: 105a, 105a, 93, 102b, 105a, 105e, 106a, 106b, 107b, 108b, 109, 119b, 123e, 137c, 138a, 139b, 139c, 140c, 159b, 160, 161, 164b, 165a, 168, 170e, 171a, 173d, 181b, 181c, 188c, 189, 196b, 197b, 210b, 211b, 212b, 213, 237, 370d, 370e, 371a, 371b, 371c, 371d, 371e
vampi: 166a, 166a, 166a, 166a, 165b, 165c, 166a, 166a, 166a, 200b, 200c, 218a, 218b, 237
vamp_integrate_grid: 138b, 139a, 139b, 139c, 140c
vamp_integrate_region: 138b, 139a, 139c
vamp_integratex_region: 140a, 140b, 140c
vampi_tests: 200b, 200c
vamp_join_grid: 95c, 15, 17, 95c, 95c, 95d, 100a, 102b, 168
vamp_join_grid_multi: 95c, 95d, 101c
vamp_join_grid_single: 95c, 95d, 98d, 101c
vamp_marshal_grid: 156b, 29, 156a, 156b, 185a, 186a, 187b
vamp_marshal_grid_size: 157, 157, 29, 156a, 157, 185a, 186a, 187b
vamp_marshal_history: 159b, 159a, 159b, 188c
vamp_marshal_history_size: 160, 159a, 160, 188c
vamp_multi_channel: 112a, 111b, 112a, 190b, 194a
vamp_multi_channel0: 112b, 111b, 112b, 203, 208b
vamp_next_event_multi: 133b, 133c, 135, 180a, 180c, 181a
vamp_next_event_single: 133b, 133c, 133d, 135, 180a, 180c, 180d
vamp_nullify_covariance: 84e, 84b, 84e, 119b, 175b, 179b, 368b, 368c, 368e
vamp_nullify_variance: 85a, 84b, 85a, 119b, 175b, 179b, 368b, 368c, 369a
vamp_parallel_mpi: 165c, 165c, 165c, 165c, 166a
vamp_print_covariance: 129d, 129e
vamp_print_histories: 106d, 107a, 108b, 170b, 170d, 171a

vamp_print_history: 106d, 106d, 107a, 170b, 170c, 170d, 196b, 197b, 210b, 211b, 212b, 213, 240a, 240b, 241, 242
vamp_print_one_history: 106d, 107a, 107b, 108b, 170b, 170d, 170e
vamp_probability: 90b, 90c, 112a, 220a, 236b
vamp_read_grid: 142c, 142a, 142c, 144b, 182a, 182b, 182c
vamp_read_grid_raw: 142b, 143a
vamp_read_grids: 142c, 142a, 142c, 148, 183c, 183d, 183e
vamp_read_grids_raw: 142b, 143a, 154b
vamp_receive_grid: 17, 185b, 30, 168, 176b, 177a, 184d, 185b, 186b
vamp_receive_history: 177a, 188b, 189
vamp_reduce_channels: 121b, 119b, 121a, 121b, 176a, 179b
vamp_refine_grid: 14, 15, 17, 92a, 85b, 92a, 93, 102b, 119b, 168, 175c
vamp_refine_grids: 85b, 92b
vamp_refine_weights: 123a, 122a, 123a, 171d, 171e, 173b, 197b, 211b, 213, 241
vamp_reshape_grid: 82b, 82b, 79d, 82a, 82b, 118b, 166b, 166c, 167c
vamp_reshape_grid_internal: 81, 82a, 82b, 92a
vamp_reshape_grids: 118b, 117b, 118a, 118b
vamp_rest: 75, 76a
vamp_rigid_divisions: 15, 17, 84c, 84b, 84c, 102b, 168
vamp_sample_grid: 93, 14, 93, 93, 93, 93, 93, 24b, 24c, 93, 93, 93, 93, 85b, 93, 93, 93, 93, 93, 137c, 139b, 166b, 166c, 168, 179b, 181b, 196b, 210b, 212b, 240a, 240b, 242
vamp_sample_grid0: 14, 15, 85c, 17, 85c, 85b, 85c, 93, 102b, 85c, 120, 85c, 137c, 138a, 168, 85c, 175d, 181b, 181c, 85c
vamp_sample_grid_parallel: 102b, 102b, 102a, 102b
vamp_sample_grids: 119b, 119a, 119b, 138a, 171d, 171e, 119b, 173d, 197b, 211b, 213, 241
vamp_send_grid: 17, 185a, 30, 168, 176b, 176c, 184d, 185a, 185a, 185a, 186a
vamp_send_history: 176c, 188b, 188c
vamp_serial_mpi: 165b, 165b, 165b, 165c, 166a
vamp_stat: 37a, 75, 132c, 291a
vamp_sum_channels: 124b, 124a, 124b
vamp_terminate_history: 106a, 105b, 105c, 106a, 120, 123b, 168, 175d, 176a, 179b, 370b, 370c, 371a
vamp_test0: 202b, 210b, 211b, 215
vamp_test0_functions: 203, 209b, 217c
vamp_tests: 194b, 198c, 194b
vamp_tests0: 209a, 217c, 218a
vamp_unmarshal_grid: 158, 29, 156a, 158, 185b, 186b, 187b

vamp_unmarshal_history: 161, 159a, 161, 189
vamp_update_weights: 117d, 117c, 117d, 123a, 171d, 171e, 173a
vamp_warmup_grid: 137c, 137c, 137b, 137c, 180a, 180b, 181b, 212b
vamp_warmup_grids: 138a, 137b, 138a, 180a, 180b, 181c, 213
vamp_write_grid: 142c, 142a, 142c, 182a, 182b, 182c, 196b, 210b, 240a, 240b
vamp_write_grid_raw: 142b, 143a
vamp_write_grids: 142c, 142a, 142c, 183c, 183d, 183e, 197b, 211b, 241
vamp_write_grids_raw: 142b, 143a
vamp_write_histories: 106d
vamp_write_history: 106d, 107a
vamp_write_one_history: 106d
var_f: 45a, 88c, 88c, 88d, 364d
volume_division: 57a, 57d, 83b, 97c, 365d, 365e, 366c
w: 51a, 96b, 190b, 194a, 197b, 203, 208b, 211b, 213, 230b, 230c
wgt: 43b, 44a, 44b, 87c, 87c, 87c, 87c, 87d, 88c, 88c, 133d, 134a, 135, 136c, 136d, 137a, 363c, 363d
wgt0: 131b, 131d
wgt1: 131b, 131d
wgts: 87c, 88c, 114, 133d, 134a
write_division: 61a, 61b, 143b
write_division_name: 61a, 61b, 63b
write_division_raw: 61a, 61b, 150
write_division_raw_name: 61a, 61b, 66a
write_division_raw_unit: 61a, 61b, 64b
write_division_unit: 61a, 61b, 61c, 63b, 66a
write_grid_name: 142a, 142c, 147b, 182a, 182c, 183a
write_grid_raw_name: 142b, 143a, 153a
write_grid_raw_unit: 142b, 143a, 150, 153a, 153c
write_grids_name: 142a, 142c, 149a, 183c, 183e, 184b
write_grids_raw_name: 142b, 143a, 155a
write_grids_raw_unit: 142b, 143a, 153c, 155a
write_grids_unit: 142a, 142c, 147d, 149a, 183c, 183e, 183f
write_grid_unit: 142a, 142c, 143b, 147b, 147d, 182a, 182c, 182d
write_histogram: 212b, 213, 295b, 295c, 298b, 301
write_histogram1: 295c, 295d, 298b
write_histogram2: 295c, 295d, 301
write_histogram1_unit: 295c, 299a, 299b
write_history: 59a, 59b, 60b, 109
write_raw_state_name: 264e, 264f, 268d
write_raw_state_unit: 264e, 264f, 265c, 266a, 268d

`write_state_array`: 265c, 266a, 266c, 266d, 267a, 267b
`write_state_name`: 264e, 264f, 268c
`write_state_unit`: 264e, 264f, 265c, 268c
`wx`: 236a, 236b, 241
`x`: 23a, 31a, 31b, 31c, 87c, 87c, 87c, 87c, 87c, 87c, 37b, 38b, 39a, 39b, 39c, 40b, 43b, 44a, 44b, 45e, 87c, 47c, 48c, 48e, 50a, 50b, 52b, 54a, 55a, 55b, 55c, 56b, 56c, 57b, 57f, 58c, 58e, 59b, 60d, 61c, 62b, 63a, 64b, 65b, 66d, 67a, 67b, 69, 70a, 87c, 87c, 87d, 88b, 88c, 90c, 112a, 112b, 113b, 114, 115b, 124b, 131a, 131d, 133d, 134a, 135, 180d, 181a, 191a, 191b, 191c, 192, 193a, 193b, 194a, 194d, 195a, 195b, 204a, 205a, 206, 207a, 207b, 207c, 208a, 208b, 209d, 212b, 213, 223b, 223c, 224b, 226b, 226d, 227b, 228, 229b, 230a, 230c, 231, 232c, 233b, 233c, 236b, 237, 248, 250f, 254b, 254d, 255d, 255e, 256a, 256b, 256c, 256d, 256e, 256f, 257a, 257c, 259c, 259e, 259f, 259g, 259h, 260a, 260b, 260d, 264a, 266a, 266b, 267c, 270c, 270d, 271a, 272a, 272b, 272c, 277b, 277c, 277d, 278a, 278b, 278c, 287c, 289b, 289c, 291c, 292a, 292b, 292d, 292e, 296b, 297b, 300d, 300e, 310c, 330a, 330b, 331d, 331e, 332d, 333a, 337b, 338a, 338d, 339a, 339b, 340a, 340b, 341a, 341b, 341c, 363c, 363d, 366a
`x5`: 226d, 228, 232c, 233b, 233c, 234c, 235a
`x_mid`: 43b, 87c, 88c, 88d, 363c
`x_new`: 47c, 48c

O.2 Refinements

⟨*API documentation* 249⟩
⟨*Accept distribution among* `n` *workers* 104a⟩
⟨*Adjust Jacobian* 224a⟩
⟨*Adjust* `grid` *and other state for new* `num_calls` 83a⟩
⟨*Adjust* `h%div` *iff necessary* 106c⟩
⟨*Allocate or resize the divisions* 98c⟩
⟨*Alternative to* `basic.f90` 24d⟩
⟨*Application in Rambo mode* 242⟩
⟨*Application in massless single channel mode* 240b⟩
⟨*Application in multi channel mode* 241⟩
⟨*Application in single channel mode* 240a⟩
⟨$A' = P^T(\phi;p,q) \cdot A \cdot P(\phi;p,q)$ 319c⟩
⟨*Bail out if* `any (d == NaN)` 47b⟩
⟨*Bail out if exception* `exc` *raised* 98a⟩
⟨*Body of* `create_*_array2_pointer` 305b⟩
⟨*Body of* `create_*_array_pointer` 305a⟩

⟨*Body of* mpi90_broadcast_*_array 354a⟩
⟨*Body of* mpi90_receive_*_array 349c⟩
⟨*Body of* mpi90_receive_*_pointer 351c⟩
⟨*Body of* mpi90_send_*_array 347b⟩
⟨*Body of* multi_channel 197b⟩
⟨*Body of* tao_random_* 274b⟩
⟨*Body of* tao_random_*_array 275d⟩
⟨*Boost and rescale the vectors* 333a⟩
⟨*Bootstrap the* x *and* xl *buffers* 259d⟩
⟨*Bootstrap the* x *buffer* 255d⟩
⟨*Check optional arguments in* vamp_sample_grid0 90a⟩
⟨*Choose a* x *and calculate* f(x) 134a⟩
⟨*Cleanup in* vamp_test0 217f⟩
⟨*Clenshaw's recurrence formula* 287b⟩
⟨*Collect integration and grid optimization data for current* cell 88d⟩
⟨*Collect integration and grid optimization data for* x *from* f 88a⟩
⟨*Collect results of* vamp_sample_grid0 89a⟩
⟨*Combine the rest of* gs *onto* g 99c⟩
⟨*Constants in* divisions 65a⟩
⟨*Constants in* vamp 151a⟩
⟨*Constants in* vamp_equivalences 72b⟩
⟨*Construct* $\hat{R}(\theta; i, j)$ 127e⟩
⟨*Copy results of* vamp_sample_grid *to dummy variables* 95a⟩
⟨*Copy results of* vamp_sample_grids *to dummy variables* 177e⟩
⟨*Copy the rest of* g *to the* gs 96c⟩
⟨*Copyleft notice* 1⟩
⟨*Count up* cell*, exit if done* 86a⟩
⟨*Declaration of 30-bit* tao_random_numbers 266d⟩
⟨*Declaration of 52-bit* tao_random_numbers 267b⟩
⟨*Declaration of 30-bit* tao_random_numbers *types* 260b⟩
⟨*Declaration of 52-bit* tao_random_numbers *types* 260d⟩
⟨*Declaration of* coordinates *procedures* 337a⟩
⟨*Declaration of* cross_section *procedures* 221d⟩
⟨*Declaration of* divisions *procedures* 38a⟩
⟨*Declaration of* divisions *procedures (removed from WHIZARD)* 60c⟩
⟨*Declaration of* divisions *types* 37b⟩
⟨*Declaration of* exceptions *procedures* 246b⟩
⟨*Declaration of* exceptions *types* 245b⟩
⟨*Declaration of* histograms *procedures* 295b⟩
⟨*Declaration of* histograms *types* 294b⟩
⟨*Declaration of* kinematics *procedures* 324b⟩

⟨*Declaration of* kinematics *types* 326g⟩
⟨*Declaration of* linalg *procedures* 313b⟩
⟨*Declaration of* mpi90 *procedures* 343b⟩
⟨*Declaration of* mpi90 *types* 348b⟩
⟨*Declaration of* phase_space *procedures* 331b⟩
⟨*Declaration of* phase_space *types* 330a⟩
⟨*Declaration of procedures in* vamp_tests0 210a⟩
⟨*Declaration of procedures in* vamp_tests 194c⟩
⟨*Declaration of procedures in* vamp_tests0 *(broken?)* 209c⟩
⟨*Declaration of* specfun *procedures* 286b⟩
⟨*Declaration of* stest_functions *procedures* 289a⟩
⟨*Declaration of* tao_random_numbers 253b⟩
⟨*Declaration of* tao_random_numbers *(unused luxury)* 282a⟩
⟨*Declaration of* utils *procedures* 304b⟩
⟨*Declaration of* vamp *procedures* 77a⟩
⟨*Declaration of* vamp *procedures (removed from WHIZARD)* 115a⟩
⟨*Declaration of* vamp *types* 105a⟩
⟨*Declaration of* vamp_equivalences *procedures* 72d⟩
⟨*Declaration of* vamp_equivalences *types* 71c⟩
⟨*Declaration of* vamp_grid_type *types* 76b⟩
⟨*Declaration of* vampi *procedures* 166b⟩
⟨*Declaration of* vampi *types* 171b⟩
⟨*Declaration of* vamp_stat *procedures* 291b⟩
⟨*Decode* channel *into* ch *and* p(:) 207b⟩
⟨*Determine* ϕ *for the Jacobi rotation* $P(\phi;p,q)$ *with* $A'_{pq}=0$ 319a⟩
⟨*Distribute complete grids among processes* 175b⟩
⟨*Distribute each grid among processes* 179b⟩
⟨*Estimate* waste *of processor time* 179a⟩
⟨*Execute* command 217b⟩
⟨*Execute* command *in* vamp_test (never defined)⟩
⟨*Execute tests in* vamp_test0 216a⟩
⟨*Exit* iterate *if* accuracy *has been reached* 95b⟩
⟨*Exit* iterate *if* accuracy *has been reached (MPI)* 178a⟩
⟨*Fill* state *from* x 257c⟩
⟨*Fork a pseudo stratified sampling division* 54a⟩
⟨*Fork a pure stratified sampling division* 52b⟩
⟨*Fork an importance sampling division* 51a⟩
⟨*Gather exceptions in* vamp_sample_grid_parallel 103a⟩
⟨*Generate isotropic null vectors* 332e⟩
⟨*Get* $\cos\theta$ *and* $\sin\theta$ *from* evecs 127d⟩
⟨*Get* x *in the current* cell 87c⟩

⟨*Handle* `g%calls_per_cell` *for* `d == 0` 96b⟩
⟨*Handle* `local_error` 344c⟩
⟨*Handle* `local_error` *(no* `mpi90_abort`*)* 344b⟩
⟨*Handle optional* `pancake` *and* `cigar` 128a⟩
⟨*Idioms* 100a⟩
⟨*Implementation of 30-bit* `tao_random_numbers` 253a⟩
⟨*Implementation of 52-bit* `tao_random_numbers` 258b⟩
⟨*Implementation of* `coordinates` *procedures* 337b⟩
⟨*Implementation of* `cross_section` *procedures* 222a⟩
⟨*Implementation of* `divisions` *procedures* 38b⟩
⟨*Implementation of* `divisions` *procedures (removed from WHIZARD)* 45b⟩
⟨*Implementation of* `exceptions` *procedures* 246c⟩
⟨*Implementation of* `histograms` *procedures* 295f⟩
⟨*Implementation of* `kinematics` *procedures* 325a⟩
⟨*Implementation of* `linalg` *procedures* 314⟩
⟨*Implementation of* `mpi90` *procedures* 344a⟩
⟨*Implementation of* `phase_space` *procedures* 331d⟩
⟨*Implementation of procedures in* `vamp_tests0` 210b⟩
⟨*Implementation of procedures in* `vamp_tests` 195a⟩
⟨*Implementation of procedures in* `vamp_tests` *(broken?)* 194d⟩
⟨*Implementation of procedures in* `vamp_tests0` *(broken?)* 209d⟩
⟨*Implementation of* `specfun` *procedures* 287c⟩
⟨*Implementation of* `stest_functions` *procedures* 289b⟩
⟨*Implementation of* `tao_random_numbers` 253f⟩
⟨*Implementation of* `utils` *procedures* 305c⟩
⟨*Implementation of* `vamp` *procedures* 77c⟩
⟨*Implementation of* `vamp` *procedures (removed from WHIZARD)* 115b⟩
⟨*Implementation of* `vamp_equivalences` *procedures* 72c⟩
⟨*Implementation of* `vampi` *procedures* 166d⟩
⟨*Implementation of* `vampi` *procedures (doesn't work with MPICH yet)* 186a⟩
⟨*Implementation of* `vamp_stat` *procedures* 291c⟩
⟨*Implementation of* `vamp_test0_functions` *procedures* 204a⟩
⟨*Implementation of* `vamp_test_functions` *procedures* 191a⟩
⟨*Increment* k *until* $\sum m_k \geq \Delta$ *and keep the surplus in* δ 48b⟩
⟨*Initialize a virginal random number generator* 278d⟩
⟨*Initialize clusters* 131a⟩
⟨*Initialize* `num_rot` 320e⟩
⟨*Initialize stratified sampling* 42⟩
⟨*Insure that* `associated (g%map) == .false.` 146b⟩
⟨*Insure that* `associated (g%mu_x) == .false.` 147a⟩
⟨*Insure that* `size (g%div) == ndim` 146a⟩

⟨*Insure that* `ubound (d%x, dim=1) == num_div` 63a⟩
⟨*Interface declaration for* `func` 22⟩
⟨*Interface declaration for* `ihp` 31b⟩
⟨*Interface declaration for* `jacobian` 31c⟩
⟨*Interface declaration for* `phi` 31a⟩
⟨*Interfaces of 30-bit* `tao_random_numbers` 279f⟩
⟨*Interfaces of 52-bit* `tao_random_numbers` 280d⟩
⟨*Interfaces of* `divisions` *procedures* 61b⟩
⟨*Interfaces of* `divisions` *procedures (removed from WHIZARD)* 364b⟩
⟨*Interfaces of* `exceptions` *procedures* 360d⟩
⟨*Interfaces of* `histograms` *procedures* 295c⟩
⟨*Interfaces of* `kinematics` *procedures* 324c⟩
⟨*Interfaces of* `mpi90` *procedures* 346c⟩
⟨*Interfaces of* `phase_space` *procedures* 331c⟩
⟨*Interfaces of* `tao_random_numbers` 257d⟩
⟨*Interfaces of* `tao_random_numbers` *(unused luxury)* 281g⟩
⟨*Interfaces of* `utils` *procedures* 304c⟩
⟨*Interfaces of* `vamp` *procedures* 94c⟩
⟨*Interfaces of* `vampi` *procedures* 170d⟩
⟨*Interpolate the new* x_i *from* x_k *and* δ 48c⟩
⟨*Join closest clusters* 131b⟩
⟨*Join importance sampling divisions* 51b⟩
⟨*Join pseudo stratified sampling divisions* 54b⟩
⟨*Join pure stratified sampling divisions* 52c⟩
⟨*Kill m4(1) builtins* 357b⟩
⟨*Load* `a` *and refresh* `state` 253c⟩
⟨*Load 52-bit* `a` *and refresh* `state` 258c⟩
⟨*Local variables in* `vamp_sample_grid0` 86c⟩
⟨*MPI communication example* 29⟩
⟨*MPI communication example'* 30⟩
⟨*Maybe accept unweighted event* 134c⟩
⟨*Maybe accept unweighted multi channel event* 136d⟩
⟨*Maybe accept unweighted multi channel event (old version)* 137a⟩
⟨*Module* `vamp_test0_functions` 203⟩
⟨*Module* `vamp_test_functions` 190b⟩
⟨*Module* `vamp_tests` 194b⟩
⟨*Modules used by* `vamp_test0` 217c⟩
⟨*Modules used by* `vamp_tests0` 209b⟩
⟨*Parallel implementation of* $S_n = S_0(rS_0)^n$ *(HPF)* 15⟩
⟨*Parallel implementation of* $S_n = S_0(rS_0)^n$ *(MPI)* 17⟩
⟨*Parallel usage of* $S_n = S_0(rS_0)^n$ *(HPF)* 16⟩

⟨*Parameters in* mpi90 (never defined)⟩
⟨*Parameters in* tao_random_numbers 252a⟩
⟨*Parameters in* tao_random_numbers *(alternatives)* 252b⟩
⟨*Parameters in* tao_random_test 282e⟩
⟨*Parameters in* utils 311c⟩
⟨*Parameters in* vampi 167a⟩
⟨*Parameters local to* tao_random_seed 255a⟩
⟨*Parse the commandline in* vamp_test *and set* command (never defined)⟩
⟨*Perform more tests of* tao_random_numbers 283d⟩
⟨*Perform simple tests of* tao_random_numbers 283a⟩
⟨*Perform the Jacobi rotation resulting in* $A'_{pq} = 0$ 318⟩
⟨*Prepare array* buffer *and* done, todo, chunk 276b⟩
⟨*Pull* u *into the intervall* $[3, 4]$ 287a⟩
⟨*Read command line and decode it as* command (never defined)⟩
⟨*Receive the result for channel* #ch *at the root* 177a⟩
⟨*Reload* buffer *or exit* 276d⟩
⟨*Reset counters in* vamp_sample_grid0 86b⟩
⟨*Resize arrays, iff necessary* 40b⟩
⟨*Return optional arguments in* lu_decompose 315d⟩
⟨*Sample* calls_per_cell *points in the current* cell 87b⟩
⟨*Sample* g%g0%grids(ch) 175d⟩
⟨*Sample the grid* g%grids(ch) 120⟩
⟨*Select* channel *from* weights 136b⟩
⟨*Serial implementation of* $S_n = S_0(rS_0)^n$ 14⟩
⟨*Set default for* domain 345b⟩
⟨*Set defaults for* source, tag *and* domain 348e⟩
⟨*Set* i, delta_x, x, *and* wgt *from* xi 44a⟩
⟨*Set* i(1), i(2) *to the axes of the optimal plane* 127a⟩
⟨*Set* i(1), i(2) *to the axes of the optimal plane (broken!)* 127b⟩
⟨*Set* iv *to the index of the optimal eigenvector* 125b⟩
⟨*Set* j *to* minloc(key) 309a⟩
⟨*Set* m *to* $(1, 1, \ldots)$ *or to rebinning weights from* d%variance 40a⟩
⟨*Set* nu *to* num *or* size(v) 276a⟩
⟨*Set* rev *to* reverse *or* .false. 308e⟩
⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ 223b⟩
⟨*Set* $(s_2, t_1, \phi, \cos\theta_3, \phi_3)$ *from* $(x_1, \ldots, x_5)$ *(massless case)* 223c⟩
⟨*Set* subspace *to the axes of the optimal plane* 129a⟩
⟨*Set up integrand and region in* vamp_test0 217e⟩
⟨*Set up* s *and* t 255f⟩
⟨*Set up* seed_value *from* seed *or* DEFAULT_SEED 255c⟩
⟨*Setup to fork a pseudo stratified sampling division* 53⟩

⟨*Setup to fork a pure stratified sampling division* 52a⟩
⟨*Shift* `s` *or* `t` *and exit if* `t` ≤ 0 257b⟩
⟨*Ship* `g%g0%grids` *from the root to the assigned processor* 176b⟩
⟨*Ship the result for channel #*`ch` *back to the root* 176c⟩
⟨*Specific procedures for 30-bit* `tao_random_number` 280a⟩
⟨*Specific procedures for 52-bit* `tao_random_number` 280e⟩
⟨*Specific procedures for* `tao_random_copy` 263f⟩
⟨*Specific procedures for* `tao_random_create` 261c⟩
⟨*Specific procedures for* `tao_random_luxury` 282c⟩
⟨*Specific procedures for* `tao_random_seed` 257f⟩
⟨*Step* `last` *and reload* `buffer` *iff necessary* 274d⟩
⟨*Test* `a(1)` = `A_2027082` 283b⟩
⟨*Trace results of* `vamp_sample_grid` 105b⟩
⟨*Trace results of* `vamp_sample_grids` 123b⟩
⟨*Trivial* `ktest.f90` 334⟩
⟨*Types in* `cross_section` 226c⟩
⟨*Unconditionally accept weighted event* 134b⟩
⟨*Unconditionally accept weighted multi channel event* 136c⟩
⟨*(Unused) Interfaces of* `phase_space` *procedures* 331g⟩
⟨*Update* `last`, `done` *and* `todo` *and set new* `chunk` 276c⟩
⟨*Update* `num_rot` 320f⟩
⟨*Variables in 30-bit* `tao_random_numbers` 252c⟩
⟨*Variables in 52-bit* `tao_random_numbers` 257g⟩
⟨*Variables in* `cross_section` 220b⟩
⟨*Variables in* `divisions` 46a⟩
⟨*Variables in* `exceptions` 245c⟩
⟨*Variables in* `histograms` 295e⟩
⟨*Variables in* `mpi90` (never defined)⟩
⟨*Variables in* `tao_random_numbers` 268a⟩
⟨*Variables in* `utils` 312b⟩
⟨*Variables in* `vamp` 78a⟩
⟨*Variables in* `vamp_test0` 217a⟩
⟨*Variables local to 52-bit* `tao_random_seed` 259b⟩
⟨$V' = V \cdot P(\phi; p, q)$ 320d⟩
⟨*XXX Implementation of* `cross_section` *procedures* 221e⟩
⟨*XXX Variables in* `cross_section` 221a⟩
⟨`application.f90` 220a⟩
⟨`basic.f90` 23a⟩
⟨*52-bit* $p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) 259g⟩
⟨*52-bit* $p(z) \to zp(z)$ (*modulo* 2 *and* $z^K + z^L + 1$) 260a⟩
⟨`call copy_division (gs%div(j), g%div(j))` 98b⟩

⟨call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 97d⟩
⟨call join_division (g%div(j), gs%div(j)) 99a⟩
⟨call sum_division (g%div(j), gs%div(j)) 99b⟩
⟨$c_0/2, c_1, c_2, \ldots, c_{15}$ *for* $\Gamma(x)$ 288a⟩
⟨constants.f90 243b⟩
⟨coordinates.f90 336⟩
⟨ctest.f90 132c⟩
⟨divisions.f90 37a⟩
⟨eps = 1 315a⟩
⟨eps = - eps 315b⟩
⟨exceptions.f90 245a⟩
⟨f = wgt * func (x, weights, channel), *iff* x *inside* true_domain 87d⟩
⟨f90.m4 357c⟩
⟨f95.m4 357a⟩
⟨histograms.f90 294a⟩
⟨kinematics.f90 324a⟩
⟨ktest.f90 333d⟩
⟨la_sample.f90 321d⟩
⟨linalg.f90 313a⟩
⟨$m_a \leftrightarrow m_b$, $m_1 \leftrightarrow m_2$ *for channel #1* 224c⟩
⟨mpi90.f90 343a⟩
⟨pivots = 0 *and* eps = 0 315c⟩
⟨$p_1 \leftrightarrow p_2$ *for channel #2* 225a⟩
⟨products.f90 323⟩
⟨$p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) 256a⟩
⟨$p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) *(DEK, C)* 256e⟩
⟨$p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) *(DEK, Fortran)* 256c⟩
⟨$p(z) \to p(z)^2$ (*modulo* 2 *and* $z^K + z^L + 1$) *(alternative)* 256d⟩
⟨$p(z) \to zp(z)$ (*modulo* 2 *and* $z^K + z^L + 1$) 257a⟩
⟨specfun.f90 286a⟩
⟨stest.f90 288b⟩
⟨tao52_random_numbers.f90 273a⟩
⟨tao_random_numbers.f90 272d⟩
⟨tao_test.f90 285⟩
⟨utils.f90 304a⟩
⟨vamp0_* => vamp_* 166c⟩
⟨vamp.f90 70c⟩
⟨vampi.f90 165b⟩
⟨vampi_test.f90 200a⟩
⟨vampi_test0.f90 218a⟩
⟨vamp_kinds.f90 243a⟩

⟨vamp_stat.f90 291a⟩
⟨vamp_test.f90 190a⟩
⟨vamp_test0.f90 202b⟩
⟨vamp_test.out 202a⟩
⟨vamp_test0.out 219⟩
⟨weights: $\alpha_i \to w_{\max,i}\alpha_i$ 136a⟩

Index

deficiencies in `Fortran90` and `F`, 74, 84
deficiencies of Fortran90 that have been fixed in Fortran95, 246
dependences on external modules, 84

Fortran problem, 68
Fortran sucks, 108
functional programming rules, 108

IEEE hacks, 45
inconvenient F constraints, 112, 313

more empirical studies helpful, 128

optimizations not implemented yet, 101

possible error by DEK, 253
Problems with MPICH, 182, 183

remove from finalized program, 331

system dependencies, 45, 265

theoretical question, 253

unfinished business, 122

Acknowledgements

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