

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

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## **Abstract**

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

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application.nw 314 2010-04-17 20:32:33Z ohl  
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constants.nw 314 2010-04-17 20:32:33Z ohl  
exceptions.nw 314 2010-04-17 20:32:33Z ohl  
specfun.nw 314 2010-04-17 20:32:33Z ohl  
vamp\_stat.nw 314 2010-04-17 20:32:33Z ohl  
histograms.nw 314 2010-04-17 20:32:33Z ohl  
utils.nw 314 2010-04-17 20:32:33Z ohl  
linalg.nw 314 2010-04-17 20:32:33Z ohl  
products.nw 314 2010-04-17 20:32:33Z ohl  
kinematics.nw 314 2010-04-17 20:32:33Z ohl  
coordinates.nw 314 2010-04-17 20:32:33Z ohl  
mpi90.nw 314 2010-04-17 20:32:33Z ohl  
postlude.nw 314 2010-04-17 20:32:33Z ohl

# CONTENTS

1	INTRODUCTION	1
2	ALGORITHMS	3
2.1	<i>Importance Sampling</i>	4
2.2	<i>Stratified Sampling</i>	5
2.3	<i>Vegas</i>	6
2.3.1	<i>Vegas' Inflexibility</i>	6
2.3.2	<i>Vegas' Dark Side</i>	7
2.4	<i>Multi Channel Sampling</i>	7
2.5	<i>Revolving</i>	8
2.6	<i>Parallelization</i>	8
2.6.1	<i>Multilinear Structure of the Sampling Algorithm</i>	8
2.6.2	<i>State and Message Passing</i>	13
2.6.3	<i>Random Numbers</i>	13
2.6.4	<i>Practice</i>	14
3	DESIGN TRADE OFFS	19
3.1	<i>Programming Language</i>	20
4	USAGE	21
4.1	<i>Basic Usage</i>	21
4.1.1	<i>Basic Example</i>	22
4.2	<i>Advanced Usage</i>	24
4.2.1	<i>Types</i>	25
4.2.2	<i>Shared Arguments</i>	25
4.2.3	<i>Single Channel Procedures</i>	27
4.2.4	<i>Inout/Output and Marshling</i>	28
4.2.5	<i>Multi Channel Procedures</i>	31
4.2.6	<i>Event Generation</i>	34
4.2.7	<i>Parallelization</i>	34
4.2.8	<i>Diagnostics</i>	35

4.2.9	<i>Other Procedures</i>	36
4.2.10	<i>(Currently) Undocumented Procedures</i>	36
5	IMPLEMENTATION	37
5.1	<i>The Abstract Datatype <b>division</b></i>	37
5.1.1	<i>Creation, Manipulation &amp; Injection</i>	38
5.1.2	<i>Grid Refinement</i>	44
5.1.3	<i>Probability Density</i>	48
5.1.4	<i>Quadrupole</i>	49
5.1.5	<i>Forking and Joining</i>	49
5.1.6	<i>Inquiry</i>	57
5.1.7	<i>Diagnostics</i>	58
5.1.8	<i>I/O</i>	61
5.1.9	<i>Marshaling</i>	66
5.1.10	<i>Boring Copying and Deleting of Objects</i>	69
5.2	<i>The Abstract Datatype <b>vamp_grid</b></i>	70
5.2.1	<i>Container for application data</i>	77
5.2.2	<i>Initialization</i>	77
5.2.3	<i>Sampling</i>	86
5.2.4	<i>Forking and Joining</i>	96
5.2.5	<i>Parallel Execution</i>	103
5.2.6	<i>Diagnostics</i>	106
5.2.7	<i>Multi Channel</i>	112
5.2.8	<i>Mapping</i>	126
5.2.9	<i>Event Generation</i>	134
5.2.10	<i>Convenience Routines</i>	139
5.2.11	<i>I/O</i>	143
5.2.12	<i>Marshaling</i>	157
5.2.13	<i>Boring Copying and Deleting of Objects</i>	163
5.3	<i>Interface to MPI</i>	166
5.3.1	<i>Parallel Execution</i>	167
5.3.2	<i>Event Generation</i>	181
5.3.3	<i>I/O</i>	183
5.3.4	<i>Communicating Grids</i>	185
6	SELF TEST	191
6.1	<i>No Mapping Mode</i>	191
6.1.1	<i>Serial Test</i>	191
6.1.2	<i>Parallel Test</i>	201
6.1.3	<i>Output</i>	203
6.2	<i>Mapped Mode</i>	203

6.2.1	<i>Serial Test</i>	203
6.2.2	<i>Parallel Test</i>	219
6.2.3	<i>Output</i>	220
7	APPLICATION	221
7.1	<i>Cross section</i>	221
A	CONSTANTS	244
A.1	<i>Kinds</i>	244
A.2	<i>Mathematical and Physical Constants</i>	244
B	ERRORS AND EXCEPTIONS	246
C	THE ART OF RANDOM NUMBERS	250
C.1	<i>Application Program Interface</i>	250
C.2	<i>Low Level Routines</i>	253
C.2.1	<i>Generation of 30-bit Random Numbers</i>	253
C.2.2	<i>Initialization of 30-bit Random Numbers</i>	254
C.2.3	<i>Generation of 52-bit Random Numbers</i>	258
C.2.4	<i>Initialization of 52-bit Random Numbers</i>	258
C.3	<i>The State</i>	260
C.3.1	<i>Creation</i>	260
C.3.2	<i>Destruction</i>	262
C.3.3	<i>Copying</i>	263
C.3.4	<i>Flushing</i>	264
C.3.5	<i>Input and Output</i>	264
C.3.6	<i>Marshaling and Unmarshaling</i>	269
C.4	<i>High Level Routines</i>	272
C.4.1	<i>Single Random Numbers</i>	273
C.4.2	<i>Arrays of Random Numbers</i>	275
C.4.3	<i>Procedures With Explicit <code>tao_random_state</code></i>	277
C.4.4	<i>Static Procedures</i>	278
C.4.5	<i>Generic Procedures</i>	279
C.4.6	<i>Luxury</i>	280
C.5	<i>Testing</i>	282
C.5.1	<i>30-bit</i>	282
C.5.2	<i>52-bit</i>	284
C.5.3	<i>Test Program</i>	285
D	SPECIAL FUNCTIONS	286
D.1	<i>Test</i>	288

E	STATISTICS	291
F	HISTOGRAMMING	294
G	MISCELLANEOUS UTILITIES	304
	<i>G.1 Memory Management</i>	304
	<i>G.2 Sorting</i>	307
	<i>G.3 Mathematics</i>	310
	<i>G.4 I/O</i>	312
H	LINEAR ALGEBRA	313
	<i>H.1 LU Decomposition</i>	313
	<i>H.2 Determinant</i>	316
	<i>H.3 Diagonalization</i>	316
	<i>H.4 Test</i>	321
I	PRODUCTS	323
J	KINEMATICS	324
	<i>J.1 Lorentz Transformations</i>	324
	<i>J.2 Massive Phase Space</i>	326
	<i>J.3 Massive 3-Particle Phase Space Revisited</i>	329
	<i>J.4 Massless n-Particle Phase Space: <b>RAMBO</b></i>	332
	<i>J.5 Tests</i>	333
K	COORDINATES	336
	<i>K.1 Angular Spherical Coordinates</i>	336
	<i>K.2 Trigonometric Spherical Coordinates</i>	340
	<i>K.3 Surface of a Sphere</i>	343
L	IDIOMATIC FORTRAN90 INTERFACE FOR MPI	344
	<i>L.1 Basics</i>	344
	<i>L.2 Point to Point</i>	347
	<i>L.3 Collective Communication</i>	353
M	IDEAS	358
	<i>M.1 Toolbox for Interactive Optimization</i>	358
	<i>M.2 Partially Non-Factorized Importance Sampling</i>	358
	<i>M.3 Correlated Importance Sampling (?)</i>	358
	<i>M.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region)</i>	359
	<i>M.5 Automagic Multi Channel</i>	359

N	CROSS REFERENCES	360
<i>N.1</i>	<i>Identifiers</i> . . . . .	360
<i>N.2</i>	<i>Refinements</i> . . . . .	380



## *Program Summary:*

- **Title of program:** VAMP, Version 1.0 (October 1999)
- **Program obtainable** by anonymous `ftp` from the host `crunch.ikp.physik.th-darmstadt.de` in the directory `pub/ohl/vamp`.
- **Licensing provisions:** Free software under the GNU General Public License.
- **Programming language used:** From version 2.2.0 of the program: Fortran2003 [8] Until version 2.1.x of the program: Fortran95 [9] (Fortran90 [7] and F [14] versions available as well)
- **Number of program lines in distributed program, including test data, etc.:**  $\approx 4300$  (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 [9, 13]<sup>1</sup> (Note that for the maintenance of the program and especially its usage within the event generator WHIZARD parts of the program have been adapted to Fortran2003). The purpose of this reimplementation is two-fold: for pedagogical reasons it is useful to employ Fortran95 features (in particular the array language) together with literate programming [4] for expressing the algorithm more concisely and more transparently. On the other hand we use a Fortran95 abstract type to separate the state from the functions. This allows multiple instances of Vegas with different adaptations to run in parallel and in paves the road for a more parallelizable implementation.

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

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---

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

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```

## —2— ALGORITHMS

 The notation has to be synchronized with [3]!

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

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

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

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

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

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

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

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

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

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

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

## 2.1 Importance Sampling

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

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

while the variance transforms non-trivially

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

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

One of the more popular approaches is to use a mapping  $\phi$  of the integration domain

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

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

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

A familiar example is given by the map

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

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

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

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

## 2.2 Stratified Sampling

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

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

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

a new estimator is

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

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

where

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

and

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

since the expectation is linear

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

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

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

This is minimized for

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

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

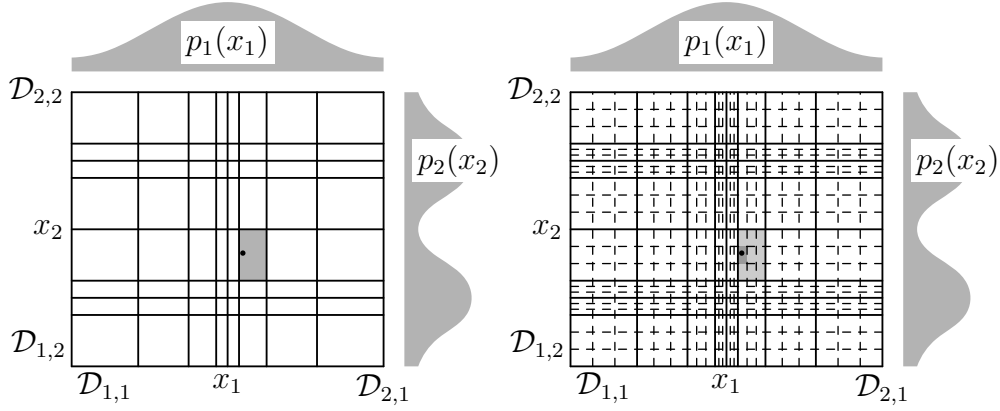


Figure 2.1: **vegas** grid structure for non-stratified sampling (left) and for genuinely stratified sampling (right), which is used in low dimensions. N.B.: the grid and the weight functions  $p_{1,2}$  are only in qualitative agreement.



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

## 2.3 Vegas



Under construction!

### 2.3.1 Vegas' Inflexibility

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

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

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

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

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

where we have used the damped standard deviation

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

instead of the spread.

### 2.3.2 Vegas’ Dark Side



Under construction!

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

## 2.4 Multi Channel Sampling

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



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



## 2.5 *Revolving*



Under construction!

## 2.6 *Parallelization*

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

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

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

### 2.6.1 *Multilinear Structure of the Sampling Algorithm*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Then

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

and a good refinement prescription  $r$ , such as Vegas, will minimize the  $\sigma$ .

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

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

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

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

However, a reordering of the random number sequence will only change the result by the statistical error, as long as the scale of the allowed reorderings is *bounded* and much smaller than the period of the random number generator<sup>1</sup> Below, we will therefore use the notation  $x \approx y$  for “equal for an appropriate finite reordering of the  $\rho$  used in calculating  $x$  and  $y$ ”. For our purposes, the relation  $x \approx y$  is strong enough and allows simple and efficient implementations.

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

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

where

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

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

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

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

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

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

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

---

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

### *Importance Sampling*

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

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

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

### *Stratified Sampling*

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

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

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

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

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

and decompositions of the  $D^j$  induce decompositions of  $G$

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

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

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

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

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

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

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

Now it remains to find a decomposition

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

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

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



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

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

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

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

### 2.6.2 State and Message Passing

### 2.6.3 Random Numbers

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

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

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

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

### 2.6.4 Practice

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

#### Serial

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

```

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

```

#### HPF

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

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

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

15  $\langle$ Parallel implementation of  $S_n = S_0(rS_0)^n$  (HPF) 15 $\rangle \equiv$

```

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

```



```

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

```

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

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

16  $\langle$ Parallel usage of  $S_n = S_0(rS_0)^n$  (HPF) 16 $\rangle \equiv$

```

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

```

## MPI

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

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

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

```

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

```

```

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

```

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

# —3—

## DESIGN TRADE OFFS

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

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

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

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

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

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

### 3.1 *Programming Language*

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

Let us consider the alternatives

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

## —4— USAGE

### 4.1 Basic Usage

`type(vamp_grid)`

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

Create a fresh grid for the integration domain

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

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

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

`subroutine vamp_delete_grid (g [, exc])`

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

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

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

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

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

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

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

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

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

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

```
22 <Interface declaration for func 22>≡
interface
  function func (xi, data, weights, channel, grids) result (f)
    use kinds
    use vamp_grid_type !NODEP!
    import vamp_data_t
    real(kind=default), dimension(:), intent(in) :: xi
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: f
  end function func
end interface
```

#### 4.1.1 Basic Example

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

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

```

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

```

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

```

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

```

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

```

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

```



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

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

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

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

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

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

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

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

## 4.2 Advanced Usage



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

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

#### 4.2.1 *Types*

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

#### 4.2.2 *Shared Arguments*

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

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

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

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

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

The average  $\chi^2$  of the iterations.

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

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

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

Collect covariance data.

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

Exceptional conditions are reported in `exc`.

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

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

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

Diagnostic information for multi channel sampling.

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

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

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

The current best estimate of the integral.

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

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

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

The number of sampling points.

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

Number of divisions of the adaptive grid in each dimension.

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

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

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

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

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

The current best estimate of the error on the integral.

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

Try to use stratified sampling.

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

```
...
```

### 4.2.3 *Single Channel Procedures*

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

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

subroutine vamp_create_empty_grid (g)

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

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

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

    func

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

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

    func

     $S_0$ 

subroutine vamp_refine_grid (g, [, exc])

     $r$ 

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

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

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

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

```

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

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

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

subroutine vamp_copy_grid (lhs, rhs)

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

subroutine vamp_delete_grid (g)

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

```

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

```

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

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

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

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

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

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

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

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

pure subroutine vamp_marshall_grid (g, integer_buffer,
double_buffer)

```

```

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

```

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



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

```

pure subroutine vamp_marshall_grid_size (g, integer_size,
    double_size)

```

```

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

```

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

```

pure subroutine vamp_unmarshal_grid (g, integer_buffer,
    double_buffer)

```

```

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

```

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

29 *<MPI communication example 29>*≡  
 call vamp\_marshall\_grid\_size (g, isize, dsize)

```

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

```

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

```

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

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

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

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

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

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

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

```

#### 4.2.5 Multi Channel Procedures

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

**31a** *Interface declaration for phi 31a*  $\equiv$

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

**31b** *Interface declaration for ihp 31b*  $\equiv$

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

**31c** *Interface declaration for jacobian 31c*  $\equiv$

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

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

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



```

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

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

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

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

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

```

Verify that

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

```

subroutine vamp_copy_grids (lhs, rhs)

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

subroutine vamp_delete_grids (g)

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

```

```

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

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

subroutine vamp_create_empty_grids (g)

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

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

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

subroutine vamp_refine_weights (g [, power)

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

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

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

subroutine vamp_reshape_grids (g, num_calls [, stratified])

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

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

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

```

```

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

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

function vamp_sum_channels (x, weights, func)

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

```

#### *4.2.6 Event Generation*

```

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

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

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

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

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

```

#### *4.2.7 Parallelization*

```

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

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

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

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

```

```

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

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

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

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

```

#### 4.2.8 *Diagnostics*

```

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

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

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

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

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

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

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

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

```



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

#### *4.2.9 Other Procedures*

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

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

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

# —5—

## IMPLEMENTATION

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

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



vamp\_apply\_equivalences from vamp accesses %variance ...

```
37b <Declaration of divisions types 37b>≡
    type, public :: division_t
    ! private
    !!! Avoiding a g95 bug
```

```

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

```

### 5.1.1 Creation, Manipulation & Injection

**38a** *<Declaration of divisions procedures 38a>*≡

```

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

```

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

```

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

```

```

else
    d%x_max_true = x_max
end if
end subroutine create_division

```

39a *⟨Implementation of divisions procedures 38b⟩*+≡  
 elemental subroutine create\_empty\_division (d)  
 type(division\_t), intent(out) :: d  
 nullify (d%x, d%integral, d%variance)  
 ! nullify (d%efficiency)  
 end subroutine create\_empty\_division

39b *⟨Implementation of divisions procedures 38b⟩*+≡  
 elemental subroutine set\_rigid\_division (d, ng)  
 type(division\_t), intent(inout) :: d  
 integer, intent(in) :: ng  
 d%stratified = ng > 1  
 d%ng = ng  
 d%dxg = real (ubound (d%x, dim=1), kind=default) / d%ng  
 end subroutine set\_rigid\_division

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

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

39c *⟨Implementation of divisions procedures 38b⟩*+≡  
 elemental subroutine reshape\_division (d, max\_num\_div, ng, use\_variance)  
 type(division\_t), intent(inout) :: d  
 integer, intent(in) :: max\_num\_div  
 integer, intent(in), optional :: ng  
 logical, intent(in), optional :: use\_variance  
 real(kind=default), dimension(:), allocatable :: old\_x, m  
 integer :: num\_div, equ\_per\_adap  
 if (present (ng)) then  
 if (max\_num\_div > 1) then  
 d%stratified = ng > 1  
 else  
 d%stratified = .false.  
 end if  
 else  
 d%stratified = .false.  
 end if  
 if (d%stratified) then



```

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

```

**40a** *<Set m to (1,1,...) or to rebinning weights from d%variance 40a>*≡

```

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

```

**40b** *<Resize arrays, iff necessary 40b>*≡

```

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

```

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

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



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



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

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

Table 5.1: To stratify or not to stratify.

the contribution to the error is largest, but to use importance sampling, i. e. concentrating the grid in the regions where the contribution to the value is largest.

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

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

and the corresponding number  $n_{\text{div}}$  of adaptive divisions

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

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

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

42 *⟨Initialize stratified sampling 42⟩*≡  
 if (d%ng >= max\_num\_div / 2) then  
   d%stratified = .true.  
   equ\_per\_adap = d%ng / max\_num\_div + 1  
   num\_div = d%ng / equ\_per\_adap  
   if (num\_div < 2) then  
     d%stratified = .false.  
     num\_div = 2  
     d%ng = 1  
 else if (mod (num\_div,2) == 1) then  
   num\_div = num\_div - 1  
   d%ng = equ\_per\_adap \* num\_div  
 else



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

```

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

```

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

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

```

43a  <Declaration of divisions procedures 38a>+≡
      public :: inject_division, inject_division_short

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

```

```

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

```

44a <Set i, delta\_x, x, and wgt from xi 44a>≡

```

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

```

44b <Implementation of divisions procedures 38b>+≡

```

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

```

### 5.1.2 Grid Refinement

44c <Declaration of divisions procedures 38a>+≡

```

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

```

44d <Implementation of divisions procedures 38b>+≡

```

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

```

45a *<Implementation of divisions procedures 38b>+≡*  
 elemental subroutine record\_variance (d, i, var\_f)  
   type(division\_t), intent(inout) :: d  
   integer, intent(in) :: i  
   real(kind=default), intent(in) :: var\_f  
   if (d%stratified) then  
     d%variance(i) = d%variance(i) + var\_f  
   end if  
end subroutine record\_variance

45b *<Implementation of divisions procedures (removed from WHIZARD) 45b>≡*  
 elemental subroutine record\_efficiency (d, i, eff)  
   type(division\_t), intent(inout) :: d  
   integer, intent(in) :: i  
   real(kind=default), intent(in) :: eff  
   ! d%efficiency(i) = d%efficiency(i) + eff  
end subroutine record\_efficiency

45c *<Implementation of divisions procedures 38b>+≡*  
 elemental subroutine clear\_integral\_and\_variance (d)  
   type(division\_t), intent(inout) :: d  
   d%integral = 0.0  
   d%variance = 0.0  
   ! d%efficiency = 0.0  
end subroutine clear\_integral\_and\_variance

45d *<Declaration of divisions procedures 38a>+≡*  
 public :: refine\_division

45e *<Implementation of divisions procedures 38b>+≡*  
 elemental subroutine refine\_division (d)  
   type(division\_t), intent(inout) :: d  
   character(len=\*), parameter :: FN = "refine\_division"  
   d%x = rebin (rebinning\_weights (d%variance), d%x, size (d%variance))  
end subroutine refine\_division

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

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

As long as the initial `num_div`  $\geq 6$ , we know that `num_div`  $\geq 3$ .

**46a** *Variables in divisions 46a*  $\equiv$   
`integer, private, parameter :: MIN_NUM_DIV = 3`

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

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

**46b** *Implementation of divisions procedures 38b*  $\equiv$   

```

pure function rebinning_weights (d) result (m)
  real(kind=default), dimension(:), intent(in) :: d
  real(kind=default), dimension(size(d)) :: m
  real(kind=default), dimension(size(d)) :: smooth_d
  real(kind=default), parameter :: ALPHA = 1.5
  integer :: nd
  Bail out if any (d == NaN) 47b
  nd = size (d)
  if (nd > 2) then
    smooth_d(1) = (d(1) + d(2)) / 2.0
    smooth_d(2:nd-1) = (d(1:nd-2) + d(2:nd-1) + d(3:nd)) / 3.0
    smooth_d(nd) = (d(nd-1) + d(nd)) / 2.0
  else
    smooth_d = d
  end if
  if (all (smooth_d < tiny (1.0_default))) then

```

---

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

```

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

```

47a *<Declaration of divisions procedures 38a>+≡*  
 private :: rebinning\_weights



The NaN test is probably not portable:

47b *<Bail out if any (d == NaN) 47b>≡*  
 if (any (d /= d)) then  
 m = 1.0  
 return  
 end if

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

47c *<Implementation of divisions procedures 38b>+≡*  
 pure function rebin (m, x, num\_div) result (x\_new)  
 real(kind=default), dimension(:), intent(in) :: m  
 real(kind=default), dimension(0:), intent(in) :: x  
 integer, intent(in) :: num\_div  
 real(kind=default), dimension(0:num\_div) :: x\_new  
 integer :: i, k  
 real(kind=default) :: step, delta  
 step = sum (m) / num\_div  
 k = 0  
 delta = 0.0  
 x\_new(0) = x(0)  
 do i = 1, num\_div - 1  
*<Increment k until  $\sum m_k \geq \Delta$  and keep the surplus in  $\delta$  48b>*  
*<Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c>*  
 end do  
 x\_new(num\_div) = 1.0  
 end function rebin





Figure 5.4: Typical weights used in the rebinning algorithm.

48a  $\langle$ Declaration of divisions procedures 38a $\rangle + \equiv$   
`private :: rebin`

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

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

48c  $\langle$ Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c $\rangle \equiv$   
`x_new(i) = x(k) - (x(k) - x(k-1)) * delta / m(k)`

### 5.1.3 Probability Density

48d  $\langle$ Declaration of divisions procedures 38a $\rangle + \equiv$   
`public :: probability`

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

and

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

48e  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$   
`elemental function probability (d, x) result (p)`  
`type(division_t), intent(in) :: d`  
`real(kind=default), intent(in) :: x`

```

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

```

#### 5.1.4 *Quadrupole*

- 49a *<Declaration of divisions procedures 38a>+≡*  
 public :: quadrupole\_division
- 49b *<Implementation of divisions procedures 38b>+≡*  
 elemental function quadrupole\_division (d) result (q)  
 type(division\_t), intent(in) :: d  
 real(kind=default) :: q  
 !!! q = value\_spread\_percent (rebinning\_weights (d%variance))  
 q = standard\_deviation\_percent (rebinning\_weights (d%variance))  
 end function quadrupole\_division

#### 5.1.5 *Forking and Joining*

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

- 49c *<Declaration of divisions procedures 38a>+≡*  
 public :: fork\_division, join\_division, sum\_division



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

50a *<Implementation of divisions procedures 38b>+≡*

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

50b *<Implementation of divisions procedures 38b>+≡*

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

```

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

```

### *Importance Sampling*

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

```

51a Fork an importance sampling division 51a≡
  if (d%stratified) then
    call raise_exception (exc, EXC_FATAL, FN, &
      "ng == 1 incompatible w/ stratification")
  else
    call copy_division (ds, d)
    num_calls(2:) = ceiling (real (sum_calls) / num_forks)
    num_calls(1) = sum_calls - sum (num_calls(2:))
  end if

```

and sum up the results in the end:

```

51b Join importance sampling divisions 51b≡
  call sum_division (d, ds)

```

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

### *Stratified Sampling*

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

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

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

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

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

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

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

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

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



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

### *Pseudo Stratified Sampling*

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

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

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

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

**53** *<Setup to fork a pseudo stratified sampling division 53>*  $\equiv$   
`nx = lcm (d%ng / gcd (num_forks, d%ng), num_div)  
ds_ng = (d%ng * (/ (j, j=0,num_forks) /)) / num_forks  
n = (nx * ds_ng) / d%ng  
n0(1:num_forks) = n(0:num_forks-1)  
n1(1:num_forks) = n(1:num_forks)`

```

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

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

54c <Declaration of divisions procedures 38a>+≡
    private :: subdivide
    private :: distribute

```

```
private :: collect
```

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

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

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

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

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

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

### *Trivia*

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

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



```

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

```

56a *<Declaration of divisions procedures 38a>+≡*

```

public :: debug_division
public :: dump_division

```

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

```

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

```

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

```

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

```

```
end subroutine dump_division
```

### 5.1.6 Inquiry

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

- 57a *<Declaration of divisions procedures 38a>+≡*  
public :: inside\_division, stratified\_division  
public :: volume\_division, rigid\_division, adaptive\_division
- 57b *<Implementation of divisions procedures 38b>+≡*  
elemental function inside\_division (d, x) result (theta)  
type(division\_t), intent(in) :: d  
real(kind=default), intent(in) :: x  
logical :: theta  
theta = (x >= d%x\_min\_true) .and. (x <= d%x\_max\_true)  
end function inside\_division
- 57c *<Implementation of divisions procedures 38b>+≡*  
elemental function stratified\_division (d) result (yorn)  
type(division\_t), intent(in) :: d  
logical :: yorn  
yorn = d%stratified  
end function stratified\_division
- 57d *<Implementation of divisions procedures 38b>+≡*  
elemental function volume\_division (d) result (vol)  
type(division\_t), intent(in) :: d  
real(kind=default) :: vol  
vol = d%dx  
end function volume\_division
- 57e *<Implementation of divisions procedures 38b>+≡*  
elemental function rigid\_division (d) result (n)  
type(division\_t), intent(in) :: d  
integer :: n  
n = d%ng  
end function rigid\_division
- 57f *<Implementation of divisions procedures 38b>+≡*  
elemental function adaptive\_division (d) result (n)  
type(division\_t), intent(in) :: d  
integer :: n  
n = ubound (d%x, dim=1)  
end function adaptive\_division

### 5.1.7 Diagnostics

- 58a *<Declaration of divisions types 37b>+≡*  
type, public :: div\_history  
private  
logical :: stratified  
integer :: ng, num\_div  
real(kind=default) :: x\_min, x\_max, x\_min\_true, x\_max\_true  
real(kind=default) :: &  
spread\_f\_p, stddev\_f\_p, spread\_p, stddev\_p, spread\_m, stddev\_m  
end type div\_history
- 58b *<Declaration of divisions procedures 38a>+≡*  
public :: copy\_history, summarize\_division
- 58c *<Implementation of divisions procedures 38b>+≡*  
elemental function summarize\_division (d) result (s)  
type(division\_t), intent(in) :: d  
type(div\_history) :: s  
real(kind=default), dimension(:), allocatable :: p, m  
allocate (p(ubound(d%x,dim=1)), m(ubound(d%x,dim=1)))  
p = probabilities (d%x)  
m = rebinning\_weights (d%variance)  
s%ng = d%ng  
s%num\_div = ubound (d%x, dim=1)  
s%stratified = d%stratified  
s%x\_min = d%x\_min  
s%x\_max = d%x\_max  
s%x\_min\_true = d%x\_min\_true  
s%x\_max\_true = d%x\_max\_true  
s%spread\_f\_p = value\_spread\_percent (d%integral)  
s%stddev\_f\_p = standard\_deviation\_percent (d%integral)  
s%spread\_p = value\_spread\_percent (p)  
s%stddev\_p = standard\_deviation\_percent (p)  
s%spread\_m = value\_spread\_percent (m)  
s%stddev\_m = standard\_deviation\_percent (m)  
deallocate (p, m)  
end function summarize\_division
- 58d *<Declaration of divisions procedures 38a>+≡*  
private :: probabilities
- 58e *<Implementation of divisions procedures 38b>+≡*  
pure function probabilities (x) result (p)  
real(kind=default), dimension(0:), intent(in) :: x  
real(kind=default), dimension(ubound(x,dim=1)) :: p

```

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

```

59a *<Implementation of divisions procedures 38b>+≡*

```

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

```

59b *<Implementation of divisions procedures 38b>+≡*

```

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

```

```

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

60a  <Variables in divisions 46a>+≡
    integer, private, parameter :: BUFFER_SIZE = 50

60b  <Declaration of divisions procedures 38a>+≡
    public :: print_history, write_history

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

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

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

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

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

```

```

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

```

### 5.1.8 I/O

61a *<Declaration of divisions procedures 38a>+≡*

```

public :: write_division
private :: write_division_unit, write_division_name
public :: read_division
private :: read_division_unit, read_division_name
public :: write_division_raw
private :: write_division_raw_unit, write_division_raw_name
public :: read_division_raw
private :: read_division_raw_unit, read_division_raw_name

```

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

```

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

```

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

61c *<Implementation of divisions procedures 38b>+≡*

```

subroutine write_division_unit (d, unit, write_integrals)
    type(division_t), intent(in) :: d
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    logical :: write_integrals0
    integer :: i
    write_integrals0 = .false.
    if (present(write_integrals)) write_integrals0 = write_integrals
    write (unit = unit, fmt = descr_fmt) "begin type(division_t) :: d"
    write (unit = unit, fmt = integer_fmt) "ubound(d%x,1) = ", ubound (d%x, dim=1)
    write (unit = unit, fmt = integer_fmt) "d%ng = ", d%ng
    write (unit = unit, fmt = logical_fmt) "d%stratified = ", d%stratified

```

```

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

```

62a *<Variables in divisions 46a>+≡*

```

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

```

62b *<Implementation of divisions procedures 38b>+≡*

```

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

```

```

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

```



What happened to d%efficiency?

- 63a** *⟨Insure that ubound (d%x, dim=1) == num\_div 63a⟩*≡
- ```

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

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

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

```



```

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

```

64a *<Implementation of divisions procedures 38b>+≡*

```

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

```

64b *<Implementation of divisions procedures 38b>+≡*

```

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

```

```

65a  <Constants in divisions 65a>≡
      integer, parameter, private :: MAGIC_DIVISION = 11111111
      integer, parameter, private :: MAGIC_DIVISION_BEGIN = MAGIC_DIVISION + 1
      integer, parameter, private :: MAGIC_DIVISION_END = MAGIC_DIVISION + 2

65b  <Implementation of divisions procedures 38b>+≡
      subroutine read_division_raw_unit (d, unit, read_integrals)
        type(division_t), intent(inout) :: d
        integer, intent(in) :: unit
        logical, intent(in), optional :: read_integrals
        logical :: read_integrals0
        integer :: i, num_div, magic
        character(len=*), parameter :: FN = "read_division_raw_unit"
        read_integrals0 = .false.
        if (present(read_integrals)) read_integrals0 = read_integrals
        read (unit = unit) magic
        if (magic /= MAGIC_DIVISION_BEGIN) then
          print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_BEGIN, &
            ", found ", magic
          stop
        end if
        read (unit = unit) num_div
        <Insure that ubound (d%x, dim=1) == num_div 63a>
        read (unit = unit) d%ng
        read (unit = unit) d%stratified
        read (unit = unit) d%dx
        read (unit = unit) d%dxg
        read (unit = unit) d%x_min
        read (unit = unit) d%x_max
        read (unit = unit) d%x_min_true
        read (unit = unit) d%x_max_true
        do i = 0, ubound (d%x, dim=1)
          if (read_integrals0 .and. i/=0) then
            read (unit = unit) d%x(i), d%integral(i), d%variance(i)
          else
            read (unit = unit) d%x(i)
          end if
        end do
        if (.not.read_integrals0) then
          d%integral = 0.0
          d%variance = 0.0
        !   d%efficiency = 0.0
        end if
        read (unit = unit) magic

```

```

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

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

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

```

### 5.1.9 Marshaling

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

```

66c  <Declaration of divisions procedures 38a>+≡
    public :: marshal_division_size, marshal_division, unmarshal_division

66d  <Implementation of divisions procedures 38b>+≡
    pure subroutine marshal_division (d, ibuf, dbuf)
        type(division_t), intent(in) :: d

```

```

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

```

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

```

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

```

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

```

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

```

```

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

68a <Declaration of divisions procedures 38a>+≡
    public :: marshal_div_history_size, marshal_div_history, unmarshal_div_history

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

68c <Implementation of divisions procedures 38b>+≡
    pure subroutine marshal_div_history_size (h, iwords, dwords)
        type(div_history), intent(in) :: h
        integer, intent(out) :: iwords, dwords
        iwords = 3
        dwords = 10
    end subroutine marshal_div_history_size

68d <Implementation of divisions procedures 38b>+≡
    pure subroutine unmarshal_div_history (h, ibuf, dbuf)

```

```

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

```

### 5.1.10 Boring Copying and Deleting of Objects

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

```

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

```

```

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

```

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

```

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

```

70b  $\langle$ Implementation of divisions procedures 38b $\rangle + \equiv$

```

elemental subroutine copy_history (lhs, rhs)
  type(div_history), intent(out) :: lhs
  type(div_history), intent(in) :: rhs
  lhs%stratified = rhs%stratified
  lhs%ng = rhs%ng
  lhs%num_div = rhs%num_div
  lhs%x_min = rhs%x_min
  lhs%x_max = rhs%x_max
  lhs%x_min_true = rhs%x_min_true
  lhs%x_max_true = rhs%x_max_true
  lhs%spread_f_p = rhs%spread_f_p
  lhs%stddev_f_p = rhs%stddev_f_p
  lhs%spread_p = rhs%spread_p
  lhs%stddev_p = rhs%stddev_p
  lhs%spread_m = rhs%spread_m
  lhs%stddev_m = rhs%stddev_m
end subroutine copy_history

```

## 5.2 The Abstract Datatype *vamp\_grid*

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

```
! vamp.f90 --
<Copyleft notice 1>
```

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

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

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

⚡ By WK for WHIZARD.

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

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



```

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

72b  <Constants in vamp_equivalences 72b>≡
      integer, parameter, public :: &
         VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3

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

72d  <Declaration of vamp_equivalences procedures 72d>≡
      public :: vamp_equivalences_init

72e  <Implementation of vamp_equivalences procedures 72c>+≡
      subroutine vamp_equivalences_init (eq, n_eq, n_ch, n_dim)
         type(vamp_equivalences_t), intent(inout) :: eq
         integer, intent(in) :: n_eq, n_ch, n_dim
         integer :: i
         eq%n_eq = n_eq
         eq%n_ch = n_ch
         allocate (eq%eq(n_eq))
         allocate (eq%pointer(n_ch+1))
         do i=1, n_eq
            call vamp_equivalence_init (eq%eq(i), n_dim)
         end do
         allocate (eq%independent(n_ch), eq%equivalent_to_ch(n_ch))
         allocate (eq%multiplicity(n_ch), eq%symmetry(n_ch))
         allocate (eq%div_is_invariant(n_ch, n_dim))
         eq%independent = .true.
         eq%equivalent_to_ch = 0
         eq%multiplicity = 0
         eq%symmetry = 0
         eq%div_is_invariant = .false.

```

```

        end subroutine vamp_equivalences_init

73a  <Implementation of vamp_equivalences procedures 72c>+≡
      subroutine vamp_equivalence_final (eq)
        type(vamp_equivalence_t), intent(inout) :: eq
        deallocate (eq%permutation, eq%mode)
      end subroutine vamp_equivalence_final

73b  <Declaration of vamp_equivalences procedures 72d>+≡
      public :: vamp_equivalences_final

73c  <Implementation of vamp_equivalences procedures 72c>+≡
      subroutine vamp_equivalences_final (eq)
        type(vamp_equivalences_t), intent(inout) :: eq
        ! integer :: i
        ! do i=1, eq%n_eq
        !   call vamp_equivalence_final (eq%eq(i))
        ! end do
        if (allocated (eq%eq)) deallocate (eq%eq)
        if (allocated (eq%pointer)) deallocate (eq%pointer)
        if (allocated (eq%multiplicity)) deallocate (eq%multiplicity)
        if (allocated (eq%symmetry)) deallocate (eq%symmetry)
        if (allocated (eq%independent)) deallocate (eq%independent)
        if (allocated (eq%equivalent_to_ch)) deallocate (eq%equivalent_to_ch)
        if (allocated (eq%div_is_invariant)) deallocate (eq%div_is_invariant)
        eq%n_eq = 0
        eq%n_ch = 0
      end subroutine vamp_equivalences_final

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

73e  <Declaration of vamp_equivalences procedures 72d>+≡
      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, "(1x,A)") "Inequivalent channels:"
if (allocated (eq%independent)) then
  do ch=1, eq%n_ch
    if (eq%independent(ch)) then
      write (u, "(3x,A,1x,I0,A,4x,A,I0,4x,A,I0,4x,A,999(L1))") &
        "Channel", ch, ":", &
        "Mult. = ", eq%multiplicity(ch), &
        "Symm. = ", eq%symmetry(ch), &
        "Invar.: ", eq%div_is_invariant(ch,:)
    end if
  end do
else
  write (u, "(3x,A)") "[not allocated]"
end if
write (u, "(1x,A)") "Equivalence list:"
if (allocated (eq%eq)) then
  do i=1, size (eq%eq)
    call vamp_equivalence_write (eq%eq(i), u)
  end do
else
  write (u, "(3x,A)") "[not allocated]"
end if
end subroutine vamp_equivalences_write

```

**74a** *<Declaration of vamp\_equivalences procedures 72d>+≡*  
 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

75a *<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

```

75b *<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 95c>
  <Constants in vamp 152a>
  <Declaration of vamp types 77b>
  <Variables in vamp 79a>
  character(len=*), public, parameter :: VAMP_RCS_ID = &
    "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
contains
  <Implementation of vamp procedures 78>
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 estimate 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**  $\langle$ Declaration of `vamp` procedures **77a** $\rangle \equiv$   

```

public :: vamp_copy_grid, vamp_delete_grid

```

### 5.2.1 Container for application data



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

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

**77b**  $\langle$ Declaration of `vamp` types **77b** $\rangle \equiv$   

```

type, public :: vamp_data_t
end type vamp_data_t

```

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

**77c**  $\langle$ Declaration of `vamp` types **77b** $\rangle + \equiv$   

```

type(vamp_data_t), parameter, public :: NO_DATA = vamp_data_t ()

```

### 5.2.2 Initialization

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

```

public :: vamp_create_grid, vamp_create_empty_grid

```

Create a fresh grid for the integration domain

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

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

78 *⟨Implementation of vamp procedures 78⟩*≡

```

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

```

```

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

```

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

**79a**  $\langle \text{Variables in vamp 79a} \rangle \equiv$

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

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

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

**79b**  $\langle \text{Declaration of vamp procedures 77a} \rangle + \equiv$

```
private :: map_domain
```

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

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

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

**79c**  $\langle \text{Implementation of vamp procedures 78} \rangle + \equiv$

```

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

```



```

        xmax = maxval (corners, dim=1)
    end subroutine map_domain
80a  <Implementation of vamp procedures 78>+≡
        elemental subroutine vamp_create_empty_grid (g)
            type(vamp_grid), intent(inout) :: g
            nullify (g%div, g%num_div, g%map, g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
        end subroutine vamp_create_empty_grid
80b  <Declaration of vamp procedures 77a>+≡
        public :: vamp_discard_integral
        Keep the current optimized grid, but drop the accumulated results for the
        integral (value and errors). Iff the second variable is given, it will be the new
        number of sampling points for the next call to vamp_sample_grid.
80c  <Implementation of vamp procedures 78>+≡
        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

81a  <Declaration of vamp procedures 77a>+≡
    private :: set_grid_options

81b  <Implementation of vamp procedures 78>+≡
    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`.

82a *⟨Implementation of vamp procedures 78⟩*+≡

```
pure subroutine vamp_reshape_grid_internal &
  (g, num_calls, num_div, &
   stratified, quadrupole, covariance, exc, use_variance, &
   independent, equivalent_to_ch, multiplicity)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
logical, intent(in), optional :: use_variance
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
integer :: ndim, num_cells
integer, dimension(size(g%div)) :: ng
character(len=*), parameter :: FN = "vamp_reshape_grid_internal"
ndim = size (g%div)
call set_grid_options &
  (g, num_calls, num_div, stratified, quadrupole, &
   & independent, equivalent_to_ch, multiplicity)
⟨Adjust grid and other state for new num_calls 84a⟩
g%all_stratified = all (stratified_division (g%div))
if (present (covariance)) then
  ndim = size (g%div)
  if (covariance .and. (.not. associated (g%mu_x))) then
    allocate (g%mu_x(ndim), g%mu_xx(ndim,ndim))
    allocate (g%sum_mu_x(ndim), g%sum_mu_xx(ndim,ndim))
    g%sum_mu_x = 0.0
    g%sum_mu_xx = 0.0
  else if ((.not. covariance) .and. (associated (g%mu_x))) then
    deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
  end if
end if
end subroutine vamp_reshape_grid_internal
```

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

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

```

private :: vamp_reshape_grid_internal
public :: vamp_reshape_grid
83  <Implementation of vamp procedures 78>+≡
pure subroutine vamp_reshape_grid &
    (g, num_calls, num_div, stratified, quadrupole, covariance, exc, &
     independent, equivalent_to_ch, multiplicity)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
logical, intent(in), optional :: independent
integer, intent(in), optional :: equivalent_to_ch, multiplicity
call vamp_reshape_grid_internal &
    (g, num_calls, num_div, stratified, quadrupole, covariance, &
     exc, use_variance = .false., &
     independent=independent, equivalent_to_ch=equivalent_to_ch, &
     multiplicity=multiplicity)
end subroutine vamp_reshape_grid

```

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

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

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

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

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

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

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

NB:

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

84a *Adjust grid and other state for new num\_calls 84a*  $\equiv$

```

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

```

(5.15)

and

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

84b *Adjust grid and other state for new num\_calls 84a*  $+\equiv$

```

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

```

84c *Adjust grid and other state for new num\_calls 84a*  $+\equiv$

```

  call vamp_nullify_f_limits (g)

```

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

84d *Declaration of vamp procedures 77a*  $+\equiv$

```

  public :: vamp_nullify_f_limits

```

84e *Implementation of vamp procedures 78*  $+\equiv$

```

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

```

```

85a  <Declaration of vamp procedures 77a>+≡
      public :: vamp_rigid_divisions
      public :: vamp_get_covariance, vamp_nullify_covariance
      public :: vamp_get_variance, vamp_nullify_variance

85b  <Implementation of vamp procedures 78>+≡
      pure function vamp_rigid_divisions (g) result (ng)
        type(vamp_grid), intent(in) :: g
        integer, dimension(size(g%div)) :: ng
        ng = rigid_division (g%div)
      end function vamp_rigid_divisions

85c  <Implementation of vamp procedures 78>+≡
      pure function vamp_get_covariance (g) result (cov)
        type(vamp_grid), intent(in) :: g
        real(kind=default), dimension(size(g%div),size(g%div)) :: cov
        if (associated (g%mu_x)) then
          if (abs (g%sum_weights) <= tiny (cov(1,1))) then
            where (g%sum_mu_xx == 0.0_default)
              cov = 0.0
            elsewhere
              cov = huge (cov(1,1))
            endwhere
          else
            cov = g%sum_mu_xx / g%sum_weights &
                  - outer_product (g%sum_mu_x, g%sum_mu_x) / g%sum_weights**2
          end if
        else
          cov = 0.0
        end if
      end function vamp_get_covariance

85d  <Implementation of vamp procedures 78>+≡
      elemental subroutine vamp_nullify_covariance (g)
        type(vamp_grid), intent(inout) :: g
        if (associated (g%mu_x)) then
          g%sum_mu_x = 0
          g%sum_mu_xx = 0
        end if
      end subroutine vamp_nullify_covariance

85e  <Implementation of vamp procedures 78>+≡
      elemental function vamp_get_variance (g) result (v)
        type(vamp_grid), intent(in) :: g
        real(kind=default) :: v
        if (abs (g%sum_weights) <= tiny (v)) then

```

```

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

```

86a *⟨Implementation of vamp procedures 78⟩*+≡  
 elemental subroutine vamp\_nullify\_variance (g)  
   type(vamp\_grid), intent(inout) :: g  
   g%sum\_mu\_gi = 0  
end subroutine vamp\_nullify\_variance

### 5.2.3 Sampling

86b *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_sample\_grid  
 public :: vamp\_sample\_grid0  
 public :: vamp\_refine\_grid  
 public :: vamp\_refine\_grids

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

86c *⟨Implementation of vamp procedures 78⟩*+≡  
 subroutine vamp\_sample\_grid0 &  
   (rng, g, func, data, channel, weights, grids, exc, &  
   negative\_weights)  
 type(tao\_random\_state), intent(inout) :: rng  
 type(vamp\_grid), intent(inout) :: g  
 class(vamp\_data\_t), intent(in) :: data  
 integer, intent(in), optional :: channel  
 real(kind=default), dimension(:), intent(in), optional :: weights  
 type(vamp\_grid), dimension(:), intent(in), optional :: grids  
 type(exception), intent(inout), optional :: exc  
*⟨Interface declaration for func 22⟩*  
 character(len=\*), parameter :: FN = "vamp\_sample\_grid0"  
 logical, intent(in), optional :: negative\_weights  
*⟨Local variables in vamp\_sample\_grid0 87c⟩*  
 integer :: ndim  
 logical :: neg\_w

```

ndim = size (g%div)
neg_w = .false.
if (present (negative_weights)) neg_w = negative_weights
<Check optional arguments in vamp_sample_grid0 91a>
<Reset counters in vamp_sample_grid0 87b>
loop_over_cells: do
    <Sample calls_per_cell points in the current cell 88a>
    <Collect integration and grid optimization data for current cell 89d>
    <Count up cell, exit if done 87a>
end do loop_over_cells
<Collect results of vamp_sample_grid0 90a>
end subroutine vamp_sample_grid0

```

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

```

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

87b <Reset counters in vamp_sample_grid0 87b>≡
    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

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

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

```



```

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

```

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

```

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

```

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

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

```

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

```

```
end if
```

89a *Collect integration and grid optimization data for x from f 89a*≡

```
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
```

89b *Collect integration and grid optimization data for x from f 89a*+≡

```
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
```

89c *Local variables in vamp\_sample\_grid0 87c*+≡

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

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

89d *Collect integration and grid optimization data for current cell 89d*≡

```
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

```

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

where the  $N_{\text{calls}}^2$  cancels the corresponding factor in the Jacobian and the  $N_{\text{cells}}^{-2}$  is the result of stratification.

90a  $\langle \text{Collect results of vamp\_sample\_grid0 90a} \rangle \equiv$

```

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

```

90b  $\langle \text{Collect results of vamp\_sample\_grid0 90a} \rangle + \equiv$

```

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

```

```

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

```

91a *⟨Check optional arguments in vamp\_sample\_grid0 91a⟩*≡  
 if (present (channel) .neqv. present (weights)) then  
 call raise\_exception (exc, EXC\_FATAL, FN, &  
 "channel and weights required together")  
 return  
end if

91b *⟨Declaration of vamp procedures 77a⟩*+≡  
 public :: vamp\_probability

91c *⟨Implementation of vamp procedures 78⟩*+≡  
 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

91d *⟨Implementation of vamp procedures 78⟩*+≡  
 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

```

$$\begin{aligned}
& \text{Grid Refinement: } r \\
n_{\text{div},j} & \rightarrow \frac{Q_j n_{\text{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\text{dim}}}} \quad (5.19)
\end{aligned}$$

where

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

- 93a *⟨Implementation of vamp procedures 78⟩* +=
- ```

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

```
- 93b *⟨Implementation of vamp procedures 78⟩* +=
- ```

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

```
- 93c *⟨Variables in vamp 79a⟩* +=
- ```

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

```

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

94 *⟨Implementation of vamp procedures 78⟩*+≡

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

Assuming that the iterations have been statistically independent, we can

combine them with the usual formulae.

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

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

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

**95a** *Implementation of vamp procedures 78*)+≡  
 elemental subroutine vamp\_average\_iterations\_grid &  
   (g, iteration, integral, std\_dev, avg\_chi2)  
   type(vamp\_grid), intent(in) :: g  
   integer, intent(in) :: iteration  
   real(kind=default), intent(out) :: integral, std\_dev, avg\_chi2  
   real(kind=default), parameter :: eps = 1000 \* epsilon (1.\_default)  
   if (g%sum\_weights>0) then  
     integral = g%sum\_integral / g%sum\_weights  
     std\_dev = sqrt (1.0 / g%sum\_weights)  
     avg\_chi2 = &  
       max ((g%sum\_chi2 - g%sum\_integral \* integral) / (iteration-0.99), &  
         0.0\_default)  
     if (avg\_chi2 < eps \* g%sum\_chi2) avg\_chi2 = 0  
   else  
     integral = 0  
     std\_dev = 0  
     avg\_chi2 = 0  
   end if  
end subroutine vamp\_average\_iterations\_grid

**95b** *Declaration of vamp procedures 77a*)+≡  
 public :: vamp\_average\_iterations  
 private :: vamp\_average\_iterations\_grid

**95c** *Interfaces of vamp procedures 95c*)+≡  
 interface vamp\_average\_iterations  
   module procedure vamp\_average\_iterations\_grid  
 end interface

Lepage suggests [1] to reweight the contributions as in the following improved



formulae, which we might implement as an option later.

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

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

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

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

```

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

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

```

#### 5.2.4 Forking and Joining

```

96c  <Declaration of vamp procedures 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

96d  <Interfaces of vamp procedures 95c>+≡
      interface vamp_fork_grid
        module procedure vamp_fork_grid_single, vamp_fork_grid_multi
      end interface

```

```

interface vamp_join_grid
  module procedure vamp_join_grid_single, vamp_join_grid_multi
end interface

```

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

97a *⟨Implementation of vamp procedures 78⟩* +=

```

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

```

Divide the sampling points among identical grids

97b *⟨Handle g%calls\_per\_cell for d == 0 97b⟩* ≡

```

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

```

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

```

do i = 1, num_grids
  call copy_array_pointer (gs(i)%num_div, g%num_div)

```

```

        if (associated (g%map)) then
            call copy_array_pointer (gs(i)%map, g%map)
        end if
        if (associated (g%mu_x)) then
            call create_array_pointer (gs(i)%mu_x, ndim)
            call create_array_pointer (gs(i)%sum_mu_x, ndim)
            call create_array_pointer (gs(i)%mu_xx, (/ ndim, ndim /))
            call create_array_pointer (gs(i)%sum_mu_xx, (/ ndim, ndim /))
        end if
    end do
Reset results
98a  <Copy the rest of g to the gs 97c>+≡
      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

98b  <Copy the rest of g to the gs 97c>+≡
      gs%stratified = g%stratified
      gs%all_stratified = g%all_stratified
      gs%quadrupole = g%quadrupole

98c  <Copy the rest of g to the gs 97c>+≡
      do i = 1, num_grids
          num_cells = product (rigid_division (gs(i)%div))
          gs(i)%calls = gs(i)%calls_per_cell * num_cells
          gs(i)%num_calls = gs(i)%calls
          gs(i)%jacobi = product (volume_division (gs(i)%div)) / gs(i)%calls
          gs(i)%dv2g = (gs(i)%calls / num_cells)**2 &
              / gs(i)%calls_per_cell / gs(i)%calls_per_cell / (gs(i)%calls_per_cell - 1.0)
      end do
      gs%f_min = g%f_min * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)
      gs%f_max = g%f_max * (gs%jacobi * gs%calls) / (g%jacobi * g%calls)
This could be self-explaining, if the standard would allow .... Note that we
can get away with copying just the pointers, because fork_division does
the dirty work for the memory management.
98d  <call fork_division (g%div(j), gs%div(j), g%calls_per_cell, ...) 98d>≡
      allocate (d_tmp(num_grids))
      do i = 1, num_grids
          d_tmp(i) = gs(i)%div(j)

```

```

end do
call fork_division (g%div(j), d_tmp, g%calls_per_cell, gs%calls_per_cell, exc)
do i = 1, num_grids
  gs(i)%div(j) = d_tmp(i)
end do
deallocate (d_tmp)
<Bail out if exception exc raised 99a>

```

**99a** *<Bail out if exception exc raised 99a>*≡

```

  if (present (exc)) then
    if (exc%level > EXC_WARN) then
      return
    end if
  end if

```

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

**99b** *<call copy\_division (gs%div(j), g%div(j)) 99b>*≡

```

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

```

**99c** *<Allocate or resize the divisions 99c>*≡

```

  num_div = size (g%div)
  do i = 1, size (gs)
    if (associated (gs(i)%div)) then
      if (size (gs(i)%div) /= num_div) then
        allocate (gs(i)%div(num_div))
        call create_empty_division (gs(i)%div)
      end if
    else
      allocate (gs(i)%div(num_div))
      call create_empty_division (gs(i)%div)
    end if
  end do

```

**99d** *<Implementation of vamp procedures 78>*+≡

```

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

```

```

        if (j == d) then
            <call join_division (g%div(j), gs%div(j)) 100a>
        else
            <call sum_division (g%div(j), gs%div(j)) 100b>
        end if
    end do
    <Combine the rest of gs onto g 100c>
end subroutine vamp_join_grid_single

100a <call join_division (g%div(j), gs%div(j)) 100a>≡
    allocate (d_tmp(num_grids))
    do i = 1, num_grids
        d_tmp(i) = gs(i)%div(j)
    end do
    call join_division (g%div(j), d_tmp, exc)
    deallocate (d_tmp)
    <Bail out if exception exc raised 99a>

100b <call sum_division (g%div(j), gs%div(j)) 100b>≡
    allocate (d_tmp(num_grids))
    do i = 1, num_grids
        d_tmp(i) = gs(i)%div(j)
    end do
    call sum_division (g%div(j), d_tmp)
    deallocate (d_tmp)

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

```

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

101a *<Idioms 101a>*≡

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

101b *<Implementation of vamp procedures 78>*+≡

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

---

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

```

        end do
    end select
end subroutine vamp_fork_grid_multi

```

102a  $\langle$ Declaration of vamp procedures 77a $\rangle + \equiv$

```

public :: vamp_fork_grid_joints

```

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

102b  $\langle$ Implementation of vamp procedures 78 $\rangle + \equiv$

```

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

```

102c  $\langle$ Implementation of vamp procedures 78 $\rangle + \equiv$

```

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
            end do
        end select
    end subroutine vamp_join_grid_multi

```

```

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

```

### 5.2.5 Parallel Execution

103a *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_sample\_grid\_parallel  
 public :: vamp\_distribute\_work

HPF [10, 11, 15]:

103b *<Implementation of vamp procedures 78>+≡*  
 subroutine vamp\_sample\_grid\_parallel &  
 (rng, g, func, data, iterations, &  
 integral, std\_dev, avg\_chi2, accuracy, &  
 channel, weights, grids, exc, history)  
 type(tao\_random\_state), dimension(:), intent(inout) :: rng  
 type(vamp\_grid), intent(inout) :: g  
 class(vamp\_data\_t), intent(in) :: data  
 integer, intent(in) :: iterations  
 real(kind=default), intent(out), optional :: integral, std\_dev, avg\_chi2  
 real(kind=default), intent(in), optional :: accuracy  
 integer, intent(in), optional :: channel  
 real(kind=default), dimension(:), intent(in), optional :: weights  
 type(vamp\_grid), dimension(:), intent(in), optional :: grids  
 type(exception), intent(inout), optional :: exc  
 type(vamp\_history), dimension(:), intent(inout), optional :: history  
*<Interface declaration for func 22>*  
 character(len=\*), parameter :: FN = "vamp\_sample\_grid\_parallel"  
 real(kind=default) :: local\_integral, local\_std\_dev, local\_avg\_chi2  
 type(exception), dimension(size(rng)) :: excs  
 type(vamp\_grid), dimension(:), allocatable :: gs, gx  
 !hpf\$ processors p(number\_of\_processors())  
 !hpf\$ distribute gs(cyclic(1)) onto p  
 integer, dimension(:,:), pointer :: d  
 integer :: iteration, i  
 integer :: num\_workers  
 nullify (d)  
 call clear\_exception (excs)  
 iterate: do iteration = 1, iterations



```

call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
num_workers = max (1, product (d(2,:)))
if (num_workers > 1) then
  allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
  call vamp_create_empty_grid (gs)
  ! vamp_fork_grid is certainly not local. Speed freaks might
  ! want to tune it to the processor topology, but the gain will be small.
  call vamp_fork_grid (g, gs, gx, d, exc)
  !hpf$ independent
  do i = 1, num_workers
    call vamp_sample_grid0 &
      (rng(i), gs(i), func, data, &
       channel, weights, grids, exc)
  end do
  <Gather exceptions in vamp_sample_grid_parallel 104a>
  call vamp_join_grid (g, gs, gx, d, exc)
  call vamp_delete_grid (gs)
  deallocate (gs, gx)
else
  call vamp_sample_grid0 &
    (rng(1), g, func, data, channel, weights, grids, exc)
end if
<Bail out if exception exc raised 99a>
call vamp_average_iterations &
  (g, iteration, local_integral, local_std_dev, local_avg_chi2)
<Trace results of vamp_sample_grid 106b>
<Exit iterate if accuracy has been reached 96b>
if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
deallocate (d)
<Copy results of vamp_sample_grid to dummy variables 96a>
end subroutine vamp_sample_grid_parallel
104a <Gather exceptions in vamp_sample_grid_parallel 104a>≡
  if ((present (exc)) .and. (any (excs(1:num_workers)%level > 0))) then
    call gather_exceptions (exc, excs(1:num_workers))
  end if
104b <Implementation of vamp procedures 78>+≡
  pure subroutine vamp_distribute_work (num_workers, ng, d)

```

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

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

but the gain will be negligible.

```

104b <Implementation of vamp procedures 78>+≡
  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 105a>
end do try
end subroutine vamp_distribute_work
105a <Accept distribution among n workers 105a>≡
    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
105b <Accept distribution among n workers 105a>+≡
    j = 1
    do i = 1, size (ng)
        if (num_forks(i) > 1) then
            d(:,j) = (/ i, num_forks(i) /)
            j = j + 1
        end if
    end do
    return

```

## 5.2.6 Diagnostics

- 106a *⟨Declaration of vamp types 77b⟩*+≡  

```

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

```
- 106b *⟨Trace results of vamp\_sample\_grid 106b⟩*≡  

```

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

```
- 106c *⟨Declaration of vamp procedures 77a⟩*+≡  

```

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

```
- 106d *⟨Interfaces of vamp procedures 95c⟩*+≡  

```

interface vamp_get_history
  module procedure vamp_get_history_single
end interface

```
- 106e *⟨Implementation of vamp procedures 78⟩*+≡  

```

elemental subroutine vamp_create_history (h, ndim, verbose)
  type(vamp_history), intent(out) :: h
  integer, intent(in), optional :: ndim
  logical, intent(in), optional :: verbose
  if (present (verbose)) then
    h%verbose = verbose
  else
    h%verbose = .false.
  end if
  h%calls = 0.0

```

```

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

107a <Implementation of vamp procedures 78>+≡
    elemental subroutine vamp_terminate_history (h)
        type(vamp_history), intent(inout) :: h
        h%calls = 0.0
    end subroutine vamp_terminate_history

107b <Implementation of vamp procedures 78>+≡
    pure subroutine vamp_get_history_single (h, g, integral, std_dev, avg_chi2)
        type(vamp_history), intent(inout) :: h
        type(vamp_grid), intent(in) :: g
        real(kind=default), intent(in) :: integral, std_dev, avg_chi2
        h%calls = g%calls
        h%stratified = g%all_stratified
        h%integral = g%mu(1)
        h%std_dev = sqrt (g%mu(2))
        h%avg_integral = integral
        h%avg_std_dev = std_dev
        h%avg_chi2 = avg_chi2
        h%f_min = g%f_min
        h%f_max = g%f_max
        if (h%verbose) then
            <Adjust h%div iff necessary 107c>
            call copy_history (h%div, summarize_division (g%div))
        end if
    end subroutine vamp_get_history_single

107c <Adjust h%div iff necessary 107c>≡
    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

107d <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
108a <Interfaces of vamp procedures 95c>+≡
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
108b <Implementation of vamp procedures 78>+≡
subroutine vamp_print_one_history (h, tag)
  type(vamp_history), dimension(:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  type(div_history), dimension(:), allocatable :: h_tmp
  character(len=BUFFER_SIZE) :: pfx
  character(len=1) :: s
  integer :: i, imax, j
  if (present (tag)) then
    pfx = tag
  else
    pfx = "[vamp]"
  end if
  print "(1X,A78)", repeat("-", 78)
  print "(1X,A8,1X,A2,A9,A1,1X,A11,1X,8X,1X," &
    // "1X,A13,1X,8X,1X,A5,1X,A5)", &
    pfx, "it", "#calls", "", "integral", "average", "chi2", "eff."
  imax = size (h)
  iterations: do i = 1, imax
    if (h(i)%calls <= 0) then
      imax = i - 1
      exit iterations
    end if
    ! *JR: Skip zero channel
    if (h(i)%f_max==0) cycle
    if (h(i)%stratified) then
      s = "*"
    else
      s = ""
    end if
    print "(1X,A8,1X,I2,I9,A1,1X,E11.4,A1,E8.2,A1," &
      // "1X,E13.6,A1,E8.2,A1,F5.1,1X,F5.3)", pfx, &
      i, h(i)%calls, s, h(i)%integral, "(", h(i)%std_dev, ")", &
      h(i)%avg_integral, "(", h(i)%avg_std_dev, ")", h(i)%avg_chi2, &

```

```

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

```

109a *<Variables in vamp 79a>+≡*  
integer, private, parameter :: BUFFER\_SIZE = 50

109b *<Implementation of vamp procedures 78>+≡*  
subroutine vamp\_print\_histories (h, tag)  
type(vamp\_history), dimension(:,,:), intent(in) :: h  
character(len=\*), intent(in), optional :: tag  
character(len=BUFFER\_SIZE) :: pfx  
integer :: i  
print "(1X,A78)", repeat ("=", 78)  
channels: do i = 1, size (h, dim=2)  
 if (present (tag)) then  
 write (unit = pfx, fmt = "(A4,A1,I3.3)") tag, "#", i  
 else  
 write (unit = pfx, fmt = "(A4,A1,I3.3)") "chan", "#", i  
 end if  
 call vamp\_print\_one\_history (h(:,i), pfx)  
end do channels  
print "(1X,A78)", repeat ("=", 78)  
flush (output\_unit)

```
end subroutine vamp_print_histories
```

 WK

110 *Implementation of vamp procedures 78*  $\rightarrow$

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

```

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

```



### 5.2.7 Multi Channel

[23]

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

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

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

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

Therefore...

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

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

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

112a  $\langle$ Declaration of **vamp** types 77b $\rangle + \equiv$

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

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

112b  $\langle$ Declaration of **vamp** procedures 77a $\rangle + \equiv$

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

113a *<Implementation of vamp procedures 78>+≡*

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

113b *<Implementation of vamp procedures 78>+≡*

```
function vamp_multi_channel0 &
  (func, data, phi, jacobian, x, weights, channel) result (w_x)
  class(vamp_data_t), intent(in) :: data
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in) :: channel
  <Interface declaration for func 22>
  <Interface declaration for phi 31a>
  <Interface declaration for jacobian 31c>
  real(kind=default) :: w_x
  real(kind=default), dimension(size(x)) :: x_prime
  real(kind=default), dimension(size(weights)) :: g_phi_x
```

```

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

```



WK

114a *<Declaration of vamp procedures 77a>+≡*

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

114b *<Implementation of vamp procedures 78>+≡*

```

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

```

```

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

```

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

115 *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

```
end subroutine vamp_check_jacobian
```

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

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

```
private :: numeric_jacobian
```

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

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

116c *⟨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 [9]) even if the dummy argument is optional itself.

117a *Implementation of vamp procedures 78* +=

```
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
```

117b *Implementation of vamp procedures 78* +=

```
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
```

118a *<Declaration of vamp procedures 77a>+≡*  
`public :: vamp_discard_integrals`

118b *<Implementation of vamp procedures 78>+≡*  
`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`

118c *<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:

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

```

end if
if (present (num_calls)) then
    call vamp_discard_integrals (g, num_calls, num_div, &
                                stratified, quadrupole, exc)
else
    call vamp_discard_integrals (g, sum (g%num_calls), num_div, &
                                stratified, quadrupole, exc)
end if
end subroutine vamp_update_weights
119a <Declaration of vamp procedures 77a>+≡
    public :: vamp_reshape_grids
119b <Implementation of vamp procedures 78>+≡
    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
            end do

```



```

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

```

120a *<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.

120b *<Implementation of vamp procedures 78>+≡*

```

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

```

```

endwhere
if (sum (weights) /= 0) weights = weights / sum (weights)
call clear_exception (excs)
iterate: do iteration = 1, iterations
  do ch = 1, size (g%grids)
    if (active(ch)) then
      call vamp_discard_integral (g%grids(ch))
      <Sample the grid g%grids(ch) 121>
    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 124b>
  <Exit iterate if accuracy has been reached 96b>
end do iterate
<Copy results of vamp_sample_grid to dummy variables 96a>
end subroutine vamp_sample_grids

```

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

```

121 <Sample the grid g%grids(ch) 121>≡
  call vamp_sample_grid0 &
    (rng, g%grids(ch), func, data, &
     ch, weights, g%grids, excs(ch), neg_w)
  if (present (exc) .and. present (warn_error)) then
    if (warn_error) call handle_exception (excs(ch))
  end if

```

```

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

```

122a  $\langle$ Declaration of vamp procedures 77a $\rangle + \equiv$   
 public :: vamp\_reduce\_channels

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

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

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

where (5.30b) is actually

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

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

122b  $\langle$ Implementation of vamp procedures 78 $\rangle + \equiv$   
 pure subroutine vamp\_reduce\_channels (g, integrals, std\_devs, active)  
 type(vamp\_grids), intent(inout) :: g  
 real(kind=default), dimension(:), intent(in) :: integrals, std\_devs  
 logical, dimension(:), intent(in) :: active  
 real(kind=default) :: this\_integral, this\_weight, total\_calls  
 real(kind=default) :: total\_variance  
 if (.not.any(active)) return  
 total\_calls = sum (g%num\_calls, mask=active)  
 if (total\_calls > 0) then  
 this\_integral = sum (g%num\_calls \* integrals, mask=active) / total\_calls

```

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

```

123a *<Declaration of vamp procedures 77a>+≡*

```

public :: vamp_refine_weights

```

123b *<Implementation of vamp procedures 78>+≡*

```

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

```

123c *<Declaration of vamp procedures 77a>+≡*

```

private :: vamp_average_iterations_grids

```

123d *<Interfaces of vamp procedures 95c>+≡*

```

interface vamp_average_iterations
    module procedure vamp_average_iterations_grids
end interface

```

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

124a *⟨Implementation of vamp procedures 78⟩*+≡

```
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
```

124b *⟨Trace results of vamp\_sample\_grids 124b⟩*≡

```
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
```

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

```
private :: vamp_get_history_multi
```

124d *⟨Interfaces of vamp procedures 95c⟩*+≡

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

124e *⟨Implementation of vamp procedures 78⟩*+≡

```
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

125a *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_sum\_channels

125b *<Implementation of vamp procedures 78>+≡*  
 function vamp\_sum\_channels (x, weights, func, data, grids) result (g)  
 real(kind=default), dimension(:), intent(in) :: x, weights  
 class(vamp\_data\_t), intent(in) :: data  
 type(vamp\_grid), dimension(:), intent(in), optional :: grids  
 interface  
 function func (xi, data, weights, channel, grids) result (f)  
 use kinds  
 use vamp\_grid\_type !NODEP!  
 import vamp\_data\_t  
 real(kind=default), dimension(:), intent(in) :: xi  
 class(vamp\_data\_t), intent(in) :: data  
 real(kind=default), dimension(:), intent(in), optional :: weights  
 integer, intent(in), optional :: channel  
 type(vamp\_grid), dimension(:), intent(in), optional :: grids  
 real(kind=default) :: f  
 end function func  
 end interface  
 real(kind=default) :: g  
 integer :: ch  
 g = 0.0  
 do ch = 1, size (weights)  
 g = g + weights(ch) \* func (x, data, weights, ch, grids)  
 end do  
end function vamp\_sum\_channels

### 5.2.8 Mapping

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

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

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

where

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

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

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

After call `diagonalize_real_symmetric (cov, evals, evecs)`, we have `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 isotropic in these directions. In this case the benefit from the rotation is rather small and offset by the negative effects from the misalignment of the integration region.

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

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

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

```

126a <Declaration of vamp procedures 77a>+≡
    public :: select_rotation_axis
    public :: select_rotation_subspace

126b <Set iv to the index of the optimal eigenvector 126b>≡
    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
end if

```

127a *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

127b *⟨Declaration of vamp procedures 77a⟩*+≡

```

private :: more_pancake_than_cigar

```

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

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



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

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

```
abs_evec = abs (evecs(:,iv))
i(1) = sum (maxloc (abs_evec))
abs_evec(i(1)) = -1.0
i(2) = sum (maxloc (abs_evec))
```

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

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

```
abs_evec = abs (evecs(:,iv))
i(1) = sum (maxloc (abs_evec))
i(2) = sum (maxloc (abs_evec, mask = abs_evec < abs_evec(i(1))))
```

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

```
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)
```

128d  $\langle$ Get  $\cos \theta$  and  $\sin \theta$  from evecs 128d $\rangle \equiv$

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

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

128e  $\langle$ Construct  $\hat{R}(\theta; i, j)$  128e $\rangle \equiv$

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

128f  $\langle$ Implementation of vamp procedures 78 $\rangle + \equiv$

```
subroutine select_rotation_axis (cov, r, pancake, cigar)
  real(kind=default), dimension(:, :), intent(in) :: cov
  real(kind=default), dimension(:, :), intent(out) :: r
```

---

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

```

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 129a>
call diagonalize_real_symmetric (cov, evals, evecs)
<Set iv to the index of the optimal eigenvector 126b>
<Set i(1), i(2) to the axes of the optimal plane 128a>
<Get cos  $\theta$  and sin  $\theta$  from evecs 128d>
<Construct  $\hat{R}(\theta; i, j)$  128e>
end subroutine select_rotation_axis
129a <Handle optional pancake and cigar 129a>≡
  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:

```

129b <Implementation of vamp procedures 78>+≡
  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
129c <Implementation of vamp procedures 78>+≡

```

```

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 129a>
  call diagonalize_real_symmetric (cov, evals, evecs)
  <Set iv to the index of the optimal eigenvector 126b>
  <Set subspace to the axes of the optimal plane 130a>
  call select_subspace_explicit (cov, r, subspace)
end subroutine select_subspace_guess

130a <Set subspace to the axes of the optimal plane 130a>≡
  abs_evec = abs (evecs(:,iv))
  subspace(1) = sum (maxloc (abs_evec))
  do i = 2, ndim
    abs_evec(subspace(i-1)) = -1.0
    subspace(i) = sum (maxloc (abs_evec))
  end do

130b <Interfaces of vamp procedures 95c>+≡
  interface select_rotation_subspace
    module procedure select_subspace_explicit, select_subspace_guess
  end interface

130c <Declaration of vamp procedures 77a>+≡
  private :: select_subspace_explicit
  private :: select_subspace_guess

130d <Declaration of vamp procedures 77a>+≡
  public :: vamp_print_covariance

130e <Implementation of vamp procedures 78>+≡
  subroutine vamp_print_covariance (cov)
    real(kind=default), dimension(:,:), intent(in) :: cov
    real(kind=default), dimension(size(cov,dim=1)) :: &
      evals, abs_evals, tmp
    real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: &
      evecs, abs_evecs
    integer, dimension(size(cov,dim=1)) :: idx

```

```

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

```

### *Condensing Eigenvalues*

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

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

```

! private :: condense
public :: condense

```

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



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

132a  $\langle \text{Initialize clusters 132a} \rangle \equiv$   
`cl_pos = x`  
`cl_num = size (cl_pos)`  
`cl = spread ((/ (i, i=1,cl_num) /), dim = 2, ncopies = 2)`

It appears that the logarithmic metric

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

performs better than the linear metric

$$d_1(x, y) = |x - y| \quad (5.37b)$$

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

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

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

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

132b  $\langle \text{Join closest clusters 132b} \rangle \equiv$   
`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)`

132c  $\langle \text{Join closest clusters 132b} \rangle + \equiv$   
`cl_pos(gap+1:cl_num-1) = cl_pos(gap+2:cl_num)`  
`cl(gap+1:cl_num-1,:) = cl(gap+2:cl_num,:)`

132d  $\langle \text{Implementation of vamp procedures 78} \rangle + \equiv$   
`subroutine condense (x, cluster_pos, clusters, linear)`  
`real(kind=default), dimension(:), intent(in) :: x`  
`real(kind=default), dimension(:), intent(out) :: cluster_pos`  
`integer, dimension(:,:), intent(out) :: clusters`  
`logical, intent(in), optional :: linear`

```

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

```

133a *<Declaration of vamp procedures 77a>*+≡  
! private :: condense\_action  
public :: condense\_action

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

133b *<Implementation of vamp procedures 78>*+≡  
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

133c *<ctest.f90 133c>*≡  
program ctest  
 use kinds  
 use utils  
 use vamp\_stat  
 use tao\_random\_numbers

```

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

```

### 5.2.9 Event Generation

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

134a *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_next\_event

134b *<Interfaces of vamp procedures 95c>+≡*  
 interface vamp\_next\_event  
 module procedure vamp\_next\_event\_single, vamp\_next\_event\_multi  
 end interface

134c *<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.

134d *<Implementation of vamp procedures 78>+≡*

```

subroutine vamp_next_event_single &
  (x, rng, g, func, data, &
   weight, channel, weights, grids, exc)
  real(kind=default), dimension(:), intent(out) :: x
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grid), intent(inout) :: g
  real(kind=default), intent(out), optional :: weight
  class(vamp_data_t), intent(in) :: data
  integer, intent(in), optional :: channel
  real(kind=default), dimension(:), intent(in), optional :: weights
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  type(exception), intent(inout), optional :: exc
  <Interface declaration for func 22>
  character(len=*), parameter :: FN = "vamp_next_event_single"
  real(kind=default), dimension(size(g%div)):: wgts
  real(kind=default), dimension(size(g%div)):: r
  integer, dimension(size(g%div)):: ia
  real(kind=default) :: f, wgt
  real(kind=default) :: r0
  rejection: do
    <Choose a x and calculate f(x) 135a>
    if (present (weight)) then
      <Unconditionally accept weighted event 135b>
    else
      <Maybe accept unweighted event 135c>
    end if
  end do rejection
end subroutine vamp_next_event_single

135a <Choose a x and calculate f(x) 135a>≡
  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 88c>
  ! call record_efficiency (g%div, ia, f/g%f_max)

135b <Unconditionally accept weighted event 135b>≡
  weight = f
  exit rejection

135c <Maybe accept unweighted event 135c>≡

```



```

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

```

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

$$f(x) = \sum_i \alpha_i g_i(x) w(x) \quad (5.39)$$

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

136 *<Implementation of vamp procedures 78>+≡*

```

subroutine vamp_next_event_multi &
  (x, rng, g, func, data, phi, weight, excess, exc)
  real(kind=default), dimension(:), intent(out) :: x
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grids), intent(inout) :: g
  class(vamp_data_t), intent(in) :: data
  real(kind=default), intent(out), optional :: weight
  real(kind=default), intent(out), optional :: excess
  type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>
<Interface declaration for phi 31a>
  character(len=*), parameter :: FN = "vamp_next_event_multi"
  real(kind=default), dimension(size(x)) :: xi
  real(kind=default) :: r, wgt
  real(kind=default), dimension(size(g%weights)) :: weights
  integer :: channel
<weights:  $\alpha_i \rightarrow w_{\max,i} \alpha_i$  137a>
  rejection: do
    <Select channel from weights 137b>
    call vamp_next_event_single &
      (xi, rng, g%grids(channel), func, data, wgt, &
       channel, g%weights, g%grids, exc)
    if (present (weight)) then
      <Unconditionally accept weighted multi channel event 137c>

```

```

else
    ⟨Maybe accept unweighted multi channel event 137d⟩
end if
end do rejection
x = phi (xi, channel)
end subroutine vamp_next_event_multi

```

We can either reject with the weights

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

after using the apriori weights  $\alpha_i$  to select a channel  $i$  or we can reject with the weights

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

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

```

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

137b ⟨Select channel from weights 137b⟩≡
    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

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

137d ⟨Maybe accept unweighted multi channel event 137d⟩≡
    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

```

138a *<Maybe accept unweighted multi channel event (old version) 138a>≡*

```

if (wgt > g%grids(channel)%f_max) then
    g%grids(channel)%f_max = wgt
    <weights:  $\alpha_i \rightarrow w_{\max,i}\alpha_i$  137a>
    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.

138b *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_warmup\_grid, vamp\_warmup\_grids

138c *<Implementation of vamp procedures 78>+≡*  
 subroutine vamp\_warmup\_grid &  
 (rng, g, func, data, iterations, exc, history)  
 type(tao\_random\_state), intent(inout) :: rng  
 type(vamp\_grid), intent(inout) :: g  
 class(vamp\_data\_t), intent(in) :: data  
 integer, intent(in) :: iterations  
 type(exception), intent(inout), optional :: exc  
 type(vamp\_history), dimension(:), intent(inout), optional :: history  
*<Interface declaration for func 22>*

```

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

```



WHERE ... END WHERE alert!

139a *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

### 5.2.10 Convenience Routines

139b *⟨Declaration of vamp procedures 77a⟩*+≡

```

public :: vamp_integrate
private :: vamp_integrate_grid, vamp_integrate_region

140a <Interfaces of vamp procedures 95c>+≡
interface vamp_integrate
    module procedure vamp_integrate_grid, vamp_integrate_region
end interface

140b <Implementation of vamp procedures 78>+≡
subroutine vamp_integrate_grid &
    (rng, g, func, data, calls, integral, std_dev, avg_chi2, num_div, &
     stratified, quadrupole, accuracy, exc, history)
type(tao_random_state), intent(inout) :: rng
type(vamp_grid), intent(inout) :: g
class(vamp_data_t), intent(in) :: data
integer, dimension(:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_integrate_grid"
integer :: step, last_step, it
last_step = size (calls, dim = 2)
it = 1
do step = 1, last_step - 1
    call vamp_discard_integral (g, calls(2,step), num_div, &
                               stratified, quadrupole, exc = exc)
    call vamp_sample_grid (rng, g, func, data, calls(1,step), &
                           exc = exc, history = history(it:))
    <Bail out if exception exc raised 99a>
    it = it + calls(1,step)
end do
call vamp_discard_integral (g, calls(2,last_step), exc = exc)
call vamp_sample_grid (rng, g, func, data, calls(1,last_step), &
                       integral, std_dev, avg_chi2, accuracy, exc = exc, &
                       history = history(it:))
end subroutine vamp_integrate_grid

140c <Implementation of vamp procedures 78>+≡
subroutine vamp_integrate_region &
    (rng, region, func, data, calls, &
     integral, std_dev, avg_chi2, num_div, &

```

```

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

141a <Declaration of vamp procedures 77a>+≡
    public :: vamp_integratex
    private :: vamp_integratex_region

141b <Interfaces of vamp procedures 95c>+≡
    interface vamp_integratex
        module procedure vamp_integratex_region
    end interface

141c <Implementation of vamp procedures 78>+≡
    subroutine vamp_integratex_region &
        (rng, region, func, data, calls, integral, std_dev, avg_chi2, &
         num_div, stratified, quadrupole, accuracy, pancake, cigar, &
         exc, history)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region

```

```

class(vamp_data_t), intent(in) :: data
integer, dimension(:,:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: pancake, cigar
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
real(kind=default), dimension(size(region,dim=2)) :: eval
real(kind=default), dimension(size(region,dim=2),size(region,dim=2)) :: evec
type(vamp_grid) :: g
integer :: step, last_step, it
it = 1
call vamp_create_grid &
    (g, region, calls(2,1,1), num_div, &
    stratified, quadrupole, covariance = .true., exc = exc)
call vamp_integrate_grid &
    (rng, g, func, data, calls(:, :, 1), num_div = num_div, &
    exc = exc, history = history(it:))
<Bail out if exception exc raised 99a>
it = it + sum (calls(1, :, 1))
last_step = size (calls, dim = 3)
do step = 2, last_step - 1
    call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
    call sort (eval, evec)
    call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
    call vamp_delete_grid (g)
    call vamp_create_grid &
        (g, region, calls(2,1,step), num_div, stratified, quadrupole, &
        covariance = .true., map = evec, exc = exc)
    call vamp_integrate_grid &
        (rng, g, func, data, calls(:, :, step), num_div = num_div, &
        exc = exc, history = history(it:))
    <Bail out if exception exc raised 99a>
    it = it + sum (calls(1, :, step))
end do
call diagonalize_real_symmetric (vamp_get_covariance(g), eval, evec)
call sort (eval, evec)
call select_rotation_axis (vamp_get_covariance(g), evec, pancake, cigar)
call vamp_delete_grid (g)
call vamp_create_grid &

```

```

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

```

### 5.2.11 I/O

143a *<Declaration of vamp procedures 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

```

143b *<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

```

143c *<Interfaces of vamp procedures 95c>+≡*

```

interface vamp_write_grid
    module procedure write_grid_unit, write_grid_name
end interface
interface vamp_read_grid
    module procedure read_grid_unit, read_grid_name
end interface
interface vamp_write_grids
    module procedure write_grids_unit, write_grids_name
end interface
interface vamp_read_grids
    module procedure read_grids_unit, read_grids_name
end interface

```



144a *<Interfaces of vamp procedures 95c>+≡*

```
interface vamp_write_grid_raw
  module procedure write_grid_raw_unit, write_grid_raw_name
end interface
interface vamp_read_grid_raw
  module procedure read_grid_raw_unit, read_grid_raw_name
end interface
interface vamp_write_grids_raw
  module procedure write_grids_raw_unit, write_grids_raw_name
end interface
interface vamp_read_grids_raw
  module procedure read_grids_raw_unit, read_grids_raw_name
end interface
```

144b *<Implementation of vamp procedures 78>+≡*

```
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

```

145a *<Variables in vamp 79a>+≡*

```

character(len=*), parameter, private :: &
    descr_fmt =          "(1x,a)", &
    integer_fmt =        "(1x,a17,1x,i15)", &
    integer_array_fmt =  "(1x,i17,1x,i15)", &
    logical_fmt =        "(1x,a17,1x,l1)", &
    double_fmt =         "(1x,a17,1x,e30.22e4)", &
    double_array_fmt =   "(1x,i17,1x,e30.22e4)", &
    double_array2_fmt =  "(2(1x,i8),1x,e30.22e4)"

```

145b *<Implementation of vamp procedures 78>+≡*

```

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 147a>
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. 147b>
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. 148a>
end if
read (unit = unit, fmt = descr_fmt) chdum
end subroutine read_grid_unit

147a <Insure that size (g%div) == ndim 147a>≡
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

147b <Insure that associated (g%map) == .false. 147b>≡
if (associated (g%map)) then
    deallocate (g%map)

```

```

        end if
148a  <Insure that associated (g%mu_x) == .false. 148a>≡
        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
148b  <Implementation of vamp procedures 78>+≡
        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
148c  <Implementation of vamp procedures 78>+≡
        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
148d  <Implementation of vamp procedures 78>+≡
        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

```

149 *⟨Implementation of vamp procedures 78⟩*+≡

```

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
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

```

150a *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

150b *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

151 *<Implementation of vamp procedures 78>+≡*

```

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
  end if

```



```

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

```

152a *<Constants in vamp 152a>*≡

```

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

```

152b *<Implementation of vamp procedures 78>*+≡

```

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 147a>
  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. 147b⟩
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
end if

```

```

        end do
    end do
else if (magic == MAGIC_GRID_EMPTY) then
    <Insure that associated (g%mu_x) == .false. 148a>
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

154a <Implementation of vamp procedures 78>+≡
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

154b <Implementation of vamp procedures 78>+≡
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

154c <Implementation of vamp procedures 78>+≡
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

```

155a *<Constants in vamp 152a>+≡*

```

integer, parameter, private :: MAGIC_GRIDS = 33333333
integer, parameter, private :: MAGIC_GRIDS_BEGIN = MAGIC_GRIDS + 1
integer, parameter, private :: MAGIC_GRIDS_END = MAGIC_GRIDS + 2

```

155b *<Implementation of vamp procedures 78>+≡*

```

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

```

156a *⟨Implementation of vamp procedures 78⟩*+≡

```

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

```

156b *⟨Implementation of vamp procedures 78⟩*+≡

```

subroutine read_grids_raw_name (g, name, read_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: read_integrals
    integer :: unit

```

```

call find_free_unit (unit)
open (unit = unit, action = "read", status = "old", &
      form = "unformatted", file = name)
call read_grids_raw_unit (g, unit, read_integrals)
close (unit = unit)
end subroutine read_grids_raw_name

```

### 5.2.12 Marshaling

157a *<Declaration of vamp procedures 77a>+≡*  
 public :: vamp\_marshall\_grid\_size, vamp\_marshall\_grid, vamp\_unmarshal\_grid

157b *<Implementation of vamp procedures 78>+≡*  
 pure subroutine vamp\_marshall\_grid (g, ibuf, dbuf)  
 type(vamp\_grid), intent(in) :: g  
 integer, dimension(:), intent(inout) :: ibuf  
 real(kind=default), dimension(:), intent(inout) :: dbuf  
 integer :: i, iwords, dwords, iidx, didx, ndim  
 ndim = size (g%div)  
 ibuf(1) = g%num\_calls  
 ibuf(2) = g%calls\_per\_cell  
 ibuf(3) = ndim  
 if (g%stratified) then  
 ibuf(4) = 1  
 else  
 ibuf(4) = 0  
 end if  
 if (g%all\_stratified) then  
 ibuf(5) = 1  
 else  
 ibuf(5) = 0  
 end if  
 if (g%quadrupole) then  
 ibuf(6) = 1  
 else  
 ibuf(6) = 0  
 end if  
 dbuf(1:2) = g%mu  
 dbuf(3) = g%sum\_integral  
 dbuf(4) = g%sum\_weights  
 dbuf(5) = g%sum\_chi2  
 dbuf(6) = g%calls  
 dbuf(7) = g%dv2g

```

dbuf(8) = g%jacobi
dbuf(9) = g%f_min
dbuf(10) = g%f_max
dbuf(11) = g%mu_gi
dbuf(12) = g%sum_mu_gi
ibuf(7:6+ndim) = g%num_div
iidx = 7 + ndim
didx = 13
do i = 1, ndim
  call marshal_division_size (g%div(i), iwords, dwords)
  ibuf(iidx) = iwords
  ibuf(iidx+1) = dwords
  iidx = iidx + 2
  call marshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
                        dbuf(didx:didx-1+dwords))

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

```

158 *⟨Implementation of vamp procedures 78⟩*+≡

```
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

```

159 *⟨Implementation of vamp procedures 78⟩+≡*

```

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 147a>
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. 147b>
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. 148a>
end if
iidx = iidx + 1
end subroutine vamp_unmarshal_grid
160a <Declaration of vamp procedures 77a>+≡
public :: vamp_marshal_history_size, vamp_marshal_history
public :: vamp_unmarshal_history
160b <Implementation of vamp procedures 78>+≡
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

```

161 *⟨Implementation of vamp procedures 78⟩+≡*

```

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

```

162 *⟨Implementation of vamp procedures 78⟩+≡*

```

pure subroutine vamp_unmarshal_history (h, ibuf, dbuf)
    type(vamp_history), intent(inout) :: h
    integer, dimension(:), intent(in) :: ibuf
    real(kind=default), dimension(:), intent(in) :: dbuf
    integer :: j, ndim, iidx, didx, iwords, dwords
    ndim = ibuf(1)
    h%calls = ibuf(2)
    h%stratified = ibuf(3) /= 0
    h%integral = dbuf(1)
    h%std_dev = dbuf(2)
    h%avg_integral = dbuf(3)
    h%avg_std_dev = dbuf(4)
    h%avg_chi2 = dbuf(5)
    h%f_min = dbuf(6)
    h%f_max = dbuf(7)
    if (ndim > 0) then
        if (associated (h%div)) then
            if (size (h%div) /= ndim) then
                deallocate (h%div)
                allocate (h%div(ndim))
            end if
        else
            allocate (h%div(ndim))
        end if
        iidx = 4
        didx = 8
        do j = 1, ndim
            iwords = ibuf(iidx)
            dwords = ibuf(iidx+1)
            iidx = iidx + 2
            call unmarshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                                     dbuf(didx:didx-1+dwords))

```

```

        iidx = iidx + iwords
        didx = didx + dwords
    end do
end if
end subroutine vamp_unmarshal_history

```

### 5.2.13 Boring Copying and Deleting of Objects

163 *<Implementation of vamp procedures 78>+≡*

```

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)
    end if
end subroutine vamp_copy_grid

```

```

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

```

164a *<Implementation of vamp procedures 78>+≡*

```

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

```

164b *<Implementation of vamp procedures 78>+≡*

```

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

```

165a *⟨Implementation of vamp procedures 78⟩*+≡

```

    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

```

165b *⟨Implementation of vamp procedures 78⟩*+≡

```

    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

```

```

166a <Implementation of vamp procedures 78>+≡
      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 re-define them:

```

166b <vampi.f90 166b>≡
      ! vampi.f90 --
      <Copyleft notice 1>
      module vamp_serial_mpi
        use vamp, &
          <vamp0_* => vamp_* 167c>
          VAMPO_RCS_ID => VAMP_RCS_ID
        public
      end module vamp_serial_mpi

```

`vamp_parallel_mpi` contains the non trivial MPI code and will be discussed in detail below.

```

166c <vampi.f90 166b>+≡
      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 167b>
  <Interfaces of vampi procedures 171d>
  <Parameters in vampi 168a>
  <Declaration of vampi types 172b>
  character(len=*), public, parameter :: VAMPI_RCS_ID = &
    "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of vampi procedures 167d>
end module vamp_parallel_mpi

```

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

```

167a <vampi.f90 166b>+≡
  module vampi
    use vamp_serial_mpi !NODEP!
    use vamp_parallel_mpi !NODEP!
    public
  end module vampi

```

### 5.3.1 Parallel Execution

#### Single Channel

```

167b <Declaration of vampi procedures 167b>≡
  public :: vamp_create_grid
  public :: vamp_discard_integral
  public :: vamp_reshape_grid
  public :: vamp_sample_grid
  public :: vamp_delete_grid

167c <vamp0_* => vamp_* 167c>≡
  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, &

167d <Implementation of vampi procedures 167d>≡
  subroutine vamp_create_grid &
    (g, domain, num_calls, num_div, &
     stratified, quadrupole, covariance, map, exc)
    type(vamp_grid), intent(inout) :: g
  end subroutine

```



```

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

168a <Parameters in vampi 168a>≡
integer, public, parameter :: VAMP_ROOT = 0

168b <Implementation of vampi procedures 167d>+≡
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

168c <Implementation of vampi procedures 167d>+≡
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.

169 *<Implementation of vampi procedures 167d>+≡*

```

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
171a <Implementation of vampi procedures 167d>+≡
    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
171b <Declaration of vampi procedures 167b>+≡
    public :: vamp_print_history
    private :: vamp_print_one_history, vamp_print_histories
171c <vamp0_* => vamp_* 167c>+≡
    vamp0_print_history => vamp_print_history, &
171d <Interfaces of vampi procedures 171d>≡
    interface vamp_print_history
        module procedure vamp_print_one_history, vamp_print_histories
    end interface
171e <Implementation of vampi procedures 167d>+≡
    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

```

172a *⟨Implementation of vampi procedures 167d⟩*+≡

```

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*

172b *⟨Declaration of vampi types 172b⟩*≡

```

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

```

172c *⟨vamp0\_\* => vamp\_\* 167c⟩*+≡

```

vamp0_grids => vamp_grids, &

```

Partially duplicate the API of vamp:

172d *⟨Declaration of vampi procedures 167b⟩*+≡

```

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

```

172e *⟨vamp0\_\* => vamp\_\* 167c⟩*+≡

```

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

173a *⟨Implementation of vampi procedures 167d⟩+≡*

```

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

```

173b *⟨Implementation of vampi procedures 167d⟩+≡*

```

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
174a <Implementation of vampi procedures 167d>+≡
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
174b <Implementation of vampi procedures 167d>+≡
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
174c <Implementation of vampi procedures 167d>+≡
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.
174d <Implementation of vampi procedures 167d>+≡
subroutine vamp_sample_grids &
    (rng, g, func, iterations, integral, std_dev, avg_chi2, &
    accuracy, history, histories, exc)
type(tao_random_state), intent(inout) :: rng

```

```

type(vamp_grids), intent(inout) :: g
integer, intent(in) :: iterations
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
real(kind=default), intent(in), optional :: accuracy
type(vamp_history), dimension(:), intent(inout), optional :: history
type(vamp_history), dimension(:, :), intent(inout), optional :: histories
type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_sample_grids"
integer :: num_proc, proc_id, nch, ch, iteration
real(kind=default), dimension(size(g%g0%weights)) :: weights
real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
real(kind=default) :: current_accuracy, waste
logical :: distribute_complete_grids
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
nch = size (g%g0%weights)
if (proc_id == VAMP_ROOT) then
    g%active = (g%g0%num_calls >= 2)
    where (g%active)
        weights = g%g0%num_calls
    elsewhere
        weights = 0.0
    endwhere
    weights = weights / sum (weights)
    call schedule (weights, num_proc, g%proc, waste)
    distribute_complete_grids = (waste <= VAMP_MAX_WASTE)
end if
call mpi90_broadcast (weights, VAMP_ROOT)
call mpi90_broadcast (g%active, VAMP_ROOT)
call mpi90_broadcast (distribute_complete_grids, VAMP_ROOT)
if (distribute_complete_grids) then
    call mpi90_broadcast (g%proc, VAMP_ROOT)
end if
iterate: do iteration = 1, iterations
    if (distribute_complete_grids) then
        call vamp_broadcast_grid (g%g0%grids, VAMP_ROOT)
        <Distribute complete grids among processes 176b>
    else
        <Distribute each grid among processes 180b>
    end if
    <Exit iterate if accuracy has been reached (MPI) 179a>
end do iterate

```



```

    <Copy results of vamp_sample_grids to dummy variables 178e>
end subroutine vamp_sample_grids
Setting VAMP_MAX_WASTE to 1 disables the splitting of grids, which doesn't
work yet.
176a <Parameters in vampi 168a>+≡
    real(kind=default), private, parameter :: VAMP_MAX_WASTE = 1.0
    ! real(kind=default), private, parameter :: VAMP_MAX_WASTE = 0.3
176b <Distribute complete grids among processes 176b>≡
    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) 176d>
            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:

```

176c <Distribute complete grids among processes 176b>+≡
    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 177c>
            end if
        end if
    end do

```

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

```

176d <Sample g%g0%grids(ch) 176d>≡
    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

177a <Distribute complete grids among processes 176b>+≡
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 178a>
        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:

177b <Ship g%g0%grids from the root to the assigned processor 177b>≡
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

177c <Ship the result for channel #ch back to the root 177c>≡
call mpi90_send (g%integrals(ch), VAMP_ROOT, object (ch, TAG_INTEGRAL))
call mpi90_send (g%std_devs(ch), VAMP_ROOT, object (ch, TAG_STD_DEV))

```

```

call vamp_send_grid (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
if (present (histories)) then
    call vamp_send_history &
        (histories(iteration,ch), VAMP_ROOT, object (ch, TAG_HISTORY))
end if

178a <Receive the result for channel #ch at the root 178a>≡
call mpi90_receive (g%integrals(ch), g%proc(ch), object (ch, TAG_INTEGRAL))
call mpi90_receive (g%std_devs(ch), g%proc(ch), object (ch, TAG_STD_DEV))
call vamp_receive_grid (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
if (present (histories)) then
    call vamp_receive_history &
        (histories(iteration,ch), g%proc(ch), object (ch, TAG_HISTORY))
end if

178b <Declaration of vampi procedures 167b>+≡
private :: object

178c <Implementation of vampi procedures 167d>+≡
pure function object (ch, obj) result (tag)
    integer, intent(in) :: ch, obj
    integer :: tag
    tag = 100 * ch + obj
end function object

178d <Parameters in vampi 168a>+≡
integer, public, parameter :: &
    TAG_INTEGRAL = 1, &
    TAG_STD_DEV = 2, &
    TAG_GRID = 3, &
    TAG_HISTORY = 6, &
    TAG_NEXT_FREE = 9

178e <Copy results of vamp_sample_grids to dummy variables 178e>≡
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

```

179a *<Exit iterate if accuracy has been reached (MPI) 179a>*≡

```

    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
end if

```

A very simple minded scheduler: maximizes processor utilization and, does not pay attention to communication costs.

179b *<Declaration of vampi procedures 167b>*+≡

```

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.

179c *<Implementation of vampi procedures 167d>*+≡

```

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 180a>
end subroutine schedule

```

Assuming equivalent processors and uniform computation costs, the waste is

given by the fraction of the time that it spent by the other processors waiting for the processor with the biggest assignment:

180a *⟨Estimate waste of processor time 180a⟩*≡  
 if (present (waste)) then  
   waste = 1.0 - sum (fill) / (num\_procs \* maxval (fill))  
end if

Accordingly, if the waste caused by distributing only complete grids, we switch to splitting the grids, just like in single channel sampling. This is *not* the default, because the communication costs are measurably higher for many grids and many processors.



This version is broken!

180b *⟨Distribute each grid among processes 180b⟩*≡  
 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 ...

```

181a <Declaration of vampi procedures 167b>+≡
    public :: vamp_warmup_grid
    public :: vamp_warmup_grids
    public :: vamp_next_event
    private :: vamp_next_event_single, vamp_next_event_multi

181b <vamp0_* => vamp_* 167c>+≡
    vamp0_warmup_grid => vamp_warmup_grid, &
    vamp0_warmup_grids => vamp_warmup_grids, &
    vamp0_next_event => vamp_next_event, &

181c <Interfaces of vampi procedures 171d>+≡
    interface vamp_next_event
        module procedure vamp_next_event_single, vamp_next_event_multi
    end interface

181d <Implementation of vampi procedures 167d>+≡
    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

```

182a *<Implementation of vampi procedures 167d>+≡*

```
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
```

182b *<Implementation of vampi procedures 167d>+≡*

```
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
```

182c *<Implementation of vampi procedures 167d>+≡*

```
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

- 183a *<Declaration of vampi procedures 167b>+≡*
- ```

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

```
- 183b *<vamp0\_\* => vamp\_\* 167c>+≡*
- ```

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

```
- 183c *<Interfaces of vampi procedures 171d>+≡*
- ```

    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

```
- 183d *<Implementation of vampi procedures 167d>+≡*
- ```

    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

```
- 183e *<Implementation of vampi procedures 167d>+≡*
- ```

    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

```



```

184a  <Implementation of vampi procedures 167d>+≡
      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

184b  <Implementation of vampi procedures 167d>+≡
      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

184c  <Declaration of vampi procedures 167b>+≡
      public :: vamp_write_grids, vamp_read_grids
      private :: write_grids_unit, write_grids_name
      private :: read_grids_unit, read_grids_name

184d  <vamp0_* => vamp_* 167c>+≡
      vamp0_write_grids => vamp_write_grids, &
      vamp0_read_grids => vamp_read_grids, &

184e  <Interfaces of vampi procedures 171d>+≡
      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

184f  <Implementation of vampi procedures 167d>+≡
      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

```

185a *⟨Implementation of vampi procedures 167d⟩*+≡

```

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

```

185b *⟨Implementation of vampi procedures 167d⟩*+≡

```

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

```

185c *⟨Implementation of vampi procedures 167d⟩*+≡

```

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

185d *⟨Declaration of vampi procedures 167b⟩*+≡

```

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`:

186a *<Implementation of vampi procedures 167d>+≡*

```

subroutine vamp_send_grid (g, target, tag, domain, error)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: target, tag
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call vamp_marshall_grid_size (g, words(1), words(2))
  allocate (ibuf(words(1)), dbuf(words(2)))
  call vamp_marshall_grid (g, ibuf, dbuf)
  call mpi90_send (words, target, tag, domain, error)
  call mpi90_send (ibuf, target, tag+1, domain, error)
  call mpi90_send (dbuf, target, tag+2, domain, error)
  deallocate (ibuf, dbuf)
end subroutine vamp_send_grid

```

186b *<Implementation of vampi procedures 167d>+≡*

```

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_unmarshall_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`:

187a *Implementation of vampi procedures (doesn't work with MPICH yet)* 187a)≡

```
subroutine vamp_send_grid (g, target, tag, domain, error)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: target, tag
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: iwords, dwords
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call vamp_marshall_grid_size (g, iwords, dwords)
  allocate (ibuf(iwords), dbuf(dwords))
  call vamp_marshall_grid (g, ibuf, dbuf)
  call mpi90_send (ibuf, target, tag, domain, error)
  call mpi90_send (dbuf, target, tag+1, domain, error)
  deallocate (ibuf, dbuf)
end subroutine vamp_send_grid
```

⚠ There's something wrong with MPICH: if I call `mpi90_receive_pointer` in the opposite order, the low level call to `mpi_get_count` bombs for no apparent reason!

⚠ There are also funky things going on with tag: `mpi90_receive_pointer` should leave it alone, but ...

187b *Implementation of vampi procedures (doesn't work with MPICH yet)* 187a)+≡

```
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_unmarshall_grid (g, ibuf, dbuf)
  deallocate (ibuf, dbuf)
end subroutine vamp_receive_grid
```

This is not a good idea, with respect to communication costs. For SMP machines, it appears to be negligible however.

188a *⟨Interfaces of vampi procedures 171d⟩+≡*

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

188b *⟨Implementation of vampi procedures 167d⟩+≡*

```
subroutine vamp_broadcast_one_grid (g, root, domain, error)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  integer :: iwords, dwords, me
  call mpi90_rank (me)
  if (me == root) then
    call vamp_marshall_grid_size (g, iwords, dwords)
  end if
  call mpi90_broadcast (iwords, root, domain, error)
  call mpi90_broadcast (dwords, root, domain, error)
  allocate (ibuf(iwords), dbuf(dwords))
  if (me == root) then
    call vamp_marshall_grid (g, ibuf, dbuf)
  end if
  call mpi90_broadcast (ibuf, root, domain, error)
  call mpi90_broadcast (dbuf, root, domain, error)
  if (me /= root) then
    call vamp_unmarshal_grid (g, ibuf, dbuf)
  end if
  deallocate (ibuf, dbuf)
end subroutine vamp_broadcast_one_grid
```

188c *⟨Implementation of vampi procedures 167d⟩+≡*

```
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

```

189a *⟨Implementation of vampi procedures 167d⟩+≡*

```

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

```

189b *⟨Declaration of vampi procedures 167b⟩+≡*

```

public :: vamp_send_history
public :: vamp_receive_history

```

189c *⟨Implementation of vampi procedures 167d⟩+≡*

```

subroutine vamp_send_history (g, target, tag, domain, error)

```

```

type(vamp_history), intent(in) :: g
integer, intent(in) :: target, tag
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
integer, dimension(2) :: words
integer, dimension(:), allocatable :: ibuf
real(kind=default), dimension(:), allocatable :: dbuf
call vamp_marshall_history_size (g, words(1), words(2))
allocate (ibuf(words(1)), dbuf(words(2)))
call vamp_marshall_history (g, ibuf, dbuf)
call mpi90_send (words, target, tag, domain, error)
call mpi90_send (ibuf, target, tag+1, domain, error)
call mpi90_send (dbuf, target, tag+2, domain, error)
deallocate (ibuf, dbuf)
end subroutine vamp_send_history

```

190 *⟨Implementation of vampi procedures 167d⟩*+≡

```

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

```

## —6— SELF TEST

### 6.1 No Mapping Mode

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

#### 6.1.1 Serial Test

```
191a <vamp_test.f90 191a>≡
      ! vamp_test.f90 --
      <Copyleft notice 1>
      <Module vamp_test_functions 191b>
      <Module vamp_tests 195b>

191b <Module vamp_test_functions 191b>≡
      module vamp_test_functions
        use kinds
        use constants, only: PI
        use coordinates
        use vamp, only: vamp_grid, vamp_multi_channel
        use vamp, only: vamp_data_t
        implicit none
        private
        public :: f, j, phi, ihp, w
        public :: lorentzian
        private :: lorentzian_normalized
        real(kind=default), public :: width
      contains
        <Implementation of vamp_test_functions procedures 192a>
```



$$\begin{aligned} &\text{end module vamp\_test\_functions} \\ &\int_{x_1}^{x_2} dx \frac{1}{(x - x_0)^2 + a^2} = \frac{1}{a} \left( \text{atan} \left( \frac{x_2 - x_0}{a} \right) - \text{atan} \left( \frac{x_1 - x_0}{a} \right) \right) = N(x_0, x_1, x_2, a) \end{aligned} \quad (6.1)$$

192a  $\langle$ Implementation of vamp\_test\_functions procedures 192a $\rangle \equiv$

```

pure function lorentzian_normalized (x, x0, x1, x2, a) result (f)
  real(kind=default), intent(in) :: x, x0, x1, x2, a
  real(kind=default) :: f
  if (x1 <= x .and. x <= x2) then
    f = 1 / ((x - x0)**2 + a**2) &
      * a / (atan2 (x2 - x0, a) - atan2 (x1 - x0, a))
  else
    f = 0
  end if
end function lorentzian_normalized

```

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

192b  $\langle$ Implementation of vamp\_test\_functions procedures 192a $\rangle + \equiv$

```

pure function lorentzian (x, x0, x1, x2, r0, a) result (f)
  real(kind=default), dimension(:), intent(in) :: x, x0, x1, x2
  real(kind=default), intent(in) :: r0, a
  real(kind=default) :: f
  real(kind=default) :: r, r1, r2
  integer :: n
  n = size (x)
  if (n > 1) then
    r = sqrt (dot_product (x-x0, x-x0))
    r1 = 0.4_default
    r2 = min (minval (x2-x0), minval (x0-x1))
    if (r1 <= r .and. r <= r2) then
      f = lorentzian_normalized (r, r0, r1, r2, a) * r**(1-n) / surface (n)
    else
      f = 0
    end if
  else
    f = lorentzian_normalized (x(1), x0(1), x1(1), x2(1), a)
  endif
end function lorentzian

```

192c  $\langle$ Implementation of vamp\_test\_functions procedures 192a $\rangle + \equiv$

```

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

```

```

real(kind=default), dimension(:), intent(in), optional :: weights
integer, intent(in), optional :: channel
type(vamp_grid), dimension(:), intent(in), optional :: grids
real(kind=default) :: f_x
real(kind=default), dimension(size(x)) :: minus_one, plus_one, zero, w_i, f_i
integer :: n, i
n = size(x)
minus_one = -1
zero = 0
plus_one = 1
w_i = 1
do i = 1, n
  if (all (abs (x(i+1:)) <= 1)) then
    f_i = lorentzian (x(1:i), zero(1:i), minus_one(1:i), plus_one(1:i), &
      0.7_default, width) &
      / 2.0_default**(n-i)
  else
    f_i = 0
  end if
end do
f_x = dot_product (w_i, f_i) / sum (w_i)
end function f

```

193 *⟨Implementation of vamp\_test\_functions procedures 192a⟩* +≡

```

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

194a ⟨Implementation of vamp_test_functions procedures 192a⟩+≡
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

194b ⟨Implementation of vamp_test_functions procedures 192a⟩+≡
pure function j (x, data, channel) result (j_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: channel
    real(kind=default) :: j_x
    if (channel == 1) then
        j_x = 1
    else if (channel > 1) then
        j_x = 2 / sqrt (real (channel, kind=default)) ! 1/|dr/dξ1|
    end if
end function j

```

```

        j_x = j_x / PI ! 1/|dφ/dξ2|
        j_x = j_x * cartesian_to_spherical_cos_j (x(1:channel))
    else
        j_x = 0
    end if
end function j

```

195a *⟨Implementation of vamp\_test\_functions procedures 192a⟩*  $\equiv$

```

function w (x, data, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    w_x = vamp_multi_channel (f, data, phi, ihp, j, x, weights, channel, grids)
end function w

```

195b *⟨Module vamp\_tests 195b⟩*  $\equiv$

```

module vamp_tests
    use kinds
    use exceptions
    use histograms
    use tao_random_numbers
    use coordinates
    use vamp
    use vamp_test_functions !NODEP!
    implicit none
    private
    ⟨Declaration of procedures in vamp_tests 195c⟩
contains
    ⟨Implementation of procedures in vamp_tests 196a⟩
end module vamp_tests

```

### Verification

195c *⟨Declaration of procedures in vamp\_tests 195c⟩*  $\equiv$

```

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

```

195d *⟨Implementation of procedures in vamp\_tests (broken?) 195d⟩*  $\equiv$

```

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

```

```

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

```

196a *⟨Implementation of procedures in vamp\_tests 196a⟩*≡

```

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

```

196b *⟨Implementation of procedures in vamp\_tests 196a⟩*+≡

```

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*

197a *<Declaration of procedures in vamp\_tests 195c>+≡*  
 public :: single\_channel, multi\_channel

197b *<Implementation of procedures in vamp\_tests 196a>+≡*  
 subroutine single\_channel (rng, region, samples, iterations, &  
 integral, standard\_dev, chi\_squared)  
 type(tao\_random\_state), intent(inout) :: rng  
 real(kind=default), dimension(:,:), intent(in) :: region  
 integer, dimension(:), intent(in) :: samples, iterations  
 real(kind=default), intent(out) :: integral, standard\_dev, chi\_squared  
 type(vamp\_grid) :: gr  
 type(vamp\_history), dimension(iterations(1)+iterations(2)) :: history  
 call vamp\_create\_history (history)  
 call vamp\_create\_grid (gr, region, samples(1))  
 call vamp\_sample\_grid (rng, gr, f, NO\_DATA, iterations(1), history = history)  
 call vamp\_discard\_integral (gr, samples(2))  
 call vamp\_sample\_grid &  
 (rng, gr, f, NO\_DATA, iterations(2), &  
 integral, standard\_dev, chi\_squared, &  
 history = history(iterations(1)+1:))

```

    call vamp_write_grid (gr, "vamp_test.grid")
    call vamp_delete_grid (gr)
    call vamp_print_history (history, "single")
    call vamp_delete_history (history)
end subroutine single_channel

198a <Implementation of procedures in vamp_tests 196a> +=
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 198b>
end subroutine multi_channel

198b <Body of multi_channel 198b> =
    type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
        history
    type(vamp_history), dimension(size(history),size(weights)) :: histories
    integer :: it, nit
    nit = size (powers)
    call vamp_create_history (history)
    call vamp_create_history (histories)
    call vamp_create_grids (grs, region, samples(1), weights)
    call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
        history = history, histories = histories)
    call vamp_print_history (history, "multi")
    call vamp_print_history (histories, "multi")
    do it = 1, nit
        call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
            history = history(iterations(1)+it-1:), &
            histories = histories(iterations(1)+it-1:,:))
        call vamp_print_history (history(iterations(1)+it-1:), "multi")
        call vamp_print_history (histories(iterations(1)+it-1:,:), "multi")
        call vamp_refine_weights (grs, powers(it))
    end do
    call vamp_discard_integrals (grs, samples(2))
    call vamp_sample_grids &
        (rng, grs, w, NO_DATA, iterations(2), &
            integral, standard_dev, chi_squared, &
            history = history(iterations(1)+nit:), &

```

```

        histories = histories(iterations(1)+nit:, :)
call vamp_print_history (history(iterations(1)+nit:), "multi")
call vamp_print_history (histories(iterations(1)+nit:, :), "multi")
call vamp_write_grids (grs, "vamp_test.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)

```

### *Input/Output*

199a *<Declaration of procedures in vamp\_tests 195c>+≡*  
public :: print\_results

199b *<Implementation of procedures in vamp\_tests 196a>+≡*  
subroutine print\_results (prefix, prev\_ticks, &  
integral, std\_dev, chi2, acceptable, failures)  
character(len=\*), intent(in) :: prefix  
integer, intent(in) :: prev\_ticks  
real(kind=default), intent(in) :: integral, std\_dev, chi2, acceptable  
integer, intent(inout) :: failures  
integer :: ticks, ticks\_per\_second  
real(kind=default) :: pull  
call system\_clock (ticks, ticks\_per\_second)  
pull = (integral - 1) / std\_dev  
print "(1X,A,A,F6.2,A)", prefix, &  
": time = ", real (ticks - prev\_ticks) / ticks\_per\_second, " secs"  
print \*, prefix, ": int, err, chi2: ", &  
real (integral), real (std\_dev), real (chi2)  
if (abs (pull) > acceptable) then  
failures = failures + 1  
print \*, prefix, ": unacceptable pull:", real (pull)  
else  
print \*, prefix, ": acceptable pull:", real (pull)  
end if  
end subroutine print\_results

### *Main Program*

199c *<vamp\_test.f90 191a>+≡*  
program vamp\_test  
use kinds  
use tao\_random\_numbers



```

use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp
use vamp_test_functions !NODEP!
use vamp_tests !NODEP!
implicit none
integer :: start_ticks, status
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
failures = 0
call tao_random_create (rng, 0)
call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
if (status == 0) then
    call system_clock (start_ticks)
else
    start_ticks = 42
end if
call tao_random_seed (rng, start_ticks)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
print *, "Starting VAMP 1.0 self test..."
print *, "serial code"
print *, VAMP_RCS_ID
print *, DIVISIONS_RCS_ID
call system_clock (start_ticks)
call single_channel (rng, region, samples, iterations, &
    single_integral, single_standard_dev, single_chi_squared)
call print_results ("SINGLE", start_ticks, &
    single_integral, single_standard_dev, single_chi_squared, &
    10*ACCEPTABLE, failures)
weight_vector = 1
powers = 0.25_default
call system_clock (start_ticks)

```

```

call multi_channel (rng, region, weight_vector, samples, iterations, &
    powers, multi_integral, multi_standard_dev, multi_chi_squared)
call print_results ("MULTI", start_ticks, &
    multi_integral, multi_standard_dev, multi_chi_squared, &
    ACCEPTABLE, failures)
call system_clock (start_ticks)
! call check_jacobians (rng, region, weight_vector, samples(1))
call check_inverses (rng, region, weight_vector, samples(1))
call check_inverses3 (rng, region, samples(1))
if (failures == 0) then
    stop 0
else if (failures == 1) then
    stop 1
else
    stop 2
end if
end program vamp_test

```

### 6.1.2 Parallel Test

201a  $\langle \text{vampi\_test.f90 201a} \rangle \equiv$   
 ! vampi\_test.f90 --  
 $\langle \text{Copyleft notice 1} \rangle$   
 $\langle \text{Module vamp\_test\_functions 191b} \rangle$

The following is identical to `vamp_tests`, except for use `vampi`:

201b  $\langle \text{vampi\_test.f90 201a} \rangle + \equiv$   
 module vampi\_tests  
 use kinds  
 use exceptions  
 use histograms  
 use tao\_random\_numbers  
 use coordinates  
 use vampi  
 use vamp\_test\_functions !NODEP!  
 implicit none  
 private  
 $\langle \text{Declaration of procedures in vamp\_tests 195c} \rangle$   
 contains  
 $\langle \text{Implementation of procedures in vamp\_tests 196a} \rangle$   
 end module vampi\_tests

201c  $\langle \text{vampi\_test.f90 201a} \rangle + \equiv$   
 program vampi\_test

```

use kinds
use tao_random_numbers
use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp, only: VAMP_RCS_ID
use vampi
use mpi90
use vamp_test_functions !NODEP!
use vampi_tests !NODEP!
implicit none
integer :: num_proc, proc_id, start_ticks
logical :: perform_io
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type( tao_random_state ) :: rng
integer :: iostat, command
character(len=72) :: command_line
integer, parameter :: &
    CMD_ERROR = -1, CMD_END = 0, &
    CMD_NOP = 1, CMD_SINGLE = 2, CMD_MULTI = 3, CMD_CHECK = 4
call tao_random_create (rng, 0)
call mpi90_init ()
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
perform_io = (proc_id == 0)
call system_clock (start_ticks)
call tao_random_seed (rng, start_ticks + proc_id)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
samples = (/ 200000, 2000000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
if (perform_io) then
    print *, "Starting VAMP 1.0 self test..."
    if (num_proc > 1) then
        print *, "parallel code running on ", num_proc, " processors"
    else
        print *, "parallel code running serially"
    end if
end if

```

```

        end if
        print *, VAMP_RCS_ID
        print *, VAMPI_RCS_ID
        print *, DIVISIONS_RCS_ID
    end if
    command_loop: do
        <Parse the commandline in vamp_test and set command (never defined)>
        call mpi90_broadcast (command, 0)
        call system_clock (start_ticks)
        select case (command)
            <Execute command in vamp_test (never defined)>
            case (CMD_END)
                exit command_loop
            case (CMD_NOP)
                ! do nothing
            case (CMD_ERROR)
                ! do nothing
            end select
        end do command_loop
        call mpi90_finalize ()
    end program vampi_test

```

### 6.1.3 Output

203a *<vamp\_test.out 203a>*≡

## 6.2 Mapped Mode

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

### 6.2.1 Serial Test

203b *<vamp\_test0.f90 203b>*≡  
 ! vamp\_test0.f90 --  
*<Copyleft notice 1>*  
*<Module vamp\_test0\_functions 204>*

### Single Channel

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

```

204 <Module vamp_test0_functions 204>≡
  module vamp_test0_functions
    use kinds
    use vamp, only: vamp_grid, vamp_multi_channel0
    use vamp, only: vamp_data_t
    implicit none
    private
    public :: f, g, phi, w
    public :: create_sample, delete_sample
    private :: f0, psi, g0, f_norm
    real(kind=default), dimension(:), allocatable, private :: c, x_min, x_max
    real(kind=default), dimension(:, :, :), allocatable, public :: x0, gamma
  contains
    <Implementation of vamp_test0_functions procedures 205a>
  end module vamp_test0_functions

```

We start from a model of  $n_p$  interfering resonances in one variable (cf. section ??)

$$f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{N(x_{\min}, x_{\max}, x_0, \gamma)} \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.3)$$

where

$$N(x_{\min}, x_{\max}, x_0, \gamma) = \int_{x_{\min}}^{x_{\max}} dx \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.4)$$

such that

$$\int_{x_{\min}}^{x_{\max}} dx f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = 1 \quad (6.5)$$

NB: the  $N(x_{\min}, x_{\max}, x_0, \gamma)$  should be calculated once and tabulated to save processing time, but we are lazy here.

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

205a  $\langle$ Implementation of vamp\_test0\_functions procedures 205a $\rangle \equiv$

```

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

```

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

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

205b  $\langle$ Implementation of vamp\_test0\_functions procedures 205a $\rangle + \equiv$

```

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

```

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

convenient to take a weighted sum of products:

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

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

206a *⟨Implementation of vamp\_test0\_functions procedures 205a⟩+≡*  

```

pure function f (x, data, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  class(vamp_data_t), intent(in) :: data
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: f_x
  real(kind=default) :: fi_x
  integer :: i, j
  f_x = 0.0
  do i = 1, size (c)
    fi_x = 1.0
    do j = 1, size (x)
      if (all (gamma(:,i,j) > 0)) then
        fi_x = fi_x * f0 (x(j), x_min(j), x_max(j), &
                        x0(:,i,j), gamma(:,i,j))
      else
        fi_x = fi_x / (x_max(j) - x_min(j))
      end if
    end do
    f_x = f_x + c(i) * fi_x
  end do
  f_x = f_x / sum (c)
end function f

```

206b *⟨Implementation of vamp\_test0\_functions procedures 205a⟩+≡*  

```

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

```

206c *⟨Implementation of vamp\_test0\_functions procedures 205a⟩+≡*  

```

subroutine create_sample (num_poles, weights, region)
  integer, intent(in) :: num_poles
  real(kind=default), dimension(:), intent(in) :: weights

```

```

real(kind=default), dimension(:,,:), intent(in) :: region
integer :: nd, nc
nd = size (region, dim=2)
nc = size (weights)
allocate (c(nc), x_min(nd), x_max(nd))
allocate (x0(num_poles,nc,nd), gamma(num_poles,nc,nd))
x_min = region(1,:)
x_max = region(2,:)
c = weights
end subroutine create_sample

```

### Multi Channel

We start from the usual mapping for Lorentzian peaks

$$\begin{aligned} \psi(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ \xi \mapsto x = \psi(\xi | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.9)$$

where

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

207 *<Implementation of vamp\_test0\_functions procedures 205a>+≡*

```

pure function psi (xi, x_min, x_max, x0, gamma) result (x)
  real(kind=default), intent(in) :: xi, x_min, x_max, x0, gamma
  real(kind=default) :: x
  x = x0 + gamma &
    * tan (((xi - x_min) * atan ((x_max - x0) / gamma) &
      - (x_max - xi) * atan ((x0 - x_min) / gamma)) &
    / (x_max - x_min))
end function psi

```

The inverse mapping is

$$\begin{aligned} \psi^{-1}(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ x \mapsto \xi = \psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.11)$$

with

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



with Jacobian

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

**208a** *<Implementation of vamp\_test0\_functions procedures 205a>+≡*  

```

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:

**208b** *<Decode channel into ch and p(:) 208b>≡*  

```

ch = channel - 1
do j = 1, size (x)
  p(j) = 1 + modulo (ch, np)
  ch = ch / np
end do
ch = ch + 1

```

The map  $\phi$  is the direct product of  $\psi$ s:

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

```

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(:) 208b>
    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:

209a *⟨Implementation of vamp\_test0\_functions procedures 205a⟩*+≡

```

pure recursive function g (x, data, channel) result (g_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: channel
    real(kind=default) :: g_x
    integer, dimension(size(x)) :: p
    integer :: j, ch, np, nch, nd, channels
    np = size (x0, dim = 1)
    nch = size (x0, dim = 2)
    nd = size (x0, dim = 3)
    channels = nch * np**nd
    if (channel >= 1 .and. channel <= channels) then
        ⟨Decode channel into ch and p(:) 208b⟩
        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

```

209b *⟨Implementation of vamp\_test0\_functions procedures 205a⟩*+≡

```

function w (x, data, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel

```

```

    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    w_x = vamp_multi_channel0 (f, data, phi, g, x, weights, channel)
end function w

```

### *Driver Routines*

**210a**  $\langle \text{vamp\_test0.f90 203b} \rangle + \equiv$

```

module vamp_tests0
   $\langle \text{Modules used by vamp\_tests0 210b} \rangle$ 
  use vamp
  implicit none
  private
   $\langle \text{Declaration of procedures in vamp\_tests0 211a} \rangle$ 
contains
   $\langle \text{Implementation of procedures in vamp\_tests0 211b} \rangle$ 
end module vamp_tests0

```

**210b**  $\langle \text{Modules used by vamp\_tests0 210b} \rangle \equiv$

```

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

```

### *Verification*

**210c**  $\langle \text{Declaration of procedures in vamp\_tests0 (broken?) 210c} \rangle \equiv$

```

public :: check_jacobians

```

**210d**  $\langle \text{Implementation of procedures in vamp\_tests0 (broken?) 210d} \rangle \equiv$

```

subroutine check_jacobians (do_print, region, samples, rng)
  logical, intent(in) :: do_print
  real(kind=default), dimension(:, :), intent(in) :: region
  integer, dimension(:), intent(in) :: samples
  type( tao_random_state ), intent(inout) :: rng
  real(kind=default), dimension(size(region,dim=2)) :: x
  real(kind=default) :: d
  integer :: ch
  do ch = 1, size(x0,dim=2) * size(x0,dim=1)**size(x0,dim=3) + 1
    call vamp_check_jacobian (rng, samples(1), g, phi, ch, region, d, x)
    if (do_print) then
      print *, ch, ": ", d, ", x = ", real (x)
    end if
  end do

```

```

        end do
    end subroutine check_jacobians

```

### *Integration*

**211a** *<Declaration of procedures in vamp\_tests0 211a>*≡  
 public :: single\_channel, multi\_channel

**211b** *<Implementation of procedures in vamp\_tests0 211b>*≡  
 subroutine single\_channel (do\_print, region, iterations, samples, rng, &  
 acceptable, failures)  
 logical, intent(in) :: do\_print  
 real(kind=default), dimension(:,:), intent(in) :: region  
 integer, dimension(:), intent(in) :: iterations, samples  
 type(tao\_random\_state), intent(inout) :: rng  
 real(kind=default), intent(in) :: acceptable  
 integer, intent(inout) :: failures  
 type(vamp\_grid) :: gr  
 type(vamp\_history), dimension(iterations(1)+iterations(2)) :: history  
 real(kind=default) :: integral, standard\_dev, chi\_squared, pull  
 call vamp\_create\_history (history)  
 call vamp\_create\_grid (gr, region, samples(1))  
 call vamp\_sample\_grid (rng, gr, f, NO\_DATA, iterations(1), history = history)  
 call vamp\_discard\_integral (gr, samples(2))  
 call vamp\_sample\_grid &  
 (rng, gr, f, NO\_DATA, iterations(2), &  
 integral, standard\_dev, chi\_squared, &  
 history = history(iterations(1)+1:))  
 call vamp\_write\_grid (gr, "vamp\_test0.grid")  
 call vamp\_delete\_grid (gr)  
 call vamp\_print\_history (history, "single")  
 call vamp\_delete\_history (history)  
 pull = (integral - 1) / standard\_dev  
 if (do\_print) then  
 print \*, " int, err, chi2:", integral, standard\_dev, chi\_squared  
 end if  
 if (abs (pull) > acceptable) then  
 failures = failures + 1  
 print \*, " unacceptable pull:", pull  
 else  
 print \*, " acceptable pull:", pull  
 end if  
 end subroutine single\_channel

212a *⟨Implementation of procedures in vamp\_tests0 211b⟩*+≡

```
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 198b⟩
end subroutine multi_channel
```

212b *⟨Body of multi\_channel 198b⟩*+≡

```
real(kind=default), &
    dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
    weight_vector
type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
real(kind=default) :: integral, standard_dev, chi_squared, pull
integer :: it
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
    history = history, histories = histories)
do it = 1, 5
    call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
        history = history(iterations(1)+it-1:), &
        histories = histories(iterations(1)+it-1:,:))
    call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
    (rng, grs, w, NO_DATA, iterations(2), &
    integral, standard_dev, chi_squared, &
    history = history(iterations(1)+5:), &
    histories = histories(iterations(1)+5:,:))
call vamp_write_grids (grs, "vamp_test0.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
```

```

call vamp_delete_history (histories)
if (do_print) then
    print *, integral, standard_dev, chi_squared
end if
pull = (integral - 1) / standard_dev
if (abs (pull) > acceptable) then
    failures = failures + 1
    print *, " unacceptable pull:", pull
else
    print *, "    acceptable pull:", pull
end if

```

### *Event Generation*

213a *<Declaration of procedures in vamp\_tests0 211a>+≡*

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

213b *<Implementation of procedures in vamp\_tests0 211b>+≡*

```

subroutine single_channel_generator (do_print, region, iterations, samples, rng)
    logical, intent(in) :: do_print
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: iterations, samples
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid) :: gr
    type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
    type(histogram) :: unweighted, reweighted, weighted, weights
    type(exception) :: exc
    real(kind=default) :: weight, integral, standard_dev
    integer :: i
    real(kind=default), dimension(size(region,dim=2)) :: x
    call vamp_create_grid (gr, region, samples(1))
    call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
    call vamp_discard_integral (gr, samples(2))
    call vamp_warmup_grid &
        (rng, gr, f, NO_DATA, iterations(2), history = history(iterations(1)+1:))
    call vamp_print_history (history, "single")
    call vamp_delete_history (history)
    call create_histogram (unweighted, region(1,1), region(2,1), 100)
    call create_histogram (reweighted, region(1,1), region(2,1), 100)
    call create_histogram (weighted, region(1,1), region(2,1), 100)
    call create_histogram (weights, 0.0_default, 10.0_default, 100)
    ! do i = 1, 1000000
    do i = 1, 100
        call clear_exception (exc)
    end do
end subroutine

```

```

        call vamp_next_event (x, rng, gr, f, NO_DATA, exc = exc)
        call handle_exception (exc)
        call fill_histogram (unweighted, x(1))
        call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
    end do
    integral = 0.0
    standard_dev = 0.0
    do i = 1, 10000
        call clear_exception (exc)
        call vamp_next_event (x, rng, gr, f, NO_DATA, weight, exc = exc)
        call handle_exception (exc)
        call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
        call fill_histogram (weights, x(1), weight)
        integral = integral + weight
        standard_dev = standard_dev + weight**2
    end do
    if (do_print) then
        print *, integral / (i-1), sqrt (standard_dev) / (i-1)
        call write_histogram (unweighted, "u_s.d")
        call write_histogram (reweighted, "r_s.d")
        call write_histogram (weighted, "w_s.d")
        call write_histogram (weights, "ws_s.d")
    end if
    call delete_histogram (unweighted)
    call delete_histogram (reweighted)
    call delete_histogram (weighted)
    call delete_histogram (weights)
    call vamp_delete_grid (gr)
end subroutine single_channel_generator

```

214 *<Implementation of procedures in vamp\_tests0 211b>+≡*

```

subroutine multi_channel_generator (do_print, region, iterations, samples, rng)
    logical, intent(in) :: do_print
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: iterations, samples
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids) :: grs
    real(kind=default), &
        dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
        weight_vector
    type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
    type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
    type(histogram) :: unweighted, reweighted, weighted, weights
    type(exception) :: exc

```

```

real(kind=default) :: weight, integral, standard_dev
real(kind=default), dimension(size(region,dim=2)) :: x
character(len=5) :: pfx
integer :: it, i, j
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
    call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
                            history = history(iterations(1)+it-1:), &
                            histories = histories(iterations(1)+it-1:,:))
    call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_warmup_grids &
    (rng, grs, w, NO_DATA, iterations(2), &
     history = history(iterations(1)+5:), &
     histories = histories(iterations(1)+5:,:))
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
!!! do i = 1, size (grs%grids)
!!!     do j = 1, size (grs%grids(i)%div)
!!!         write (pfx, "(I2.2,'/',I2.2)") i, j
!!!         call dump_division (grs%grids(i)%div(j), pfx)
!!!     end do
!!! end do
call create_histogram (unweighted, region(1,1), region(2,1), 100)
call create_histogram (reweighted, region(1,1), region(2,1), 100)
call create_histogram (weighted, region(1,1), region(2,1), 100)
call create_histogram (weights, 0.0_default, 10.0_default, 100)
! do i = 1, 1000000
do i = 1, 100
    call clear_exception (exc)
    call vamp_next_event (x, rng, grs, f, NO_DATA, phi, exc = exc)
    call handle_exception (exc)
    call fill_histogram (unweighted, x(1))
    call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
end do

```



```

integral = 0.0
standard_dev = 0.0
do i = 1, 10000
  call clear_exception (exc)
  call vamp_next_event (x, rng, grs, f, NO_DATA, phi, weight, exc = exc)
  call handle_exception (exc)
  call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
  call fill_histogram (weights, x(1), weight)
  integral = integral + weight
  standard_dev = standard_dev + weight**2
end do
if (do_print) then
  print *, integral / (i-1), sqrt (standard_dev) / (i-1)
  call write_histogram (unweighted, "u_m.d")
  call write_histogram (reweighted, "r_m.d")
  call write_histogram (weighted, "w_m.d")
  call write_histogram (weights, "ws_m.d")
end if
call delete_histogram (unweighted)
call delete_histogram (reweighted)
call delete_histogram (weighted)
call delete_histogram (weights)
call vamp_delete_grids (grs)
end subroutine multi_channel_generator

```

### *Main Program*

```

216 <vamp_test0.f90 203b>+≡
  program vamp_test0
    <Modules used by vamp_test0 218d>
    implicit none
    <Variables in vamp_test0 218b>
    do_print = .true.
    print *, "Starting VAMP 1.0 self test..."
    print *, "serial code"
    print *, VAMP_RCS_ID
    print *, DIVISIONS_RCS_ID
    call tao_random_create (rng, 0)
    call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
    if (status == 0) then
      call system_clock (ticks0)
    else
      ticks0 = 42
    end if
  end program

```

```

end if
call tao_random_seed (rng, ticks0)
<Set up integrand and region in vamp_test0 218f>
<Execute tests in vamp_test0 217a>
<Cleanup in vamp_test0 219a>
if (failures == 0) then
    stop 0
else if (failures == 1) then
    stop 1
else
    stop 2
end if
end program vamp_test0

217a <Execute tests in vamp_test0 217a>≡
failures = 0
call system_clock (ticks0)
call single_channel (do_print, region, iterations, samples, rng, 10*ACCEPTABLE, failures)
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
    "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

217b <Execute tests in vamp_test0 217a>+≡
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"

217c <Execute tests in vamp_test0 217a>+≡
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"

217d <Execute tests in vamp_test0 217a>+≡
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"

```

```

218a  <Execute tests in vamp_test0 217a>+≡
      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"

218b  <Variables in vamp_test0 218b>≡
      logical :: do_print

218c  <Execute command 218c>≡

218d  <Modules used by vamp_test0 218d>≡
      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!

218e  <Variables in vamp_test0 218b>+≡
      integer :: i, j, ticks, ticks_per_second, ticks0, status
      integer, dimension(2) :: iterations, samples
      real(kind=default), dimension(:,,:), allocatable :: region
      type( tao_random_state ) :: rng
      real(kind=default), parameter :: ACCEPTABLE = 4
      integer :: failures

218f  <Set up integrand and region in vamp_test0 218f>≡
      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

```

219a *<Cleanup in vamp\_test0 219a>*≡  
     call delete\_sample ()  
     deallocate (region)

## 6.2.2 Parallel Test

219b *<vampi\_test0.f90 219b>*≡  
     ! vampi\_test0.f90 --  
     *<Copyleft notice 1>*  
     *<Module vamp\_test0\_functions 204>*  
     module vamp\_tests0  
         *<Modules used by vamp\_tests0 210b>*  
         use vampi  
         use mpi90  
         implicit none  
         private  
         *<Declaration of procedures in vamp\_tests0 211a>*  
     contains  
         *<Implementation of procedures in vamp\_tests0 211b>*  
     end module vamp\_tests0

219c *<vampi\_test0.f90 219b>*+≡  
     program vampi\_test0  
         *<Modules used by vamp\_test0 218d>*  
         use mpi90  
         use vampi, only: VAMPI\_RCS\_ID  
         implicit none  
         *<Variables in vamp\_test0 218b>*  
         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  
         end if

```

else
    do_print = .false.
end if
call tao_random_create (rng, 0)
call system_clock (ticks0)
call tao_random_seed (rng, ticks0 + proc_id)
<Set up integrand and region in vamp_test0 218f>
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 218c>
    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 219a>
call mpi90_finalize ()
if (proc_id == 0) then
    print *, "bye."
end if
end program vampi_test0

```

### 6.2.3 Output

220 *<vamp\_test0.out 220>*≡

# —7—

## APPLICATION

### 7.1 *Cross section*

```
221a <application.f90 221a>≡
    ! 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 222d>
        <Types in cross_section 227c>
        <Variables in cross_section 221b>
    contains
        <Implementation of cross_section procedures 223a>
    end module cross_section

221b <Variables in cross_section 221b>≡
    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
```

222a *<XXX Variables in cross\_section 222a>*≡

```
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
```

222b *<XXX Variables in cross\_section 222a>*+≡

```
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
```

222c *<Variables in cross\_section 221b>*+≡

```
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
```

222d *<Declaration of cross\_section procedures 222d>*≡

```
private :: cuts
```

222e *<XXX Implementation of cross\_section procedures 222e>*≡

```
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
```

222f *<Variables in cross\_section 221b>*+≡

```
real(kind=default), private, parameter :: &
```

```

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

```

**223a** *⟨Implementation of cross\_section procedures 223a⟩*≡

```

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

```

**223b** *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

224a  $\langle$ Declaration of cross\_section procedures 222d $\rangle + \equiv$

```

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

```

where

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

224b  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  224b $\rangle \equiv$

```

! s2_min = S1_MIN_0
s2_min = (m2 + m3)**2
s2_max = (sqrt(s) - m1)**2
s2 = s2_max * x(1) + s2_min * (1 - x(1))
t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
+ sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
- sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1 = t1_max * x(2) + t1_min * (1 - x(2))
phi = 2*PI * x(3)
cos_theta3 = 2 * x(4) - 1
phi3 = 2*PI * x(5)

```

224c  $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 224c $\rangle \equiv$

```

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

```

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

i.e.

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

```

225a  <Adjust Jacobian 225a>≡
      p%jacobian = p%jacobian &
        * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))

225b  <Implementation of cross_section procedures 223a>+≡
      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
      <ma ↔ mb, m1 ↔ m2 for channel #1 225c>
      <Set (s2, t1, φ, cos θ3, φ3) from (x1, ..., x5) 224b>
      p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
      <Adjust Jacobian 225a>
      <p1 ↔ p2 for channel #2 226a>
      end function phase_space

225c  <ma ↔ mb, m1 ↔ m2 for channel #1 225c>≡
      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

```

226a  $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 226a} \rangle \equiv$

```

    select case (channel)
    case (1)
        ! OK
    case (2)
        call swap (p%p(1,:), p%p(2,:))
    case (3)
        call swap (p%p(1,:), p%p(3,:))
    case default
        ! OK
    end select

```

226b  $\langle \text{Declaration of cross\_section procedures 222d} \rangle + \equiv$

```

    private :: jacobian

```

226c  $\langle \text{Implementation of cross\_section procedures 223a} \rangle + \equiv$

```

    pure function jacobian (k1, k2, p1, p2, q) result (jac)
    real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
    real(kind=default) :: jac
    real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
    real(kind=default) :: s, s2, s2_min, s2_max, t1_min, t1_max
    ma_2 = max (dot (k1, k1), 0.0_double)
    mb_2 = max (dot (k2, k2), 0.0_double)
    m1_2 = max (dot (p1, p1), 0.0_double)
    m2_2 = max (dot (p2, p2), 0.0_double)
    m3_2 = max (dot (q, q), 0.0_double)
    s = dot (k1 + k2, k1 + k2)
    s2 = dot (p2 + q, p2 + q)
    ! s2_min = S1_MIN_0
    s2_min = (sqrt (m2_2) + sqrt (m3_2))**2
    s2_max = (sqrt (s) - sqrt (m1_2))**2
    t1_min = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
        + sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
    t1_max = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
        - sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)

```

```

    jac = 1.0 / ((2*PI)**5 * 32 * s2) &
        * sqrt (lambda (s2, m2_2, m3_2) / lambda (s, ma_2, mb_2)) &
        * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
end function jacobian

```

227a  $\langle$ Declaration of cross\_section procedures 222d $\rangle + \equiv$

```

private :: phase_space, phase_space_massless

```

227b  $\langle$ Implementation of cross\_section procedures 223a $\rangle + \equiv$

```

pure function phase_space_massless (x, channel) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  integer, intent(in) :: channel
  type(LIPS3) :: p
  real(kind=default) :: s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s = S_0
   $\langle$ Set  $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$  from  $(x_1, \dots, x_5)$  (massless case) 224c $\rangle$ 
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3)
   $\langle$ Adjust Jacobian 225a $\rangle$ 
   $\langle p_1 \leftrightarrow p_2$  for channel #2 226a $\rangle$ 
end function phase_space_massless

```

227c  $\langle$ Types in cross\_section 227c $\rangle \equiv$

```

type, public :: LIPS3_m5i2a3
! private
  real(kind=default) :: ma, mb, m1, m2, m3
  real(kind=default) :: s, s2, t1
  real(kind=default) :: phi, cos_theta3, phi3
  real(kind=default) :: jacobian
end type LIPS3_m5i2a3

```

227d  $\langle$ Types in cross\_section 227c $\rangle + \equiv$

```

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

```

227e  $\langle$ Declaration of cross\_section procedures 222d $\rangle + \equiv$

```

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

```

227f  $\langle$ Implementation of cross\_section procedures 223a $\rangle + \equiv$

```

pure function invariants_from_p (p, k1, k2) result (q)
  type(LIPS3), intent(in) :: p

```

```

real(kind=default), dimension(0:), intent(in) :: k1, k2
type(LIPS3_m5i2a3) :: q
real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
real(kind=default), dimension(0:3) :: k1k2, p2p3, k1p1, p3_23
k1k2 = k1 + k2
k1p1 = - k1 + p%p(1,:)
p2p3 = p%p(2,:) + p%p(3,:)
ma_2 = max (dot (k1, k1), 0.0_double)
mb_2 = max (dot (k2, k2), 0.0_double)
m1_2 = max (dot (p%p(1,:), p%p(1:)), 0.0_double)
m2_2 = max (dot (p%p(2,:), p%p(2:)), 0.0_double)
m3_2 = max (dot (p%p(3,:), p%p(3:)), 0.0_double)
q%ma = sqrt (ma_2)
q%mb = sqrt (mb_2)
q%m1 = sqrt (m1_2)
q%m2 = sqrt (m2_2)
q%m3 = sqrt (m3_2)
q%s = dot (k1k2, k1k2)
q%s2 = dot (p2p3, p2p3)
q%t1 = dot (k1p1, k1p1)
q%phi = atan2 (p%p(1,2), p%p(1,1))
if (q%phi < 0) then
    q%phi = q%phi + 2*PI
end if
p3_23 = boost_momentum (p%p(3,:), p2p3)
q%cos_theta3 = p3_23(3) / sqrt (dot_product (p3_23(1:3), p3_23(1:3)))
q%phi3 = atan2 (p3_23(2), p3_23(1))
if (q%phi3 < 0) then
    q%phi3 = q%phi3 + 2*PI
end if
q%jacobian = 1.0 / ((2*PI)**5 * 32 * q%s2) &
    * sqrt (lambda (q%s2, m2_2, m3_2) / lambda (q%s, ma_2, mb_2))
end function invariants_from_p

```

**228a** *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

**228b** *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

229 *⟨Implementation of cross\_section procedures 223a⟩* +≡

```

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

```

230a *<Declaration of cross\_section procedures 222d>+≡*

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

230b *<Implementation of cross\_section procedures 223a>+≡*

```

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

```

230c *<Implementation of cross\_section procedures 223a>+≡*

```

function sigma_raw (k1, k2, p1, p2, q) result (xs)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  real(kind=default) :: xs
  if (cuts (k1, k2, p1, p2, q)) then
    xs = xsect (k1, k2, p1, p2, q)
  end if
end function sigma_raw

```

```

else
  xs = 0.0
end if
end function sigma_raw

```

231a *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

231b *⟨Declaration of cross\_section procedures 222d⟩*+≡

```

public :: w

```



231c *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

**232** *⟨Implementation of cross\_section procedures 223a⟩+≡*

```

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

```

```

233a  <Declaration of cross_section procedures 222d>+≡
      public :: sigma_rambo

233b  <Declaration of cross_section procedures 222d>+≡
      public :: check_kinematics
      private :: print_LIPS3_m5i2a3

233c  <Implementation of cross_section procedures 223a>+≡
      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

233d  <Implementation of cross_section procedures 223a>+≡
      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

```

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

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

234b *⟨Implementation of cross\_section procedures 223a⟩*+≡

```
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
```

234c *⟨Implementation of cross\_section procedures 223a⟩*+≡

```
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

```

235a *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

235b *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

235c *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

236a *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

236b *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

236c *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

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

```

237a *⟨Declaration of cross\_section procedures 222d⟩*+≡

```

public :: wx

```

237b *⟨Implementation of cross\_section procedures 223a⟩*+≡

```

function wx (x, weights, channel, grids) result (w_x)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in) :: weights
  integer, intent(in) :: channel
  type(vamp_grid), dimension(:), intent(in) :: grids
  real(kind=default) :: w_x
  real(kind=default), dimension(size(weights)) :: g_x, p_q
  real(kind=default), dimension(size(x)) :: x1, x2
  real(kind=default), dimension(2,0:3) :: k
  type(LIPS3) :: q
  k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
  k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  select case (abs (channel))
  case (1)
    x1 = x
    x2 = phi12 (x, 0)
    q = phi1 (x1)
  case (2)
    x1 = phi21 (x, 0)
    x2 = x
    q = phi2 (x2)
  end select
  p_q(1) = vamp_probability (grids(1), x1)
  p_q(2) = vamp_probability (grids(2), x2)
  g_x(1) = p_q(1) * g1 (x1)
  g_x(2) = p_q(2) * g2 (x2)
  g_x = g_x / p_q(abs(channel))
  if (channel > 0) then
    w_x = sigma_raw (k(1,:), k(2,:), q%p(1,:), q%p(2,:), q%p(3,:)) &
      / dot_product (weights, g_x)
  else if (channel < 0) then
    w_x = vamp_probability (grids(-channel), x) / dot_product (weights, g_x)
  else
    w_x = 0
  end if
end function wx

```

```

        end if
    end function wx

```

238 <application.f90 221a>+≡

```

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 241a
case (CMD_MASSLESS)
  Application in massless single channel mode 241b
case (CMD_MULTI)
  Application in multi channel mode 242
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 243>
case (CMD_COMPARE)
  <Application in single channel mode 241a>
  single_integral = integral
  single_standard_dev = standard_dev
  <Application in Rambo mode 243>
  if (proc_id == 0) then
    rambo_integral = integral
    rambo_standard_dev = standard_dev
    integral = &
      (single_integral / single_standard_dev**2 &
       + rambo_integral / rambo_standard_dev**2) &
      / (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    standard_dev = 1.0_double &
      / sqrt (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    chi_squared = &
      ((single_integral - integral)**2 / single_standard_dev**2) &
      + ((rambo_integral - integral)**2 / rambo_standard_dev**2)
    print *, "S&R:   ", integral, standard_dev, chi_squared
  end if
case default
  if (proc_id == 0) then
    print *, "???: ", command
    !!! TO BE REMOVED !!!
    call check_kinematics (rng)
    allocate (region(2,5))
    region(1,:) = 0
    region(2,:) = 1
    do i = 1, 10
      call tao_random_number (rng, x)
      call vamp_jacobian (phi12, 0, x, region, jac)
      print *, "12:  ", jac, 1 / g12 (x), jac * g12 (x) - 1
      call vamp_jacobian (phi21, 0, x, region, jac)
      print *, "21:  ", jac, 1 / g21 (x), jac * g21 (x) - 1
      print *, "1:   ", real(x)
      print *, "2:   ", real(phi12(phi21(x,0),0))
      print *, "2':  ", real(phi12(phi21(x,-1),-1))
      print *, "3:   ", real(phi21(phi12(x,0),0))
      print *, "3':  ", real(phi21(phi12(x,-1),-1))
      print *, "2-1: ", real(phi12(phi21(x,0),0) - x)
    end do
  end if
end

```

```

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

```

**241a** *⟨Application in single channel mode 241a⟩≡*

```

    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)

```

**241b** *⟨Application in massless single channel mode 241b⟩≡*

```

    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)

```

242 *Application in multi channel mode 242*≡

```

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)

```

243 *Application in Rambo mode 243*≡

```

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.

```
244a <vamp_kinds.f90 244a>≡
      ! vamp_kinds.f90 --
      <Copyleft notice 1>
      module kinds
        implicit none
        integer, parameter, private :: single = &
          & selected_real_kind (precision(1.0), range(1.0))
        integer, parameter, private :: double = &
          & selected_real_kind (precision(1.0_single) + 1, range(1.0_single) + 1)
        integer, parameter, private :: extended = &
          & selected_real_kind (precision (1.0_double) + 1, range (1.0_double))
        integer, parameter, public :: default = double
        character(len=*), public, parameter :: KINDS_RCS_ID = &
          "$Id: kinds.nw 314 2010-04-17 20:32:33Z ohl $"
      end module kinds
```

### *A.2 Mathematical and Physical Constants*

```
244b <constants.f90 244b>≡
      ! 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

```
246a <exceptions.f90 246a>≡
      ! exceptions.f90 --
      <Copyleft notice 1>
      module exceptions
        use kinds
        implicit none
        private
        <Declaration of exceptions procedures 247b>
        <Interfaces of exceptions procedures (never defined)>
        <Variables in exceptions 246c>
        <Declaration of exceptions types 246b>
        character(len=*, public, parameter :: EXCEPTIONS_RCS_ID = &
          "$Id: exceptions.nw 314 2010-04-17 20:32:33Z ohl $"
        contains
          <Implementation of exceptions procedures 247c>
        end module exceptions

246b <Declaration of exceptions types 246b>≡
      type, public :: exception
        integer :: level = EXC_NONE
        character(len=NAME_LENGTH) :: message = ""
        character(len=NAME_LENGTH) :: origin = ""
      end type exception

246c <Variables in exceptions 246c>≡
      integer, public, parameter :: &
        EXC_NONE = 0, &
        EXC_INFO = 1, &
        EXC_WARN = 2, &
```

```

    EXC_ERROR = 3, &
    EXC_FATAL = 4

```

247a *<Variables in exceptions 246c>+≡*

```

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

```

247b *<Declaration of exceptions procedures 247b>≡*

```

    public :: handle_exception

```

247c *<Implementation of exceptions procedures 247c>≡*

```

    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

```

247d *<Declaration of exceptions procedures 247b>+≡*

```

    public :: raise_exception, clear_exception, gather_exceptions

```

Raise an exception, but don't overwrite the messages in `exc` if it holds a more severe exception. This way we can accumulate error codes across procedure calls. We have `exc` optional to simplify life for the calling procedures, which might have it optional themselves.

247e *<Implementation of exceptions procedures 247c>+≡*

```

    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

```

248a *⟨Implementation of exceptions procedures 247c⟩*+≡

```

elemental subroutine clear_exception (exc)
  type(exception), intent(inout) :: exc
  exc%level = 0
  exc%message = ""
  exc%origin = ""
end subroutine clear_exception

```

248b *⟨Implementation of exceptions procedures 247c⟩*+≡

```

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`

249 *⟨Idioms 101a⟩*+≡

```
call clear_exception (excs)
call elemental_procedure_1 (y, x, excs)
call elemental_procedure_2 (b, a, excs)
if (any (excs%level > 0)) then
  call gather_exceptions (exc, excs)
  return
end if
```

# —C—

## THE ART OF RANDOM NUMBERS

Volume two of Donald E. Knuth' *The Art of Computer Programming* [16] has always been celebrated as a prime reference for random number generation. Recently, the third edition has been published and it contains a gem of a *portable* random number generator. It generates 30-bit integers with the following desirable properties

- they pass all the tests from George Marsaglia's "diehard" suite of tests for random number generators [24] (but see [16] for a caveat regarding the "birthday-spacing" test)
- they can be generated with portable signed 32-bit arithmetic (Fortran can't do unsigned arithmetic)
- it is faster than other lagged Fibonacci generators
- it can create at least  $2^{30} - 2$  independent sequences

We implement the improved versions available as FORTRAN77 code from

<http://www-cs-faculty.stanford.edu/~uno/programs.html#rng>

that contain a streamlined seeding algorithm with better independence of substreams.

### *C.1 Application Program Interface*

A function returning single reals and integers. Note that the static version without the `tao_random_state` argument does not require initialization. It will behave as if `call tao_random_seed(0)` had been executed. On the other hand, the parallelizable version with the explicit `tao_random_state` will fail if none of the `tao_random_create` have been called for the state. (This is a deficiency of Fortran90 that can be fixed in Fortran95).

250  $\langle$ API documentation 250 $\rangle \equiv$   
     call tao\_random\_number (r)  
     call tao\_random\_number (s, r)

The state of the random number generator comes in two varieties: buffered and raw. The former is much more efficient, but it can be beneficial to flush the buffers and to pass only the raw state in order to save of interprocess communication (IPC) costs.

251a  $\langle$ API documentation 250 $\rangle + \equiv$   
     type(tao\_random\_state) :: s  
     type(tao\_random\_raw\_state) :: rs

Subroutines filling arrays of reals and integers:

251b  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_number (a, num = n)  
     call tao\_random\_number (s, a, num = n)

Subroutine for changing the seed:

251c  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_seed (seed = seed)  
     call tao\_random\_seed (s, seed = seed)

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

251d  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_luxury ()  
     call tao\_random\_luxury (s)

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

251e  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_luxury (n)  
     call tao\_random\_luxury (s, n)

With a floating point argument, use that fraction of each fill of the buffer:

251f  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_luxury (x)  
     call tao\_random\_luxury (s, x)

Create a tao\_random\_state

251g  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_create (s, seed, buffer\_size = buffer\_size)  
     call tao\_random\_create (s, raw\_state, buffer\_size = buffer\_size)  
     call tao\_random\_create (s, state)

Create a tao\_random\_raw\_state

251h  $\langle$ API documentation 250 $\rangle + \equiv$   
     call tao\_random\_create (rs, seed)  
     call tao\_random\_create (rs, raw\_state)  
     call tao\_random\_create (rs, state)

Destroy a `tao_random_state` or `tao_random_raw_state`

252a  $\langle$ API documentation 250 $\rangle + \equiv$   
    call `tao_random_destroy (s)`

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

252b  $\langle$ API documentation 250 $\rangle + \equiv$   
    call `tao_random_copy (lhs, rhs)`  
    lhs = rhs

252c  $\langle$ API documentation 250 $\rangle + \equiv$   
    call `tao_random_flush (s)`

252d  $\langle$ API documentation 250 $\rangle + \equiv$   
    call `tao_random_read (s, unit)`  
    call `tao_random_write (s, unit)`

252e  $\langle$ API documentation 250 $\rangle + \equiv$   
    call `tao_random_test (name = name)`

Here is a sample application of random number states:

252f  $\langle$ API documentation 250 $\rangle + \equiv$   
    subroutine `threads (args, y, state)`  
        real, dimension(:), intent(in) :: args  
        real, dimension(:), intent(out) :: y  
        type(`tao_random_state`) :: state  
        integer :: seed  
        type(`tao_random_raw_state`), dimension(size(y)) :: states  
        integer :: s  
        call `tao_random_number (state, seed)`  
        call `tao_random_create (states, (/ (s, s=seed,size(y)-1) /))`  
        y = `thread (args, states)`  
    end function `thread`

In this example, we could equivalently pass an integer seed, instead of `raw_state`. But in more complicated cases it can be beneficial to have the option of reusing `raw_state` in the calling routine.

252g  $\langle$ API documentation 250 $\rangle + \equiv$   
    elemental function `thread (arg, raw_state) result (y)`  
        real, dimension, intent(in) :: arg  
        type(`tao_random_raw_state`) :: raw\_state  
        real :: y  
        type(`tao_random_state`) :: state  
        real :: r  
        call `tao_random_create (state, raw_state)`  
    do

```

...
call tao_random_number (state, r)
...
end do
end function thread

```

## C.2 Low Level Routines

Here the low level routines are *much* more interesting than the high level routines. The latter contain a lot of duplication (made necessary by Fortran's lack of parametric polymorphism) and consist mostly of bookkeeping. We will therefore start with the former.

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

The generator is a subtractive lagged Fibonacci

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

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

**253a**  $\langle$ Parameters in tao\_random\_numbers **253a** $\rangle \equiv$

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

Other good choices for  $K$  and  $L$  are (cf. [16], table 1 in section 3.2.2, p. 29)

**253b**  $\langle$ Parameters in tao\_random\_numbers (alternatives) **253b** $\rangle \equiv$

```
integer, parameter, private :: K = 55, L = 24
integer, parameter, private :: K = 89, L = 38
integer, parameter, private :: K = 100, L = 37
integer, parameter, private :: K = 127, L = 30
integer, parameter, private :: K = 258, L = 83
integer, parameter, private :: K = 378, L = 107
integer, parameter, private :: K = 607, L = 273
```

A modulus of  $2^{30}$  is the largest we can handle in *portable* (i.e. *signed*) 32-bit arithmetic

**253c**  $\langle$ Variables in 30-bit tao\_random\_numbers **253c** $\rangle \equiv$

```
integer(kind=tao_i32), parameter, private :: M = 2**30
```

**generate** fills the array  $a_1, \dots, a_n$  with random integers  $0 \leq a_i < 2^{30}$ . We *must* have at least  $n \geq K$ . Higher values don't change the results, but make **generate** more efficient (about a factor of two, asymptotically). For  $K = 100$ , DEK recommends  $n \geq 1000$ . Best results are obtained using the first 100

random numbers out of 1009. Let's therefore use 1009 as a default buffer size. The user can call `tao_random_luxury (100)` him/herself:

254a  $\langle$ Parameters in `tao_random_numbers` 253a $\rangle + \equiv$

```
integer, parameter, private :: DEFAULT_BUFFER_SIZE = 1009
```

Since users are not expected to call `generate` directly, we do *not* check for  $n \geq K$  and assume that the caller knows what (s)he's doing ...

254b  $\langle$ Implementation of 30-bit `tao_random_numbers` 254b $\rangle \equiv$

```
pure subroutine generate (a, state)
  integer(kind=tao_i32), dimension(:), intent(inout) :: a, state
  integer :: j, n
  n = size (a)
   $\langle$ Load a and refresh state 254d $\rangle$ 
end subroutine generate
```

254c  $\langle$ Declaration of `tao_random_numbers` 254c $\rangle \equiv$

```
private :: generate
```

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

254d  $\langle$ Load a and refresh state 254d $\rangle \equiv$

```
a(1:K) = state(1:K)
```

The remaining  $n - K$  random numbers can be gotten directly from the recursion (C.1). Note that Fortran90's `modulo` intrinsic does the right thing, since it guarantees (unlike Fortran77's `mod`) that  $0 \leq \text{modulo}(a, m) < a$  if  $m > 0$ ).

254e  $\langle$ Load a and refresh state 254d $\rangle + \equiv$

```
do j = K+1, n
  a(j) = modulo (a(j-K) - a(j-L), M)
end do
```

Do the recursion (C.1)  $K$  more times to prepare `state(1:K)` for the next invocation of `generate`.

254f  $\langle$ Load a and refresh state 254d $\rangle + \equiv$

```
state(1:L) = modulo (a(n+1-K:n+L-K) - a(n+1-L:n), M)
do j = L+1, K
  state(j) = modulo (a(n+j-K) - state(j-L), M)
end do
```

### C.2.2 Initialization of 30-bit Random Numbers

The non-trivial and most beautiful part is the algorithm to initialize the random number generator state `state` with the first  $K$  numbers. I haven't studied algebra over finite fields in sufficient depth to consider the mathematics behind it straightforward. The commentary below is rather verbose

and reflects my understanding of DEK's rather terse remarks (solution to exercise 3.6-9 [16]).

255a *⟨Implementation of tao\_random\_numbers 255a⟩*≡  
 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:

255b *⟨Variables in 30-bit tao\_random\_numbers 253c⟩*+≡  
 integer(kind=tao\_i32), dimension(K), save, private :: s\_state  
 logical, save, private :: s\_virginal = .true.

255c *⟨Implementation of tao\_random\_numbers 255a⟩*+≡  
 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

255d *⟨Implementation of tao\_random\_numbers 255a⟩*+≡  
 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.

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



```

        end do
        ⟨Fill state from x 257e⟩
        ⟨Warm up state 257f⟩
    end subroutine seed_stateless
Any default will do
256a ⟨Parameters local to tao_random_seed 256a⟩≡
    integer, parameter :: DEFAULT_SEED = 0
These must not be changed:
256b ⟨Parameters local to tao_random_seed 256a⟩+≡
    integer, parameter :: MAX_SEED = 2**30 - 3
    integer, parameter :: TT = 70
256c ⟨Set up seed_value from seed or DEFAULT_SEED 256c⟩≡
    if (present (seed)) then
        seed_value = modulo (seed, MAX_SEED + 1)
    else
        seed_value = DEFAULT_SEED
    end if
Fill the array  $x_1, \dots, x_K$  with even integers, shifted cyclically by 29 bits.
256d ⟨Bootstrap the x buffer 256d⟩≡
    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:
256e ⟨Bootstrap the x buffer 256d⟩+≡
    x(2) = x(2) + 1
256f ⟨Set up s and t 256f⟩≡
    s = seed_value
    t = TT - 1
Consider the polynomial

```

$$p(z) = \sum_{n=1}^K x_n z^{n-1} = x_K z^{K-1} + \dots + x_2 z + x_1 \quad (\text{C.2})$$

We have  $p(z)^2 = p(z^2) \pmod{2}$  because cross terms have an even coefficient and  $x_n^2 = x_n \pmod{2}$ . Therefore we can square the polynomial by shifting the coefficients. The coefficients for  $n > K$  will be reduced.

```
257a  ⟨p(z) → p(z)2 (modulo  $z^K + z^L + 1$ ) 257a⟩≡
      x(3:2*K-1:2) = x(2:K)
      x(2:2*K-2:2) = 0
```

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

```
257b  ⟨p(z) → p(z)2 (modulo  $z^K + z^L + 1$ ) 257a⟩+≡
      do j = 2*K-1, K+1, -1
        x(j-(K-L)) = modulo (x(j-(K-L))-x(j), M)
        x(j-K)=modulo (x(j-K)-x(j), M)
      end do
```

```
257c  ⟨p(z) → zp(z) (modulo  $z^K + z^L + 1$ ) 257c⟩≡
      if (modulo (s, 2) == 1) then
        x(2:K+1) = x(1:K)
        x(1) = x(K+1)
        x(L+1) = modulo (x(L+1) - x(K+1), M)
      end if
```

```
257d  ⟨Shift s or t and exit if t ≤ 0 257d⟩≡
      if (s /= 0) then
        s = s / 2
      else
        t = t - 1
      end if
      if (t <= 0) then
        exit
      end if
```

```
257e  ⟨Fill state from x 257e⟩≡
      state(1:K-L) = x(L+1:K)
      state(K-L+1:K) = x(1:L)
```

```
257f  ⟨Warm up state 257f⟩≡
      do j = 1, 10
        call generate (x, state)
      end do
```

```
257g  ⟨Interfaces of tao_random_numbers 257g⟩≡
      interface tao_random_seed
        module procedure ⟨Specific procedures for tao_random_seed 258b⟩
      end interface
```

258a  $\langle$ Declaration of tao\_random\_numbers 254e $\rangle + \equiv$   
       private ::  $\langle$ Specific procedures for tao\_random\_seed 258b $\rangle$   
 258b  $\langle$ Specific procedures for tao\_random\_seed 258b $\rangle \equiv$   
       seed\_static, seed\_state, seed\_raw\_state

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

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

258c  $\langle$ Variables in 52-bit tao\_random\_numbers 258c $\rangle \equiv$   
       real(kind=tao\_r64), parameter, private :: M = 1.0\_tao\_r64

The state of the internal routines

258d  $\langle$ Variables in 52-bit tao\_random\_numbers 258c $\rangle + \equiv$   
       real(kind=tao\_r64), dimension(K), save, private :: s\_state  
       logical, save, private :: s\_virginal = .true.

258e  $\langle$ Implementation of 52-bit tao\_random\_numbers 258e $\rangle \equiv$   
       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)  
          $\langle$ Load 52-bit a and refresh state 258f $\rangle$   
       end subroutine generate

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

258f  $\langle$ Load 52-bit a and refresh state 258f $\rangle \equiv$   
       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.

258g  $\langle$ Implementation of 52-bit tao\_random\_numbers 258e $\rangle + \equiv$   
       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 256a>
  <Variables local to 52-bit tao_random_seed 259b>
  <Set up seed_value from seed or DEFAULT_SEED 256c>
  <Bootstrap the 52-bit x buffer 259d>
  <Set up s and t 256f>
do
  <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  259f>
  <52-bit  $p(z) \rightarrow zp(z) \pmod{z^K + z^L + 1}$  260a>
  <Shift s or t and exit if t ≤ 0 257d>
end do
  <Fill state from x 257e>
  <Warm up state 257f>
end subroutine seed_stateless

259a <Declaration of tao_random_numbers 254c>+≡
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
real(kind=tao_r64) :: ss
integer :: seed_value, t, s, j

259d <Bootstrap the 52-bit x buffer 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

259e <Bootstrap the 52-bit x buffer 259d>+≡
x(2) = x(2) + ULP

259f <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  259f>≡
x(3:2*K-1:2) = x(2:K)
x(2:2*K-2:2) = 0

This works because 2*K-1 is odd

259g <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  259f>+≡
do j = 2*K-1, K+1, -1

```

```

        x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
        x(j-K) = modulo (x(j-K) + x(j), M)
    end do
260a   $\langle 52\text{-bit } p(z) \rightarrow zp(z) \text{ (modulo } z^K + z^L + 1) \text{ 260a} \rangle \equiv$ 
    if (modulo (s, 2) == 1) THEN
        x(2:K+1) = x(1:K)
        x(1) = x(K+1)
        x(L+1) = modulo (x(L+1) + x(K+1), M)
    end if

```

### C.3 The State

```

260b   $\langle \text{Declaration of 30-bit tao\_random\_numbers types 260b} \rangle \equiv$ 
    type, public :: tao_random_raw_state
    private
        integer(kind=tao_i32), dimension(K) :: x
    end type tao_random_raw_state

260c   $\langle \text{Declaration of 30-bit tao\_random\_numbers types 260b} \rangle + \equiv$ 
    type, public :: tao_random_state
    private
        type(tao_random_raw_state) :: state
        integer(kind=tao_i32), dimension(:), pointer :: buffer => null ()
        integer :: buffer_end, last
    end type tao_random_state

260d   $\langle \text{Declaration of 52-bit tao\_random\_numbers types 260d} \rangle \equiv$ 
    type, public :: tao_random_raw_state
    private
        real(kind=tao_r64), dimension(K) :: x
    end type tao_random_raw_state

260e   $\langle \text{Declaration of 52-bit tao\_random\_numbers types 260d} \rangle + \equiv$ 
    type, public :: tao_random_state
    private
        type(tao_random_raw_state) :: state
        real(kind=tao_r64), dimension(:), pointer :: buffer => null ()
        integer :: buffer_end, last
    end type tao_random_state

```

#### C.3.1 Creation

```

260f   $\langle \text{Interfaces of tao\_random\_numbers 257g} \rangle + \equiv$ 

```

```

interface tao_random_create
  module procedure <Specific procedures for tao_random_create 261b>
end interface

```

261a *<Declaration of tao\_random\_numbers 254c>+≡*

```

  private :: <Specific procedures for tao_random_create 261b>

```

261b *<Specific procedures for tao\_random\_create 261b>≡*

```

  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.

261c *<Implementation of tao\_random\_numbers 255a>+≡*

```

  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

```

261d *<Implementation of tao\_random\_numbers 255a>+≡*

```

  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

```

261e *<Implementation of tao\_random\_numbers 255a>+≡*

```

  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 255a>+≡
    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 255a>+≡
    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 255a>+≡
    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 257g>+≡
    interface tao_random_destroy
        module procedure destroy_state, destroy_raw_state
    end interface

262e <Declaration of tao_random_numbers 254c>+≡
    private :: destroy_state, destroy_raw_state

262f <Implementation of tao_random_numbers 255a>+≡
    elemental subroutine destroy_state (s)
        type(tao_random_state), intent(inout) :: s
        deallocate (s%buffer)
    end subroutine destroy_state

```

```
end subroutine destroy_state
```

Currently, this is a no-op, but we might need a non-trivial destruction method in the future

```
263a <Implementation of tao_random_numbers 255a>+≡
      elemental subroutine destroy_raw_state (s)
        type(tao_random_raw_state), intent(inout) :: s
      end subroutine destroy_raw_state
```

### C.3.3 Copying

```
263b <Interfaces of tao_random_numbers 257g>+≡
      interface tao_random_copy
        module procedure <Specific procedures for tao_random_copy 263e>
      end interface
```

```
263c <Interfaces of tao_random_numbers 257g>+≡
      interface assignment(=)
        module procedure <Specific procedures for tao_random_copy 263e>
      end interface
```

```
263d <Declaration of tao_random_numbers 254c>+≡
      public :: assignment(=)
      private :: <Specific procedures for tao_random_copy 263e>
```

```
263e <Specific procedures for tao_random_copy 263e>≡
      copy_state, copy_raw_state, &
      copy_raw_state_to_state, copy_state_to_raw_state
```

```
263f <Implementation of tao_random_numbers 255a>+≡
      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
```

```
263g <Implementation of tao_random_numbers 255a>+≡
      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
264a  <Implementation of tao_random_numbers 255a>+≡
        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
264b  <Implementation of tao_random_numbers 255a>+≡
        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

```

264c  <Implementation of tao_random_numbers 255a>+≡
        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

```

264d  <Interfaces of tao_random_numbers 257g>+≡
        interface tao_random_write
            module procedure &
                write_state_unit, write_state_name, &
                write_raw_state_unit, write_raw_state_name
        end interface
264e  <Declaration of tao_random_numbers 254c>+≡
        private :: write_state_unit, write_state_name
        private :: write_raw_state_unit, write_raw_state_name
264f  <Interfaces of tao_random_numbers 257g>+≡
        interface tao_random_read
            module procedure &
                read_state_unit, read_state_name, &
                read_raw_state_unit, read_raw_state_name

```

```

end interface

265a  <Declaration of tao_random_numbers 254c>+≡
      private :: read_state_unit, read_state_name
      private :: read_raw_state_unit, read_raw_state_name

265b  <Implementation of tao_random_numbers 255a>+≡
      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

265c  <Implementation of tao_random_numbers 255a>+≡
      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

265d  <Implementation of tao_random_numbers 255a>+≡
      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

```

266a *<Implementation of tao\_random\_numbers 255a>+≡*

```

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

```

266b *<Implementation of 30-bit tao\_random\_numbers 254b>+≡*

```

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

```

266c *<Declaration of 30-bit tao\_random\_numbers 266c>≡*

```

private :: write_state_array

```

266d *<Implementation of 30-bit tao\_random\_numbers 254b>+≡*

```

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

```

266e *<Declaration of 30-bit tao\_random\_numbers 266c>+≡*

```

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 ...

266f *<Implementation of 52-bit tao\_random\_numbers 258e>+≡*

```

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

267a  <Declaration of 52-bit tao_random_numbers 267a>≡
    private :: write_state_array

267b  <Implementation of 52-bit tao_random_numbers 258e>+≡
    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

267c  <Declaration of 52-bit tao_random_numbers 267a>+≡
    private :: read_state_array

267d  <Implementation of tao_random_numbers 255a>+≡
    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
    end subroutine

```

```

        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 254c>+≡
        private :: find_free_unit

268c  <Implementation of tao_random_numbers 255a>+≡
        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 255a>+≡
        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 255a>+≡
        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

268f  <Implementation of tao_random_numbers 255a>+≡
        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!

269a *<Interfaces of tao\_random\_numbers 257g>+≡*

```

interface tao_random_marshall_size
  module procedure marshal_state_size, marshal_raw_state_size
end interface
interface tao_random_marshall
  module procedure marshal_state, marshal_raw_state
end interface
interface tao_random_unmarshal
  module procedure unmarshal_state, unmarshal_raw_state
end interface

```

269b *<Declaration of tao\_random\_numbers 254c>+≡*

```

public :: tao_random_marshall
private :: marshal_state, marshal_raw_state
public :: tao_random_marshall_size
private :: marshal_state_size, marshal_raw_state_size
public :: tao_random_unmarshal
private :: unmarshal_state, unmarshal_raw_state

```

269c *<Implementation of 30-bit tao\_random\_numbers 254b>+≡*

```

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 254b>+≡*

```

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 254b>+≡*

```

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 254b>+≡*

```

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 254b>+≡*

```

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

```

270e *<Implementation of 30-bit tao\_random\_numbers 254b>+≡*

```

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

271a ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
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

271b ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
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

271c ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
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

271d ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
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

```



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

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

272c *<tao\_random\_numbers.f90 272c>≡*  
 ! 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 254c>*  
*<Declaration of 30-bit tao\_random\_numbers 266c>*  
*<Interfaces of tao\_random\_numbers 257g>*  
*<Interfaces of 30-bit tao\_random\_numbers 279e>*  
*<Parameters in tao\_random\_numbers 253a>*  
*<Variables in tao\_random\_numbers 268a>*  
*<Variables in 30-bit tao\_random\_numbers 253c>*  
*<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 255a>*  
   *<Implementation of 30-bit tao\_random\_numbers 254b>*  
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 254c>
  <Declaration of 52-bit tao_random_numbers 267a>
  <Interfaces of tao_random_numbers 257g>
  <Interfaces of 52-bit tao_random_numbers 280c>
  <Parameters in tao_random_numbers 253a>
  <Variables in tao_random_numbers 268a>
  <Variables in 52-bit tao_random_numbers 258c>
  <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 255a>
    <Implementation of 52-bit tao_random_numbers 258e>
end module tao52_random_numbers

Ten functions are exported
273b <Declaration of tao_random_numbers 254c>+≡
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  $0 \leq r < 2^{30} = 1073741824$ :

```

273c <Implementation of 30-bit tao_random_numbers 254b>+≡
  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_* 274a>
end subroutine integer_stateless

```

274a <Body of tao\_random\_\* 274a>≡  
 <Step last and reload buffer iff necessary 274c>  
 r = NORM \* buffer(last)

The low level routine `generate` will fill an array  $a_1, \dots, a_n$ , which will be consumed and refilled like an input buffer. We need at least  $n \geq K$  for the call to `generate`.

274b <Variables in 30-bit tao\_random\_numbers 253c>+≡  
 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.

274c <Step last and reload buffer iff necessary 274c>≡  
 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.

274d <Implementation of 30-bit tao\_random\_numbers 254b>+≡  
 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\_\* 274a>  
end subroutine real\_stateless

A random real  $r \in [0, 1)$ .

274e <Implementation of 52-bit tao\_random\_numbers 258e>+≡  
 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_* 274a⟩
end subroutine real_stateless

```

The low level routine `generate` will fill an array  $a_1, \dots, a_N$ , which will be consumed and refilled like an input buffer.

**275a** *⟨Variables in 52-bit tao\_random\_numbers 258c⟩* +=  

```

real(kind=tao_r64), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
integer, save, private :: s_buffer_end = size (s_buffer)
integer, save, private :: s_last = size (s_buffer)

```

### C.4.2 Arrays of Random Numbers

Fill the array  $j_1, \dots, j_\nu$  with random integers  $0 \leq j_i < 2^{30} = 1073741824$ . This has to be done such that the underlying array length in `generate` is transparent to the user. At the same time we want to avoid the overhead of calling `tao_random_real`  $\nu$  times.

**275b** *⟨Implementation of 30-bit tao\_random\_numbers 254b⟩* +=  

```

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 275c⟩
end subroutine integer_array_stateless

```

**275c** *⟨Body of tao\_random\*\_array 275c⟩* =  

```

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 254b⟩*+≡

```
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 275c>
end subroutine real_array_stateless
Fill the array  $v_1, \dots, v_\nu$  with uniform deviates  $v_i \in [0, 1)$ .
277a <Implementation of 52-bit tao_random_numbers 258e>+≡
    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 275c>
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 254b>+≡
    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 254b>+≡
    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 258e>+≡
    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
277e <Implementation of 30-bit tao_random_numbers 254b>+≡
    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

278a  <Implementation of 30-bit tao_random_numbers 254b>+≡
    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

278b  <Implementation of 52-bit tao_random_numbers 258e>+≡
    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:

278c  <Initialize a virginal random number generator 278c>≡
    if (s_virginal) then
        call tao_random_seed ()
    end if

278d  <Implementation of 30-bit tao_random_numbers 254b>+≡
    subroutine integer_static (r)
        integer, intent(out) :: r
        <Initialize a virginal random number generator 278c>
        call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
    end subroutine integer_static

278e  <Implementation of 30-bit tao_random_numbers 254b>+≡
    subroutine real_static (r)
        real(kind=default), intent(out) :: r
        <Initialize a virginal random number generator 278c>
        call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
    end subroutine real_static

```

```

279a  ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
      subroutine real_static (r)
        real(kind=default), intent(out) :: r
        ⟨Initialize a virginal random number generator 278c⟩
        call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
      end subroutine real_static

279b  ⟨Implementation of 30-bit tao_random_numbers 254b⟩+≡
      subroutine integer_array_static (v, num)
        integer, dimension(:), intent(out) :: v
        integer, optional, intent(in) :: num
        ⟨Initialize a virginal random number generator 278c⟩
        call integer_array_stateless &
           (s_state, s_buffer, s_buffer_end, s_last, v, num)
      end subroutine integer_array_static

279c  ⟨Implementation of 30-bit tao_random_numbers 254b⟩+≡
      subroutine real_array_static (v, num)
        real(kind=default), dimension(:), intent(out) :: v
        integer, optional, intent(in) :: num
        ⟨Initialize a virginal random number generator 278c⟩
        call real_array_stateless &
           (s_state, s_buffer, s_buffer_end, s_last, v, num)
      end subroutine real_array_static

279d  ⟨Implementation of 52-bit tao_random_numbers 258e⟩+≡
      subroutine real_array_static (v, num)
        real(kind=default), dimension(:), intent(out) :: v
        integer, optional, intent(in) :: num
        ⟨Initialize a virginal random number generator 278c⟩
        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

```

279e  ⟨Interfaces of 30-bit tao_random_numbers 279e⟩≡
      interface tao_random_number
        module procedure ⟨Specific procedures for 30-bit tao_random_number 279f⟩
      end interface

279f  ⟨Specific procedures for 30-bit tao_random_number 279f⟩≡
      integer_static, integer_state, &
      integer_array_static, integer_array_state, &
      real_static, real_state, real_array_static, real_array_state

```



These are not exported

- 280a *<Declaration of 30-bit tao\_random\_numbers 266c>+≡*  
private :: &  
integer\_stateless, integer\_array\_stateless, &  
real\_stateless, real\_array\_stateless
- 280b *<Declaration of 30-bit tao\_random\_numbers 266c>+≡*  
private :: *<Specific procedures for 30-bit tao\_random\_number 279f>*
- 280c *<Interfaces of 52-bit tao\_random\_numbers 280c>≡*  
interface tao\_random\_number  
module procedure *<Specific procedures for 52-bit tao\_random\_number 280d>*  
end interface
- 280d *<Specific procedures for 52-bit tao\_random\_number 280d>≡*  
real\_static, real\_state, real\_array\_static, real\_array\_state

Thes are not exported

- 280e *<Declaration of 52-bit tao\_random\_numbers 267a>+≡*  
private :: real\_stateless, real\_array\_stateless
- 280f *<Declaration of 52-bit tao\_random\_numbers 267a>+≡*  
private :: *<Specific procedures for 52-bit tao\_random\_number 280d>*

#### C.4.6 *Luxury*

- 280g *<Implementation of tao\_random\_numbers 255a>+≡*  
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
- 280h *<Implementation of tao\_random\_numbers 255a>+≡*  
elemental subroutine luxury\_state (s)  
type(tao\_random\_state), intent(inout) :: s

```

        call luxury_state_integer (s, size (s%buffer))
    end subroutine luxury_state

281a  <Implementation of tao_random_numbers 255a>+≡
    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

281b  <Implementation of tao_random_numbers 255a>+≡
    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

281c  <Implementation of tao_random_numbers 255a>+≡
    subroutine luxury_static ()
        <Initialize a virginal random number generator 278c>
        call luxury_static_integer (size (s_buffer))
    end subroutine luxury_static

281d  <Implementation of tao_random_numbers 255a>+≡
    subroutine luxury_static_integer (consumption)
        integer, intent(in) :: consumption
        <Initialize a virginal random number generator 278c>
        call luxury_stateless (size (s_buffer), s_buffer_end, s_last, consumption)
    end subroutine luxury_static_integer

281e  <Implementation of tao_random_numbers 255a>+≡
    subroutine luxury_static_real (consumption)
        real(kind=default), intent(in) :: consumption
        <Initialize a virginal random number generator 278c>
        call luxury_static_integer (int (consumption * size (s_buffer)))
    end subroutine luxury_static_real

281f  <Interfaces of tao_random_numbers (unused luxury) 281f>≡
    interface tao_random_luxury
        module procedure <Specific procedures for tao_random_luxury 282a>
    end interface

281g  <Declaration of tao_random_numbers (unused luxury) 281g>≡
    private :: luxury_stateless

281h  <Declaration of tao_random_numbers (unused luxury) 281g>+≡
    private :: <Specific procedures for tao_random_luxury 282a>

```

282a  $\langle$ Specific procedures for tao\_random\_luxury 282a $\rangle \equiv$   
 luxury\_static, luxury\_state, &  
 luxury\_static\_integer, luxury\_state\_integer, &  
 luxury\_static\_real, luxury\_state\_real

## C.5 Testing

### C.5.1 30-bit

282b  $\langle$ Implementation of 30-bit tao\_random\_numbers 254b $\rangle + \equiv$   
 subroutine tao\_random\_test (name)  
   character(len=\*), optional, intent(in) :: name  
   character (len = \*), parameter :: &  
     OK = "(1x,i10,' is ok. ')", &  
     NOT\_OK = "(1x,i10,' is not ok, (expected ',i10,')!')"  
    $\langle$ Parameters in tao\_random\_test 282c $\rangle$   
   integer, parameter :: &  
     A\_2027082 = 995235265  
   integer, dimension(N) :: a  
   type(tao\_random\_state) :: s, t  
   integer, dimension(:), allocatable :: ibuf  
   real(kind=tao\_r64), dimension(:), allocatable :: dbuf  
   integer :: i, ibuf\_size, dbuf\_size  
   print \*, TAO\_RANDOM\_NUMBERS\_RCS\_ID  
   print \*, "testing the 30-bit tao\_random\_numbers ..."  
    $\langle$ Perform simple tests of tao\_random\_numbers 282d $\rangle$   
    $\langle$ Perform more tests of tao\_random\_numbers 283c $\rangle$   
 end subroutine tao\_random\_test

282c  $\langle$ Parameters in tao\_random\_test 282c $\rangle \equiv$   
 integer, parameter :: &  
   SEED = 310952, &  
   N = 2009, M = 1009, &  
   N\_SHORT = 1984

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

282d  $\langle$ Perform simple tests of tao\_random\_numbers 282d $\rangle \equiv$   
 ! 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 283a⟩*

283a *⟨Test a(1) = A\_2027082 283a⟩*≡  
if (a(1) == A\_2027082) then  
  print OK, a(1)  
else  
  print NOT\_OK, a(1), A\_2027082  
  stop 1  
end if

Deja vu all over again, but 2027081 is factored the other way around this time

283b *⟨Perform simple tests of tao\_random\_numbers 282d⟩*+≡  
  call tao\_random\_seed (SEED)  
  do i = 1, M+1  
    call tao\_random\_number (a)  
  end do  
*⟨Test a(1) = A\_2027082 283a⟩*

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

283c *⟨Perform more tests of tao\_random\_numbers 283c⟩*≡  
  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 283a⟩*

and restart the saved generator

283d *⟨Perform more tests of tao\_random\_numbers 283c⟩*+≡  
  do i = 1, N+1 - N\_SHORT  
    call tao\_random\_number (t, a, M)  
  end do  
*⟨Test a(1) = A\_2027082 283a⟩*

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

283e *⟨Perform more tests of tao\_random\_numbers 283c⟩*+≡  
  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 283a>
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 283a>
end if

```

And finally using marshaling/unmarshaling:

```

284a <Perform more tests of tao_random_numbers 283c>+≡
    print *, "testing marshaling/unmarshaling ..."
    call tao_random_seed (s, SEED)
    do i = 1, N_SHORT
        call tao_random_number (s, a, M)
    end do
    call tao_random_marshall_size (s, ibuf_size, dbuf_size)
    allocate (ibuf(ibuf_size), dbuf(dbuf_size))
    call tao_random_marshall (s, ibuf, dbuf)
    do i = 1, N+1 - N_SHORT
        call tao_random_number (s, a, M)
    end do
    <Test a(1) = A_2027082 283a>
    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 283a>

```

### C.5.2 52-bit

DEK's "official" test expects  $x_{1009 \cdot 2009 + 1} = x_{2027082} = 0.36410514377569680455$ :

```

284b <Implementation of 52-bit tao_random_numbers 258e>+≡
    subroutine tao_random_test (name)
        character(len=*), optional, intent(in) :: name
        character(len=*), parameter :: &
            OK = "(1x,f22.20,' is ok.')

```

```

real(kind=default), parameter :: &
    A_2027082 = 0.36410514377569680455_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 282d>
<Perform more tests of tao_random_numbers 283c>
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")
        stop 0
    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 [25]. It has an accuracy which is approximately one digit less than machine precision.

```

286b  <Declaration of specfun procedures 286b>≡
      public :: gamma

```

The so-called reflection formula is used for negative arguments:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \quad (\text{D.1})$$

Here's the identity transformation that pulls the argument of  $\Gamma$  into [3, 4]:

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

287a  $\langle$  Pull  $u$  into the intervall  $[3, 4]$  287a  $\rangle \equiv$

```

f = 1
if (u < 3) then
  do i = 1, int (4 - u)
    f = f / u
    u = u + 1
  end do
else
  do i = 1, int (u - 3)
    u = u - 1
    f = f * u
  end do
end if

```

A Chebyshev approximation for  $\Gamma(x)$  is used after mapping  $x \in [3, 4]$  linearly to  $h \in [-1, 1]$ . The series is 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  $\langle$  Clenshaw's recurrence formula 287b  $\rangle \equiv$

```

alpha = 2*g
b1 = 0
b2 = 0
do i = 15, 0, -1
  b0 = c(i) + alpha * b1 - b2
  b2 = b1
  b1 = b0
end do
g = f * (b0 - g * b2)

```

Note that we're assuming that  $c(0)$  is in fact  $c_0/2$ . This is for compatibility with the CERN library routines.

287c  $\langle$  Implementation of specfun procedures 287c  $\rangle \equiv$

```

pure function gamma (x) result (g)
  real(kind=default), intent(in) :: x
  real(kind=default) :: g
  integer :: i
  real(kind=default) :: u, f, alpha, b0, b1, b2
  real(kind=default), dimension(0:15), parameter :: &
    c =  $\langle c_0/2, c_1, c_2, \dots, c_{15}$  for  $\Gamma(x)$  288a  $\rangle$ 
  u = x
  if (u <= 0.0) then

```



```

        if (u == int (u)) then
            g = huge (g)
            return
        else
            u = 1 - u
        end if
    endif
    <Pull u into the intervall [3,4] 287a>
    g = 2*u - 7
    <Clenshaw's recurrence formula 287b>
    if (x < 0) then
        g = PI / (sin (PI * x) * g)
    end if
end function gamma

288a <c0/2, c1, c2, ..., c15 for  $\Gamma(x)$  288a>≡
    (/ 3.65738772508338244_default, &
       1.95754345666126827_default, &
       0.33829711382616039_default, &
       0.04208951276557549_default, &
       0.00428765048212909_default, &
       0.00036521216929462_default, &
       0.00002740064222642_default, &
       0.00000181240233365_default, &
       0.00000010965775866_default, &
       0.00000000598718405_default, &
       0.00000000030769081_default, &
       0.00000000001431793_default, &
       0.00000000000065109_default, &
       0.0000000000002596_default, &
       0.0000000000000111_default, &
       0.0000000000000004_default /)

```

## D.1 Test

```

288b <stest.f90 288b>≡
    ! stest.f90 --
    <Copyleft notice 1>
    module stest_functions
        use kinds
        use constants
        use specfun
    end module

```

```

private
  <Declaration of stest_functions procedures 289a>
contains
  <Implementation of stest_functions procedures 289b>
end module stest_functions

```

289a <Declaration of stest\_functions procedures 289a>≡  
 public :: gauss\_multiplication

Gauss' multiplication fomula can serve as a non-trivial test

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \quad (\text{D.4})$$

289b <Implementation of stest\_functions procedures 289b>≡  
 pure function gauss\_multiplication (x, n) result (delta)  
 real(kind=default), intent(in) :: x  
 integer, intent(in) :: n  
 real(kind=default) :: delta  
 real(kind=default) :: gxn  
 integer :: k  
 gxn = (2\*PI)\*\*(0.5\_double\*(1-n)) \* n\*\*(n\*x-0.5\_double)  
 do k = 0, n - 1  
 gxn = gxn \* gamma (x + real (k, kind=default) / n)  
 end do  
 delta = abs ((gamma (n\*x) - gxn) / gamma (n\*x))  
end function gauss\_multiplication

289c <stest.f90 288b>+≡  
 program stest  
 use kinds  
 use specfun  
 use stest\_functions !NODEP!  
 implicit none  
 integer :: i, steps  
 real(kind=default) :: x, g, xmin, xmax  
 xmin = -4.5  
 xmax = 4.5  
 steps = 100 ! 9  
 do i = 0, steps  
 x = xmin + ((xmax - xmin) / real (steps)) \* i  
 print "(f6.3,4(1x,e9.2))", x, &  
 gauss\_multiplication (x, 2), &  
 gauss\_multiplication (x, 3), &  
 gauss\_multiplication (x, 4), &

```
        gauss_multiplication (x, 5)
    end do
end program stest
```

# —E—

## STATISTICS

**291a**  $\langle \text{vamp\_stat.f90 291a} \rangle \equiv$   
`! vamp_stat.f90 --`  
 $\langle \text{Copyleft notice 1} \rangle$   
`module vamp_stat`  
`use kinds`  
`implicit none`  
`private`  
 $\langle \text{Declaration of vamp\_stat procedures 291b} \rangle$   
`character(len=*), public, parameter :: VAMP_STAT_RCS_ID = &`  
`"$Id: vamp_stat.nw 314 2010-04-17 20:32:33Z ohl $"`  
`contains`  
 $\langle \text{Implementation of vamp\_stat procedures 291c} \rangle$   
`end module vamp_stat`

**291b**  $\langle \text{Declaration of vamp\_stat procedures 291b} \rangle \equiv$   
`public :: average, standard_deviation, value_spread`

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

**291c**  $\langle \text{Implementation of vamp\_stat procedures 291c} \rangle \equiv$   
`pure function average (x) result (a)`  
`real(kind=default), dimension(:), intent(in) :: x`  
`real(kind=default) :: a`  
`integer :: n`  
`n = size (x)`  
`if (n == 0) then`  
`a = 0.0`  
`else`  
`a = sum (x) / n`  
`end if`  
`end function average`

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

292a *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
    s = huge (s)
  else
    s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
                  0.0_default))
  end if
end function standard_deviation

```

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

292b *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread

```

292c *<Declaration of vamp\_stat procedures 291b>+≡*

```

public :: standard_deviation_percent, value_spread_percent

```

292d *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
  else
    s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent

```

292e *<Implementation of vamp\_stat procedures 291c>+≡*

```

pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x

```

```

real(kind=default) :: s
real(kind=default) :: abs_avg
abs_avg = abs (average (x))
if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
else
    s = 100.0 * value_spread (x) / abs_avg
end if
end function value_spread_percent

```

# —F—

## HISTOGRAMMING

⚡ Merged WK's improvements for WHIZARD. TODO *after* merging:

1. bins3 is a bad undescriptive name
2. bins3 should be added to histogram2
3. write\_histogram2\_unit for symmetry.

⚡ There's almost no sanity checking. If you call one of these functions on a histogram that has not been initialized, you loose. — *Big time.*

```

294a <histograms.f90 294a>≡
    ! histograms.f90 --
    <Copyleft notice 1>
    module histograms
    use kinds
    use utils, only: find_free_unit
    implicit none
    private
    <Declaration of histograms procedures 295b>
    <Interfaces of histograms procedures 295c>
    <Variables in histograms 295e>
    <Declaration of histograms types 294b>
    character(len=*), public, parameter :: HISTOGRAMS_RCS_ID = &
        "$Id: histograms.nw 314 2010-04-17 20:32:33Z ohl $"
    contains
    <Implementation of histograms procedures 295f>
    end module histograms

294b <Declaration of histograms types 294b>≡
    type, public :: histogram
    private
    integer :: n_bins
    real(kind=default) :: x_min, x_max

```

```

        real(kind=default), dimension(:), pointer :: bins => null ()
        real(kind=default), dimension(:), pointer :: bins2 => null ()
        real(kind=default), dimension(:), pointer :: bins3 => null ()
    end type histogram

```

295a *<Declaration of histograms types 294b>+≡*

```

type, public :: histogram2
    private
    integer, dimension(2) :: n_bins
    real(kind=default), dimension(2) :: x_min, x_max
    real(kind=default), dimension(:,:), pointer :: bins => null ()
    real(kind=default), dimension(:,:), pointer :: bins2 => null ()
end type histogram2

```

295b *<Declaration of histograms procedures 295b>≡*

```

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

```

295c *<Interfaces of histograms procedures 295c>≡*

```

interface create_histogram
    module procedure create_histogram1, create_histogram2
end interface
interface fill_histogram
    module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
end interface
interface delete_histogram
    module procedure delete_histogram1, delete_histogram2
end interface
interface write_histogram
    module procedure write_histogram1, write_histogram2
    module procedure write_histogram1_unit
end interface

```

295d *<Declaration of histograms procedures 295b>+≡*

```

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

```

295e *<Variables in histograms 295e>≡*

```

integer, parameter, private :: N_BINS_DEFAULT = 10

```

295f *<Implementation of histograms procedures 295f>≡*

```

elemental subroutine create_histogram1 (h, x_min, x_max, nb)
    type(histogram), intent(out) :: h

```



```

real(kind=default), intent(in) :: x_min, x_max
integer, intent(in), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
h%bins = 0
h%bins2 = 0
allocate (h%bins3(0:h%n_bins+1))
h%bins3 = 0
end subroutine create_histogram1

```

296a *⟨Implementation of histograms procedures 295f⟩* +=

```

pure subroutine create_histogram2 (h, x_min, x_max, nb)
type(histogram2), intent(out) :: h
real(kind=default), dimension(:), intent(in) :: x_min, x_max
integer, intent(in), dimension(:), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
          h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
h%bins = 0
h%bins2 = 0
end subroutine create_histogram2

```

296b *⟨Implementation of histograms procedures 295f⟩* +=

```

elemental subroutine fill_histogram1 (h, x, weight, excess)
type(histogram), intent(inout) :: h
real(kind=default), intent(in) :: x
real(kind=default), intent(in), optional :: weight
real(kind=default), intent(in), optional :: excess
integer :: i
if (x < h%x_min) then
    i = 0
else if (x > h%x_max) then
    i = h%n_bins + 1

```

```

else
    i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
!WK! i = min (max (i, 0), h%n_bins + 1)
end if
if (present (weight)) then
    h%bins(i) = h%bins(i) + weight
    h%bins2(i) = h%bins2(i) + weight*weight
else
    h%bins(i) = h%bins(i) + 1
    h%bins2(i) = h%bins2(i) + 1
end if
if (present (excess)) h%bins3(i) = h%bins3(i) + excess
end subroutine fill_histogram1

```

297a *⟨Implementation of histograms procedures 295f⟩*+≡  
 elemental subroutine fill\_histogram2s (h, x1, x2, weight)  
 type(histogram2), intent(inout) :: h  
 real(kind=default), intent(in) :: x1, x2  
 real(kind=default), intent(in), optional :: weight  
 call fill\_histogram2v (h, (/ x1, x2 /), weight)  
 end subroutine fill\_histogram2s

297b *⟨Implementation of histograms procedures 295f⟩*+≡  
 pure subroutine fill\_histogram2v (h, x, weight)  
 type(histogram2), intent(inout) :: h  
 real(kind=default), dimension(:), intent(in) :: x  
 real(kind=default), intent(in), optional :: weight  
 integer, dimension(2) :: i  
 i = 1 + h%n\_bins \* (x - h%x\_min) / (h%x\_max - h%x\_min)  
 i = min (max (i, 0), h%n\_bins + 1)  
 if (present (weight)) then  
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight  
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight\*weight  
 else  
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1  
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1  
 end if  
 end subroutine fill\_histogram2v

297c *⟨Implementation of histograms procedures 295f⟩*+≡  
 elemental subroutine delete\_histogram1 (h)  
 type(histogram), intent(inout) :: h  
 deallocate (h%bins, h%bins2)  
 deallocate (h%bins3)  
 end subroutine delete\_histogram1

```

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

298b  <Implementation of histograms procedures 295f>+≡
      subroutine write_histogram1 (h, name, over)
        type(histogram), intent(in) :: h
        character(len=*), intent(in), optional :: name
        logical, intent(in), optional :: over
        integer :: i, iounit
        if (present (name)) then
          call find_free_unit (iounit)
          if (iounit > 0) then
            open (unit = iounit, action = "write", status = "replace", &
                  file = name)
            if (present (over)) then
              if (over) then
                write (unit = iounit, fmt = *) &
                  "underflow", h%bins(0), sqrt (h%bins2(0))
              end if
            end if
            do i = 1, h%n_bins
              write (unit = iounit, fmt = *) &
                midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
            end do
            if (present (over)) then
              if (over) then
                write (unit = iounit, fmt = *) &
                  "overflow", h%bins(h%n_bins+1), &
                  sqrt (h%bins2(h%n_bins+1))
              end if
            end if
            close (unit = iounit)
          else
            print *, "write_histogram: Can't find a free unit!"
          end if
        else
          if (present (over)) then
            if (over) then
              print *, "underflow", h%bins(0), sqrt (h%bins2(0))
            end if
          end if
        end if
      end if

```

```

do i = 1, h%n_bins
  print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
end do
if (present (over)) then
  if (over) then
    print *, "overflow", h%bins(h%n_bins+1), &
      sqrt (h%bins2(h%n_bins+1))
  end if
end if
end if
end subroutine write_histogram1

```

299a *<Declaration of histograms procedures 295b>+≡*  
 !WK! public :: write\_histogram1\_unit



I don't like the `format` statement with the line number. Use a character constant instead (after we have merged with WHIZARD's branch).

299b *<Implementation of histograms procedures 295f>+≡*

```

subroutine write_histogram1_unit (h, iounit, over, show_excess)
  type(histogram), intent(in) :: h
  integer, intent(in) :: iounit
  logical, intent(in), optional :: over, show_excess
  integer :: i
  logical :: show_exc
  show_exc = .false.; if (present(show_excess)) show_exc = show_excess
  if (present (over)) then
    if (over) then
      if (show_exc) then
        write (unit = iounit, fmt = 1) &
          "underflow", h%bins(0), sqrt (h%bins2(0)), h%bins3(0)
      else
        write (unit = iounit, fmt = 1) &
          "underflow", h%bins(0), sqrt (h%bins2(0))
      end if
    end if
  end if
  do i = 1, h%n_bins
    if (show_exc) then
      write (unit = iounit, fmt = 1) &
        midpoint (h, i), h%bins(i), sqrt (h%bins2(i)), h%bins3(i)
    else
      write (unit = iounit, fmt = 1) &
        midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
    end if
  end do
end subroutine

```

```

        end if
    end do
    if (present (over)) then
        if (over) then
            if (show_exc) then
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1)), &
                    h%bins3(h%n_bins+1)
            else
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1))
            end if
        end if
    end if
    1 format (1x,4(G16.9,2x))
end subroutine write_histogram1_unit

```

300a *<Declaration of histograms procedures 295b>+≡*  
 private :: midpoint

300b *<Interfaces of histograms procedures 295c>+≡*  
 interface midpoint  
 module procedure midpoint1, midpoint2  
 end interface

300c *<Declaration of histograms procedures 295b>+≡*  
 private :: midpoint1, midpoint2

300d *<Implementation of histograms procedures 295f>+≡*  
 elemental function midpoint1 (h, bin) result (x)  
 type(histogram), intent(in) :: h  
 integer, intent(in) :: bin  
 real(kind=default) :: x  
 x = h%x\_min + (h%x\_max - h%x\_min) \* (bin - 0.5) / h%n\_bins  
 end function midpoint1

300e *<Implementation of histograms procedures 295f>+≡*  
 elemental function midpoint2 (h, bin, d) result (x)  
 type(histogram2), intent(in) :: h  
 integer, intent(in) :: bin, d  
 real(kind=default) :: x  
 x = h%x\_min(d) + (h%x\_max(d) - h%x\_min(d)) \* (bin - 0.5) / h%n\_bins(d)  
 end function midpoint2

```

301  <Implementation of histograms procedures 295f>+≡
      subroutine write_histogram2 (h, name, over)
        type(histogram2), intent(in) :: h
        character(len=*), intent(in), optional :: name
        logical, intent(in), optional :: over
        integer :: i1, i2, iounit
        if (present (name)) then
          call find_free_unit (iounit)
          if (iounit > 0) then
            open (unit = iounit, action = "write", status = "replace", &
                  file = name)
            if (present (over)) then
              if (over) then
                write (unit = iounit, fmt = *) &
                  "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
                do i2 = 1, h%n_bins(2)
                  write (unit = iounit, fmt = *) &
                    "x1 underflow", midpoint (h, i2, 2), &
                    h%bins(0,i2), sqrt (h%bins2(0,i2))
                end do
                do i1 = 1, h%n_bins(1)
                  write (unit = iounit, fmt = *) &
                    "x2 underflow", midpoint (h, i1, 1), &
                    h%bins(i1,0), sqrt (h%bins2(i1,0))
                end do
              end if
            end if
            do i1 = 1, h%n_bins(1)
              do i2 = 1, h%n_bins(2)
                write (unit = iounit, fmt = *) &
                  midpoint (h, i1, 1), midpoint (h, i2, 2), &
                  h%bins(i1,i2), sqrt (h%bins2(i1,i2))
              end do
            end do
            if (present (over)) then
              if (over) then
                do i2 = 1, h%n_bins(2)
                  write (unit = iounit, fmt = *) &
                    "x1 overflow", midpoint (h, i2, 2), &
                    h%bins(h%n_bins(1)+1,i2), &
                    sqrt (h%bins2(h%n_bins(1)+1,i2))
                end do
                do i1 = 1, h%n_bins(1)

```

```

        write (unit = iounit, fmt = *) &
            "x2 overflow", midpoint (h, i1, 1), &
            h%bins(i1,h%n_bins(2)+1), &
            sqrt (h%bins2(i1,h%n_bins(2)+1))
    end do
    write (unit = iounit, fmt = *) "double overflow", &
        h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
        sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
    end if
end if
close (unit = iounit)
else
    print *, "write_histogram: Can't find a free unit!"
end if
else
    if (present (over)) then
        if (over) then
            print *, "double underflow", h%bins(0,0), sqrt (h%bins2(0,0))
            do i2 = 1, h%n_bins(2)
                print *, "x1 underflow", midpoint (h, i2, 2), &
                    h%bins(0,i2), sqrt (h%bins2(0,i2))
            end do
            do i1 = 1, h%n_bins(1)
                print *, "x2 underflow", midpoint (h, i1, 1), &
                    h%bins(i1,0), sqrt (h%bins2(i1,0))
            end do
        end if
    end if
    do i1 = 1, h%n_bins(1)
        do i2 = 1, h%n_bins(2)
            print *, midpoint (h, i1, 1), midpoint (h, i2, 2), &
                h%bins(i1,i2), sqrt (h%bins2(i1,i2))
        end do
    end do
    if (present (over)) then
        if (over) then
            do i2 = 1, h%n_bins(2)
                print *, "x1 overflow", midpoint (h, i2, 2), &
                    h%bins(h%n_bins(1)+1,i2), &
                    sqrt (h%bins2(h%n_bins(1)+1,i2))
            end do
            do i1 = 1, h%n_bins(1)
                print *, "x2 overflow", midpoint (h, i1, 1), &

```

```

        h%bins(i1,h%n_bins(2)+1), &
        sqrt (h%bins2(i1,h%n_bins(2)+1))
    end do
    print *, "double overflow", &
        h%bins(h%n_bins(1)+1,h%n_bins(2)+1), &
        sqrt (h%bins2(h%n_bins(1)+1,h%n_bins(2)+1))
    end if
end if
end if
end subroutine write_histogram2

```



# —G—

## MISCELLANEOUS UTILITIES

```

304a  <utils.f90 304a>≡
      ! utils.f90 --
      <Copyleft notice 1>
      module utils
        use kinds
        implicit none
        private
        <Declaration of utils procedures 304b>
        <Parameters in utils 311c>
        <Variables in utils 312b>
        <Interfaces of utils procedures 304c>
        character(len=*), public, parameter :: UTILS_RCS_ID = &
          "$Id: utils.nw 314 2010-04-17 20:32:33Z ohl $"
      contains
        <Implementation of utils procedures 305c>
      end module utils

```

### *G.1 Memory Management*

```

304b  <Declaration of utils procedures 304b>≡
      public :: create_array_pointer
      private :: create_integer_array_pointer
      private :: create_real_array_pointer
      private :: create_integer_array2_pointer
      private :: create_real_array2_pointer

304c  <Interfaces of utils procedures 304c>≡
      interface create_array_pointer
        module procedure &
          create_integer_array_pointer, &

```

```

        create_real_array_pointer, &
        create_integer_array2_pointer, &
        create_real_array2_pointer
    end interface
305a  <Body of create_*_array_pointer 305a>≡
    if (associated (lhs)) then
        if (size (lhs) /= n) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb:n+lb-1))
            else
                allocate (lhs(n))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb:n+lb-1))
        else
            allocate (lhs(n))
        end if
    end if
    lhs = 0
305b  <Body of create_*_array2_pointer 305b>≡
    if (associated (lhs)) then
        if (any (ubound (lhs) /= n)) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
            else
                allocate (lhs(n(1),n(2)))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
        else
            allocate (lhs(n(1),n(2)))
        end if
    end if
    lhs = 0
305c  <Implementation of utils procedures 305c>≡
    pure subroutine create_integer_array_pointer (lhs, n, lb)

```

```

integer, dimension(:), pointer :: lhs
integer, intent(in) :: n
integer, intent(in), optional :: lb
<Body of create_*_array_pointer 305a>
end subroutine create_integer_array_pointer

```

306a <Implementation of utils procedures 305c>+≡

```

pure subroutine create_real_array_pointer (lhs, n, lb)
  real(kind=default), dimension(:), pointer :: lhs
  integer, intent(in) :: n
  integer, intent(in), optional :: lb
  <Body of create_*_array_pointer 305a>
end subroutine create_real_array_pointer

```

306b <Implementation of utils procedures 305c>+≡

```

pure subroutine create_integer_array2_pointer (lhs, n, lb)
  integer, dimension(:,:), pointer :: lhs
  integer, dimension(:), intent(in) :: n
  integer, dimension(:), intent(in), optional :: lb
  <Body of create_*_array2_pointer 305b>
end subroutine create_integer_array2_pointer

```

306c <Implementation of utils procedures 305c>+≡

```

pure subroutine create_real_array2_pointer (lhs, n, lb)
  real(kind=default), dimension(:,:), pointer :: lhs
  integer, dimension(:), intent(in) :: n
  integer, dimension(:), intent(in), optional :: lb
  <Body of create_*_array2_pointer 305b>
end subroutine create_real_array2_pointer

```

Copy an allocatable array component of a derived type, reshaping the target if necessary. The target can be disassociated, but its association *must not* be undefined.

306d <Declaration of utils procedures 304b>+≡

```

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

```

306e <Interfaces of utils procedures 304c>+≡

```

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

```

```

        copy_real_array2_pointer
    end interface

307a  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
        integer, dimension(:), pointer :: lhs
        integer, dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_integer_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
    end subroutine copy_integer_array_pointer

307b  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_real_array_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:), pointer :: lhs
        real(kind=default), dimension(:), intent(in) :: rhs
        integer, intent(in), optional :: lb
        call create_real_array_pointer (lhs, size (rhs), lb)
        lhs = rhs
    end subroutine copy_real_array_pointer

307c  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
        integer, dimension(:, :), pointer :: lhs
        integer, dimension(:, :), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_integer_array2_pointer &
            (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
    end subroutine copy_integer_array2_pointer

307d  <Implementation of utils procedures 305c>+≡
    pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
        real(kind=default), dimension(:, :), pointer :: lhs
        real(kind=default), dimension(:, :), intent(in) :: rhs
        integer, dimension(:), intent(in), optional :: lb
        call create_real_array2_pointer &
            (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
        lhs = rhs
    end subroutine copy_real_array2_pointer

```

## G.2 Sorting

```

307e  <Declaration of utils procedures 304b>+≡
    public :: swap

```

```

        private :: swap_integer, swap_real
308a  <Interfaces of utils procedures 304c>+≡
        interface swap
            module procedure swap_integer, swap_real
        end interface
308b  <Implementation of utils procedures 305c>+≡
        elemental subroutine swap_integer (a, b)
            integer, intent(inout) :: a, b
            integer :: tmp
            tmp = a
            a = b
            b = tmp
        end subroutine swap_integer
308c  <Implementation of utils procedures 305c>+≡
        elemental subroutine swap_real (a, b)
            real(kind=default), intent(inout) :: a, b
            real(kind=default) :: tmp
            tmp = a
            a = b
            b = tmp
        end subroutine swap_real
Straight insertion:
308d  <Implementation of utils procedures 305c>+≡
        pure subroutine sort_real (key, reverse)
            real(kind=default), dimension(:), intent(inout) :: key
            logical, intent(in), optional :: reverse
            logical :: rev
            integer :: i, j
            <Set rev to reverse or .false. 308e>
            do i = 1, size (key) - 1
                <Set j to minloc(key) 309a>
                if (j /= i) then
                    call swap (key(i), key(j))
                end if
            end do
        end subroutine sort_real
308e  <Set rev to reverse or .false. 308e>≡
        if (present (reverse)) then
            rev = reverse
        else
            rev = .false.
        end if

```

```

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

309b  <Implementation of utils procedures 305c>+≡
      pure subroutine sort_real_and_real_array (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        real(kind=default), dimension(:, :), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(:, i), table(:, j))
          end if
        end do
      end subroutine sort_real_and_real_array

309c  <Implementation of utils procedures 305c>+≡
      pure subroutine sort_real_and_integer (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        integer, dimension(:), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 308e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 309a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(i), table(j))
          end if
        end do
      end subroutine sort_real_and_integer

309d  <Declaration of utils procedures 304b>+≡
      public :: sort
      private :: sort_real, sort_real_and_real_array, sort_real_and_integer

```

310a *⟨Interfaces of utils procedures 304c⟩*+≡  

```

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

```

### *G.3 Mathematics*

310b *⟨Declaration of utils procedures 304b⟩*+≡  

```

public :: outer_product

```

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

310c *⟨Implementation of utils procedures 305c⟩*+≡  

```

pure function outer_product (x, y) result (xy)
  real(kind=default), dimension(:), intent(in) :: x, y
  real(kind=default), dimension(size(x),size(y)) :: xy
  xy = spread (x, dim=2, ncopies=size(y)) &
    * spread (y, dim=1, ncopies=size(x))
end function outer_product

```

Greatest common divisor and least common multiple

310d *⟨Declaration of utils procedures 304b⟩*+≡  

```

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

```

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

310e *⟨Implementation of utils procedures 305c⟩*+≡  

```

pure recursive function gcd_internal (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
  if (n <= 0) then
    gcd_m_n = m
  else
    gcd_m_n = gcd_internal (n, modulo (m, n))
  end if
end function gcd_internal

```

Wrap an elemental procedure around the recursive procedure:

310f *⟨Implementation of utils procedures 305c⟩*+≡  

```

elemental function gcd (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n

```

```

    gcd_m_n = gcd_internal (m, n)
end function gcd

```

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

311a *<Implementation of utils procedures 305c>+≡*

```

    elemental function lcm (m, n) result (lcm_m_n)
        integer, intent(in) :: m, n
        integer :: lcm_m_n
        lcm_m_n = (m * n) / gcd (m, n)
    end function lcm

```

A very simple minded factorization procedure, that is not fool proof at all. It maintains  $n == \text{product}(\text{factors}(1:i))$ , however, and will work in all cases of practical relevance.

311b *<Implementation of utils procedures 305c>+≡*

```

    pure subroutine factorize (n, factors, i)
        integer, intent(in) :: n
        integer, dimension(:), intent(out) :: factors
        integer, intent(out) :: i
        integer :: nn, p
        nn = n
        i = 0
        do p = 1, size (PRIMES)
            try: do
                if (modulo (nn, PRIMES(p)) == 0) then
                    i = i + 1
                    factors(i) = PRIMES(p)
                    nn = nn / PRIMES(p)
                    if (i >= size (factors)) then
                        factors(i) = nn
                        return
                    end if
                else
                    exit try
                end if
            end do try
            if (nn == 1) then
                return
            end if
        end do
    end subroutine factorize

```

311c *<Parameters in utils 311c>≡*

```

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

```



## G.4 I/O

312a *<Declaration of utils procedures 304b>+≡*

```
public :: find_free_unit
```

312b *<Variables in utils 312b>≡*

```
integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99
```

312c *<Implementation of utils procedures 305c>+≡*

```
subroutine find_free_unit (u, iostat)
  integer, intent(out) :: u
  integer, intent(out), optional :: iostat
  logical :: exists, is_open
  integer :: i, status
  do i = MIN_UNIT, MAX_UNIT
    inquire (unit = i, exist = exists, opened = is_open, &
      iostat = status)
    if (status == 0) then
      if (exists .and. .not. is_open) then
        u = i
        if (present (iostat)) then
          iostat = 0
        end if
        return
      end if
    end if
  end do
  if (present (iostat)) then
    iostat = -1
  end if
  u = -1
end subroutine find_free_unit
```

# —H— LINEAR ALGEBRA

```

313a <linalg.f90 313a>≡
! linalg.f90 --
<Coyleft notice 1>
module linalg
  use kinds
  use utils
  implicit none
  private
  <Declaration of linalg procedures 313b>
  character(len=*), public, parameter :: LINALG_RCS_ID = &
    "$Id: linalg.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  <Implementation of linalg procedures 314>
end module linalg

```

## *H.1 LU Decomposition*

```

313b <Declaration of linalg procedures 313b>≡
  public :: lu_decompose

```

$$A = LU \tag{H.1a}$$

In more detail

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \dots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix} \tag{H.1b}$$

Rewriting (H.1) in block matrix notation

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

we can solve it easily

$$u_{11} = a_{11} \quad (\text{H.3a})$$

$$u_{1\cdot} = a_{1\cdot} \quad (\text{H.3b})$$

$$l_{\cdot 1} = \frac{a_{\cdot 1}}{a_{11}} \quad (\text{H.3c})$$

$$LU = A - \frac{a_{\cdot 1} \otimes a_{1\cdot}}{a_{11}} \quad (\text{H.3d})$$

and (H.3c) and (H.3d) define a simple iterative algorithm if we work from the outside in. It just remains to add pivoting.

314 *Implementation of linalg procedures 314*  $\equiv$

```

pure subroutine lu_decompose (a, pivots, eps, l, u)
  real(kind=default), dimension(:, :), intent(inout) :: a
  integer, dimension(:), intent(out), optional :: pivots
  real(kind=default), intent(out), optional :: eps
  real(kind=default), dimension(:, :), intent(out), optional :: l, u
  real(kind=default), dimension(size(a,dim=1)) :: vv
  integer, dimension(size(a,dim=1)) :: p
  integer :: j, pivot
  <eps = 1 315a>
  vv = maxval (abs (a), dim=2)
  if (any (vv == 0.0)) then
    a = 0.0
    <pivots = 0 and eps = 0 315c>
    return
  end if
  vv = 1.0 / vv
  do j = 1, size (a, dim=1)
    pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
    if (j /= pivot) then
      call swap (a(pivot,:), a(j,:))
      <eps = - eps 315b>
      vv(pivot) = vv(j)
    end if
    p(j) = pivot
    if (a(j,j) == 0.0) then
      a(j,j) = tiny (a(j,j))

```

```

        end if
        a(j+1:,j) = a(j+1:,j) / a(j,j)
        a(j+1:,j+1:) &
            = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
    end do
    <Return optional arguments in lu_decompose 315d>
end subroutine lu_decompose

315a <eps = 1 315a>≡
    if (present (eps)) then
        eps = 1.0
    end if

315b <eps = - eps 315b>≡
    if (present (eps)) then
        eps = - eps
    end if

315c <pivots = 0 and eps = 0 315c>≡
    if (present (pivots)) then
        pivots = 0
    end if
    if (present (eps)) then
        eps = 0
    end if

315d <Return optional arguments in lu_decompose 315d>≡
    if (present (pivots)) then
        pivots = p
    end if
    if (present (l)) then
        do j = 1, size (a, dim=1)
            l(1:j-1,j) = 0.0
            l(j,j) = 1.0
            l(j+1:,j) = a(j+1:,j)
        end do
        do j = size (a, dim=1), 1, -1
            call swap (l(j,:), l(p(j),:))
        end do
    end if
    if (present (u)) then
        do j = 1, size (a, dim=1)
            u(1:j,j) = a(1:j,j)
            u(j+1:,j) = 0.0
        end do
    end if

```

## H.2 Determinant

**316a**  $\langle$ Declaration of `linalg` procedures **313b** $\rangle + \equiv$   
`public :: determinant`

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

**316b**  $\langle$ Implementation of `linalg` procedures **314** $\rangle + \equiv$   
`pure subroutine determinant (a, det)`  
`real(kind=default), dimension(:, :), intent(in) :: a`  
`real(kind=default), intent(out) :: det`  
`real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu`  
`integer :: i`  
`lu = a`  
`call lu_decompose (lu, eps = det)`  
`do i = 1, size (a, dim = 1)`  
`det = det * lu(i,i)`  
`end do`  
`end subroutine determinant`

## H.3 Diagonalization

The code is an implementation of the algorithm presented in [17, 18], but independent from the code presented in [19] to avoid legal problems.

A Jacobi rotation around the angle  $\phi$  in row  $p$  and column  $q$

$$P(\phi; p, q) = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & \cos \phi & \cdots & \sin \phi \\ & & \vdots & 1 & \vdots \\ & & -\sin \phi & \cdots & \cos \phi \\ & & & & \ddots & \\ & & & & & 1 \end{pmatrix} \quad (\text{H.4})$$

results in

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

**317a** *<Declaration of linalg procedures 313b>+≡*

```
public :: diagonalize_real_symmetric
```

**317b** *<Implementation of linalg procedures 314>+≡*

```
pure subroutine diagonalize_real_symmetric (a, eval, evec, num_rot)
  real(kind=default), dimension(:, :), intent(in) :: a
  real(kind=default), dimension(:), intent(out) :: eval
  real(kind=default), dimension(:, :), intent(out) :: evec
  integer, intent(out), optional :: num_rot
  real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: aa
  real(kind=default) :: off_diagonal_norm, threshold, &
    c, g, h, s, t, tau, cot_2phi
  logical, dimension(size(eval),size(eval)) :: upper_triangle
  integer, dimension(size(eval)) :: one_to_ndim
  integer :: p, q, ndim, j, sweep
  integer, parameter :: MAX_SWEEPS = 50
  ndim = size (eval)
  one_to_ndim = (/ (j, j=1,ndim) /)
  upper_triangle = &
    spread (one_to_ndim, dim=1, ncopies=ndim) &
    > spread (one_to_ndim, dim=2, ncopies=ndim)
  aa = a
  call unit (evec)
<Initialize num_rot 320e>
  sweeps: do sweep = 1, MAX_SWEEPS
    off_diagonal_norm = sum (abs (aa), mask=upper_triangle)
    if (off_diagonal_norm == 0.0) then
      eval = diag (aa)
      return
    end if
    if (sweep < 4) then
      threshold = 0.2 * off_diagonal_norm / ndim**2
    else
```

```

        threshold = 0.0
    end if
    do p = 1, ndim - 1
        do q = p + 1, ndim
            ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  318⟩
        end do
    end do
end do sweeps
if (present (num_rot)) then
    num_rot = -1
end if
!!! print *, "linalg::diagonalize_real_symmetric: exceeded sweep count"
end subroutine diagonalize_real_symmetric
318 ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  318⟩≡
    g = 100 * abs (aa (p,q))
    if ((sweep > 4) &
        .and. (g <= min (spacing (aa(p,p)), spacing (aa(q,q)))) then
        aa(p,q) = 0.0
    else if (abs (aa(p,q)) > threshold) then
        ⟨Determine  $\phi$  for the Jacobi rotation  $P(\phi; p, q)$  with  $A'_{pq} = 0$  319a⟩
        ⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  319c⟩
        ⟨ $V' = V \cdot P(\phi; p, q)$  320d⟩
        ⟨Update num_rot 320f⟩
    end if
end if

```

We want

$$A'_{pq} = (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) = 0 \quad (\text{H.6})$$

and therefore

$$\cot 2\phi = \frac{1 - \tan^2 \phi}{2 \tan \phi} = \frac{\cos^2 \phi - \sin^2 \phi}{2 \sin \phi \cos \phi} = \frac{A_{pp} - A_{qq}}{2A_{pq}} \quad (\text{H.7})$$

i.e. with  $t = \tan \phi = s/c$

$$t^2 + 2t \cot 2\phi - 1 = 0 \quad (\text{H.8})$$

This quadratic equation has the roots

$$t = -\cot 2\phi \pm \sqrt{1 + \cot^2 2\phi} = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| \pm \epsilon(\cot 2\phi)\sqrt{1 + \cot^2 2\phi}} \quad (\text{H.9})$$

and the smaller in magnitude of these is

$$t = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| + \sqrt{1 + \cot^2 2\phi}} \quad (\text{H.10})$$

and since  $|t| \leq 1$ , it corresponds to  $|\phi| \leq \pi/4$ . For very large  $\cot 2\phi$  we will use

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

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

**319a**  $\langle \text{Determine } \phi \text{ for the Jacobi rotation } P(\phi; p, q) \text{ with } A'_{pq} = 0 \text{ 319a} \rangle \equiv$   
`h = aa(q,q) - aa(p,p)`  
`if (g <= spacing (h)) then`  
`t = aa(p,q) / h`  
`else`  
`cot_2phi = 0.5 * h / aa(p,q)`  
`t = sign (1.0_default, cot_2phi) &`  
`/ (abs (cot_2phi) + sqrt (1.0 + cot_2phi**2))`  
`end if`

Trivia

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

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

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

**319b**  $\langle \text{Determine } \phi \text{ for the Jacobi rotation } P(\phi; p, q) \text{ with } A'_{pq} = 0 \text{ 319a} \rangle + \equiv$   
`c = 1.0 / sqrt (1.0 + t**2)`  
`s = t * c`  
`tau = s / (1.0 + c)`

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

**319c**  $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) \text{ 319c} \rangle \equiv$   
`aa(p,p) = aa(p,p) - t * aa(p,q)`  
`aa(q,q) = aa(q,q) + t * aa(p,q)`  
`aa(p,q) = 0.0`

$$\begin{aligned} r \neq p < q \neq r : A'_{rp} &= cA_{rp} - sA_{rq} \\ A'_{rq} &= sA_{rp} + cA_{rq} \end{aligned} \quad (\text{H.15})$$



Here's how we cover the upper triangular region using array notation:

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

**320a**  $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  **319c**  $\rangle + \equiv$   
`call jacobi_rotation (s, tau, aa(1:p-1,p), aa(1:p-1,q))`  
`call jacobi_rotation (s, tau, aa(p,p+1:q-1), aa(p+1:q-1,q))`  
`call jacobi_rotation (s, tau, aa(p,q+1:ndim), aa(q,q+1:ndim))`

Using (H.13c), we can write the rotation as a perturbation:

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

**320b**  $\langle$ Implementation of linalg procedures **314** $\rangle + \equiv$   
`pure subroutine jacobi_rotation (s, tau, vp, vq)`  
`real(kind=default), intent(in) :: s, tau`  
`real(kind=default), dimension(:), intent(inout) :: vp, vq`  
`real(kind=default), dimension(size(vp)) :: vp_tmp`  
`vp_tmp = vp`  
`vp = vp - s * (vq + tau * vp)`  
`vq = vq + s * (vp_tmp - tau * vq)`  
`end subroutine jacobi_rotation`

**320c**  $\langle$ Declaration of linalg procedures **313b** $\rangle + \equiv$   
`private :: jacobi_rotation`

**320d**  $\langle V' = V \cdot P(\phi; p, q)$  **320d**  $\rangle \equiv$   
`call jacobi_rotation (s, tau, evec(:,p), evec(:,q))`

**320e**  $\langle$ Initialize num\_rot **320e** $\rangle \equiv$   
`if (present (num_rot)) then`  
`num_rot = 0`  
`end if`

**320f**  $\langle$ Update num\_rot **320f** $\rangle \equiv$   
`if (present (num_rot)) then`  
`num_rot = num_rot + 1`  
`end if`

321a *<Implementation of linalg procedures 314>+≡*

```
pure subroutine unit (u)
  real(kind=default), dimension(:,,:), intent(out) :: u
  integer :: i
  u = 0.0
  do i = 1, min (size (u, dim = 1), size (u, dim = 2))
    u(i,i) = 1.0
  end do
end subroutine unit
```

321b *<Implementation of linalg procedures 314>+≡*

```
pure function diag (a) result (d)
  real(kind=default), dimension(:,,:), intent(in) :: a
  real(kind=default), dimension(min(size(a,dim=1),size(a,dim=2))) :: d
  integer :: i
  do i = 1, min (size (a, dim = 1), size (a, dim = 2))
    d(i) = a(i,i)
  end do
end function diag
```

321c *<Declaration of linalg procedures 313b>+≡*

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

## H.4 Test

321d *<la\_sample.f90 321d>≡*

```
! la_sample.f90 --
<Copyleft notice 1>
program la_sample
  use kinds
  use utils
  use tao_random_numbers
  use linalg
  implicit none
  integer, parameter :: N = 200
  real(kind=default), dimension(N,N) :: a, evec, a0, l, u, NAG_bug
  real(kind=default), dimension(N) :: b, eval
  real(kind=default) :: d
  integer :: i
  call system_clock (i)
  call tao_random_seed (i)
  print *, i
  do i = 1, N
```

```

        call tao_random_number (a(:,i))
    end do
    NAG_bug = (a + transpose (a)) / 2
    a = NAG_bug
    a0 = a
    call lu_decompose (a, l=l, u=u)
    a = matmul (l, u)
    print *, maxval (abs(a-a0))
    call determinant (a, d)
    print *, d
    call diagonalize_real_symmetric (a, eval, evec)
    print *, product (eval)
    stop
    call sort (eval, evec)
    do i = 1, N
        b = matmul (a, evec(:,i)) - eval(i) * evec(:,i)
        write (unit = *, fmt = "(A,I3, 2(A,E11.4))") &
            "eval #", i, " = ", eval(i), ", |(A-lambda)V|_infty = ", &
            maxval (abs(b)) / maxval (abs(evec(:,i)))
    end do
end program la_sample

```

# —I—

## PRODUCTS

```

323 <products.f90 323>≡
    ! products.f90 --
    <Copyleft notice 1>
    module products
        use kinds
        implicit none
        private
        public :: dot, sp, spc
        character(len=*), public, parameter :: PRODUCTS_RCS_ID = &
            "$Id: products.nw 314 2010-04-17 20:32:33Z ohl $"
    contains
        pure function dot (p, q) result (pq)
            real(kind=default), dimension(0:), intent(in) :: p, q
            real(kind=default) :: pq
            pq = p(0)*q(0) - dot_product (p(1:), q(1:))
        end function dot
        pure function sp (p, q) result (sppq)
            real(kind=default), dimension(0:), intent(in) :: p, q
            complex(kind=default) :: sppq
            sppq = cmplx (p(2), p(3), kind=default) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
                - cmplx (q(2), q(3), kind=default) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
        end function sp
        pure function spc (p, q) result (spcpq)
            real(kind=default), dimension(0:), intent(in) :: p, q
            complex(kind=default) :: spcpq
            spcpq = conjg (sp (p, q))
        end function spc
    end module products

```

# —J—

## KINEMATICS

```

324a  <kinematics.f90 324a>≡
      ! kinematics.f90 --
      <Copyleft notice 1>
      module kinematics
        use kinds
        use constants
        use products, only: dot
        use specfun, only: gamma
        implicit none
        private
        <Declaration of kinematics procedures 324b>
        <Interfaces of kinematics procedures 324c>
        <Declaration of kinematics types 326g>
        character(len=*), public, parameter :: KINEMATICS_RCS_ID = &
            "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
        contains
        <Implementation of kinematics procedures 325a>
      end module kinematics

```

### *J.1 Lorentz Transformations*

```

324b  <Declaration of kinematics procedures 324b>≡
      public :: boost_velocity
      private :: boost_one_velocity, boost_many_velocity
      public :: boost_momentum
      private :: boost_one_momentum, boost_many_momentum

324c  <Interfaces of kinematics procedures 324c>≡
      interface boost_velocity
        module procedure boost_one_velocity, boost_many_velocity

```

```

end interface
interface boost_momentum
  module procedure boost_one_momentum, boost_many_momentum
end interface

```

Boost a four vector  $p$  to the inertial frame moving with the velocity  $\beta$ :

$$p'_0 = \gamma (p_0 - \vec{\beta} \vec{p}) \quad (\text{J.1a})$$

$$\vec{p}' = \gamma (\vec{p}_{\parallel} - \vec{\beta} p_0) + \vec{p}_{\perp} \quad (\text{J.1b})$$

with  $\gamma = 1/\sqrt{1 - \vec{\beta}^2}$ ,  $\vec{p}_{\parallel} = \vec{\beta}(\vec{\beta} \vec{p})/\vec{\beta}^2$  and  $\vec{p}_{\perp} = \vec{p} - \vec{p}_{\parallel}$ . Using  $1/\vec{\beta}^2 = \gamma^2/(\gamma + 1) \cdot 1/(\gamma - 1)$  and  $\vec{b} = \gamma \vec{\beta}$  this can be rewritten as

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

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

**325a**  $\langle \text{Implementation of kinematics procedures } \text{325a} \rangle \equiv$

```

pure function boost_one_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(0:3) :: p_prime
  real(kind=default), dimension(1:3) :: b
  real(kind=default) :: gamma, b_dot_p
  gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
  b = gamma * beta
  b_dot_p = dot_product (b, p(1:3))
  p_prime(0) = gamma * p(0) - b_dot_p
  p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
end function boost_one_velocity

```

**325b**  $\langle \text{Implementation of kinematics procedures } \text{325a} \rangle + \equiv$

```

pure function boost_many_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  integer :: i
  do i = 1, size (p, dim=1)
    p_prime(i,:) = boost_one_velocity (p(i,:), beta)
  end do
end function boost_many_velocity

```

Boost a four vector  $p$  to the rest frame of the four vector  $q$ . The velocity is  $\vec{\beta} = \vec{q}/|q_0|$ :

```

326a <Implementation of kinematics procedures 325a>+≡
    pure function boost_one_momentum (p, q) result (p_prime)
        real(kind=default), dimension(0:), intent(in) :: p, q
        real(kind=default), dimension(0:3) :: p_prime
        p_prime = boost_velocity (p, q(1:3) / abs (q(0)))
    end function boost_one_momentum

326b <Implementation of kinematics procedures 325a>+≡
    pure function boost_many_momentum (p, q) result (p_prime)
        real(kind=default), dimension(:,0:), intent(in) :: p
        real(kind=default), dimension(0:), intent(in) :: q
        real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
        p_prime = boost_many_velocity (p, q(1:3) / abs (q(0)))
    end function boost_many_momentum

```

## *J.2 Massive Phase Space*

$$\lambda(a, b, c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca = (a - b - c)^2 - 4bc \quad (\text{J.3})$$

and permutations

```

326c <Implementation of kinematics procedures 325a>+≡
    pure function lambda (a, b, c) result (lam)
        real(kind=default), intent(in) :: a, b, c
        real(kind=default) :: lam
        lam = a**2 + b**2 + c**2 - 2*(a*b + b*c + c*a)
    end function lambda

326d <Declaration of kinematics procedures 324b>+≡
    public :: lambda

326e <Declaration of kinematics procedures 324b>+≡
    public :: two_to_three
    private :: two_to_three_massive, two_to_three_massless

326f <Interfaces of kinematics procedures 324c>+≡
    interface two_to_three
        module procedure two_to_three_massive, two_to_three_massless
    end interface

326g <Declaration of kinematics types 326g>≡
    type, public :: LIPS3
        real(kind=default), dimension(3,0:3) :: p
        real(kind=default) :: jacobian
    end type LIPS3

```

$$dLIPS_3 = \int \frac{d^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{d^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{d^3\vec{p}_3}{(2\pi)^3 2E_3} (2\pi)^4 \delta^4(p_1 + p_2 + p_3 - p_a - p_b) \quad (J.4)$$

The jacobian is given by

$$dLIPS_3 = \frac{1}{(2\pi)^5} \int d\phi dt_1 ds_2 d\Omega_3^{[23]} \frac{1}{32\sqrt{ss_2}} \frac{|p_3^{[23]}|}{|p_a^{[ab]}|} \quad (J.5)$$

where  $\vec{p}_i^{[jk]}$  denotes the momentum of particle  $i$  in the center of mass system of particles  $j$  and  $k$ .

**327a** *⟨Implementation of kinematics procedures 325a⟩* +≡  

```

pure function two_to_three_massive &
  (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
    s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
    1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive

```

A specialized version for massless particles can be faster, because the kinematics is simpler:

**327b** *⟨Implementation of kinematics procedures 325a⟩* +≡  

```

pure function two_to_three_massless (s, t1, s2, phi, cos_theta3, phi3) &
  result (p)
  real(kind=default), intent(in) :: s, t1, s2, phi, cos_theta3, phi3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: pa_abs, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (s) / 2
  p1_abs = (s - s2) / (2 * sqrt (s))

```



```

    p3_abs = sqrt (s2) / 2
    p%jacobian = 1.0 / ((2*PI)**5 * 32 * s)
    cos_theta = 1 + t1 / (2*pa_abs*p1_abs)
    p%p(1,0) = p1_abs
    p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p23(1:3) = - p%p(1,1:3)
    p23(0) = on_shell (p23, sqrt (s2))
    p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3)
end function two_to_three_massless

328a  <Declaration of kinematics procedures 324b>+≡
      public :: one_to_two
      private :: one_to_two_massive, one_to_two_massless

328b  <Interfaces of kinematics procedures 324c>+≡
      interface one_to_two
        module procedure one_to_two_massive, one_to_two_massless
      end interface

328c  <Implementation of kinematics procedures 325a>+≡
      pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi, m1, m2
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: s, p1_abs
        s = dot (p12, p12)
        p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,1:3) = - p(1,1:3)
        p(1,0) = on_shell (p(1,:), m1)
        p(2,0) = on_shell (p(2,:), m2)
        p = boost_momentum (p, - p12)
      end function one_to_two_massive

328d  <Implementation of kinematics procedures 325a>+≡
      pure function one_to_two_massless (p12, cos_theta, phi) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: p1_abs
        p1_abs = sqrt (dot (p12, p12)) / 2
        p(1,0) = p1_abs
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,0) = p1_abs
        p(2,1:3) = - p(1,1:3)
        p = boost_momentum (p, - p12)

```

```

end function one_to_two_massless

329a <Declaration of kinematics procedures 324b>+≡
public :: polar_to_cartesian, on_shell

329b <Implementation of kinematics procedures 325a>+≡
pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
  real(kind=default), intent(in) :: v_abs, cos_theta, phi
  real(kind=default), dimension(3) :: v
  real(kind=default) :: sin_phi, cos_phi, sin_theta
  sin_theta = sqrt (1.0 - cos_theta**2)
  cos_phi = cos (phi)
  sin_phi = sin (phi)
  v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
end function polar_to_cartesian

329c <Implementation of kinematics procedures 325a>+≡
pure function on_shell (p, m) result (E)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), intent(in) :: m
  real(kind=default) :: E
  E = sqrt (m**2 + dot_product (p(1:3), p(1:3)))
end function on_shell

```

### *J.3 Massive 3-Particle Phase Space Revisited*

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

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

```

329d <kinematics.f90 324a>+≡
module phase_space
  use kinds
  use constants
  use kinematics !NODEP!
  use tao_random_numbers
  implicit none
  private

```

```

    <Declaration of phase_space procedures 331b>
    <Interfaces of phase_space procedures 331c>
    <Declaration of phase_space types 330a>
    character(len=*), public, parameter :: PHASE_SPACE_RCS_ID = &
        "$Id: kinematics.nw 314 2010-04-17 20:32:33Z ohl $"
contains
    <Implementation of phase_space procedures 331d>
end module phase_space

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

```

330a <Declaration of phase\_space types 330a>≡

```

type, public :: LIPS3_unit
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_unit

```

330b <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_unit_massless
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_unit_massless

LIPS3_s2_t1_angles : (s2, t1, φ, cos θ3, φ3) (J.9)

```

330c <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_s2_t1_angles
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles

```

330d <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_s2_t1_angles_massless
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles_massless

LIPS3_momenta : (p1, p2, p3) (J.10)

```

330e <Declaration of phase\_space types 330a>+≡

```

type, public :: LIPS3_momenta
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default), dimension(2) :: mass_in
  real(kind=default), dimension(3) :: mass_out
  real(kind=default) :: jacobian
end type LIPS3_momenta

331a <Declaration of phase_space types 330a>+≡
type, public :: LIPS3_momenta_massless
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default) :: jacobian
end type LIPS3_momenta_massless

331b <Declaration of phase_space procedures 331b>≡
public :: random_LIPS3
private :: random_LIPS3_unit, random_LIPS3_unit_massless

331c <Interfaces of phase_space procedures 331c>≡
interface random_LIPS3
  module procedure random_LIPS3_unit, random_LIPS3_unit_massless
end interface

331d <Implementation of phase_space procedures 331d>≡
pure subroutine random_LIPS3_unit (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit

331e <Implementation of phase_space procedures 331d>+≡
pure subroutine random_LIPS3_unit_massless (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit_massless), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit_massless

331f <Declaration of phase_space procedures 331b>+≡
private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0

331g <(Unused) Interfaces of phase_space procedures 331g>≡
interface assignment(=)
  module procedure &
    LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
end interface

```

```

332a <Implementation of phase_space procedures 331d>+≡
      pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
        type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
        type(LIPS3_unit), intent(in) :: unit
      end subroutine LIPS3_unit_to_s2_t1_angles

332b <Implementation of phase_space procedures 331d>+≡
      pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
        type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
        type(LIPS3_unit_massless), intent(in) :: unit
      end subroutine LIPS3_unit_to_s2_t1_angles_m0

```

## *J.4 Massless n-Particle Phase Space: RAMBO*

```

332c <Declaration of kinematics procedures 324b>+≡
      public :: massless_isotropic_decay

```

The massless RAMBO algorithm [26]:

```

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 [26]. The transformation is really a Lorentz boost (as can be seen easily).

**333a**  $\langle$ Boost and rescale the vectors **333a** $\rangle \equiv$

```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
  r = dot (q(k,:), qsum) / qabs
  z = (q(k,0) + r) / (qsum(0) + qabs)
  p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
  p(k,0) = x * r
enddo
```

**333b**  $\langle$ Declaration of kinematics procedures **324b** $\rangle + \equiv$

```
public :: phase_space_volume
```

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

**333c**  $\langle$ Implementation of kinematics procedures **325a** $\rangle + \equiv$

```
pure function phase_space_volume (n, roots) result (volume)
  integer, intent(in) :: n
  real (kind=default), intent(in) :: roots
  real (kind=default) :: volume
  real (kind=default) :: nd
  nd = n
  volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

## J.5 Tests

**333d**  $\langle$ ktest.f90 **333d** $\rangle \equiv$

```
program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default) :: &
    ma, mb, m1, m2, m3, s, t1, s2, phi, cos_theta3, phi3
  real(kind=default) :: t1_min, t1_max
  real(kind=default), dimension(5) :: r
  type(LIPS3) :: p
```

```

integer :: i
character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
ma = 1.0
mb = 1.0
m1 = 10.0
m2 = 20.0
m3 = 30.0
s = 100.0 ** 2
do i = 1, 10
  call tao_random_number (r)
  s2 = (r(1) * (sqrt (s) - m1) + (1 - r(1)) * (m2 + m3)) ** 2
  t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    + sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
    - sqrt (lambda (s, ma**2, mb**2) * lambda (s, s2, m1**2))) / (2*s)
  t1 = r(2) * t1_max + (1 - r(2)) * t1_min
  phi = 2*PI * r(3)
  cos_theta3 = 2 * r(4) - 1
  phi3 = 2*PI * r(5)
  p = two_to_three (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
  print fmt, "p1      = ", p%p(1,:)
  print fmt, "p2      = ", p%p(2,:)
  print fmt, "p3      = ", p%p(3,:)
  print fmt, "p1,2,3^2 = ", dot (p%p(1,:), p%p(1,)), &
    dot (p%p(2,:), p%p(2,)), dot (p%p(3,:), p%p(3,))
  print fmt, "sum(p)   = ", p%p(1,:) + p%p(2,:) + p%p(3,:)
  print fmt, "|J|     = ", p%jacobian
end do
end program ktest

```



Trivial check for typos, should be removed from the finalized program!

334  $\langle$  Trivial ktest.f90 334  $\rangle \equiv$

```

program ktest
  use kinds
  use constants
  use products
  use kinematics
  use tao_random_numbers
  implicit none
  real(kind=default), dimension(0:3) :: p, q, p_prime, p0
  real(kind=default) :: m
  character(len=*), parameter :: fmt = "(A,4(1X,E12.5))"
  integer :: i

```

```

do i = 1, 5
  if (i == 1) then
    p = (/ 1.0_double, 0.0_double, 0.0_double, 0.0_double /)
    m = 1.0
  else
    call tao_random_number (p)
    m = sqrt (PI)
  end if
  call tao_random_number (q(1:3))
  q(0) = sqrt (m**2 + dot_product (q(1:3), q(1:3)))
  p_prime = boost_momentum (p, q)
  print fmt, "p    = ", p
  print fmt, "q    = ", q
  print fmt, "p'   = ", p_prime
  print fmt, "p^2  = ", dot (p, p)
  print fmt, "p'^2 = ", dot (p_prime, p_prime)
  if (dot (p, p) > 0.0) then
    p0 = boost_momentum (p, p)
    print fmt, "p0   = ", p0
    print fmt, "p0^2 = ", dot (p0, p0)
  end if
end do
end program ktest

```



# —K—

## COORDINATES

```

336  <coordinates.f90 336>≡
      ! coordinates.f90 --
      <Copyleft notice 1>
      module coordinates
        use kinds
        use constants, only: PI
        use specfun, only: gamma
        implicit none
        private
        <Declaration of coordinates procedures 337a>
      contains
        <Implementation of coordinates procedures 337b>
      end module coordinates

```

### *K.1 Angular Spherical Coordinates*

$$\begin{aligned}
 x_n &= r \cos \theta_{n-2} \\
 x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
 &\dots \\
 x_3 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \cos \theta_1 \\
 x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \cos \phi \\
 x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \sin \phi
 \end{aligned} \tag{K.1}$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} (\sin \theta_i)^i \tag{K.2}$$

We can minimize the number of multiplications by computing the products

$$P_j = \prod_{i=j}^{n-2} \sin \theta_i \quad (\text{K.3})$$

Then

$$\begin{aligned} x_n &= r \cos \theta_{n-2} \\ x_{n-1} &= r P_{n-2} \cos \theta_{n-3} \\ &\dots \\ x_3 &= r P_2 \cos \theta_1 \\ x_2 &= r P_1 \cos \phi \\ x_1 &= r P_1 \sin \phi \end{aligned} \quad (\text{K.4})$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} P_i \quad (\text{K.5})$$

Note that  $\theta_i \in [0, \pi]$  and  $\phi \in [0, 2\pi]$  or  $\phi \in [-\pi, \pi]$ . Therefore  $\sin \theta_i \geq 0$  and

$$\sin \theta_i = \sqrt{1 - \cos^2 \theta_i} \quad (\text{K.6})$$

which is not true for  $\phi$ . Since `sqrt` is typically much faster than `sin` and `cos`, we use (K.6) where ever possible.

```

337a <Declaration of coordinates procedures 337a>≡
      public :: spherical_to_cartesian_2, &
               spherical_to_cartesian, spherical_to_cartesian_j

337b <Implementation of coordinates procedures 337b>≡
      pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(theta)) :: cos_theta
        real(kind=default), dimension(size(theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (theta) + 2
        cos_theta = cos (theta)
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
          product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do

```

```

    if (present (x)) then
        x(1) = r * product_sin_theta(1) * sin (phi)
        x(2) = r * product_sin_theta(1) * cos (phi)
        x(3:) = r * product_sin_theta(2:n-1) * cos_theta
    end if
    if (present (jacobian)) then
        jacobian = r**(n-1) * product (product_sin_theta)
    end if
end subroutine spherical_to_cartesian_2

```



Note that `call` inside of a function breaks F-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where `theta` could not be assumed shape ...

- 338a** *<Implementation of coordinates procedures 337b>+≡*  

```

pure function spherical_to_cartesian (r, phi, theta) result (x)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: theta
    real(kind=default), dimension(size(theta)+2) :: x
    call spherical_to_cartesian_2 (r, phi, theta, x = x)
end function spherical_to_cartesian

```
- 338b** *<Implementation of coordinates procedures 337b>+≡*  

```

pure function spherical_to_cartesian_j (r, phi, theta) &
    result (jacobian)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: theta
    real(kind=default) :: jacobian
    call spherical_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
end function spherical_to_cartesian_j

```
- 338c** *<Declaration of coordinates procedures 337a>+≡*  

```

public :: cartesian_to_spherical_2, &
    cartesian_to_spherical, cartesian_to_spherical_j

```
- 338d** *<Implementation of coordinates procedures 337b>+≡*  

```

pure subroutine cartesian_to_spherical_2 (x, r, phi, theta, jacobian)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(out), optional :: r, phi
    real(kind=default), dimension(:), intent(out), optional :: theta
    real(kind=default), intent(out), optional :: jacobian
    real(kind=default) :: local_r
    real(kind=default), dimension(size(x)-2) :: cos_theta
    real(kind=default), dimension(size(x)-1) :: product_sin_theta

```

```

integer :: n, i
n = size (x)
local_r = sqrt (dot_product (x, x))
if (local_r == 0) then
  if (present (r)) then
    r = 0
  end if
  if (present (phi)) then
    phi = 0
  end if
  if (present (theta)) then
    theta = 0
  end if
  if (present (jacobian)) then
    jacobian = 1
  end if
else
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
    if (product_sin_theta(i-1) == 0) then
      cos_theta(i-2) = 0
    else
      cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    end if
    product_sin_theta(i-2) = &
      product_sin_theta(i-1) * sqrt (1 - cos_theta(i-2)**2)
  end do
  if (present (r)) then
    r = local_r
  end if
  if (present (phi)) then
    ! Set phi = 0 for vanishing vector
    if (x(1) == 0 .and. x(2)==0) then
      phi = 0
    else
      phi = atan2 (x(1), x(2))
    end if
  end if
  if (present (theta)) then
    theta = acos (cos_theta)
  end if
  if (present (jacobian)) then
    jacobian = local_r**(1-n) / product (product_sin_theta)
  end if
end if

```

```

        end if
    end if
end subroutine cartesian_to_spherical_2
340a  Implementation of coordinates procedures 337b+≡
    pure subroutine cartesian_to_spherical (x, r, phi, theta)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out) :: r, phi
        real(kind=default), dimension(:), intent(out) :: theta
        call cartesian_to_spherical_2 (x, r, phi, theta)
    end subroutine cartesian_to_spherical
340b  Implementation of coordinates procedures 337b+≡
    pure function cartesian_to_spherical_j (x) result (jacobian)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default) :: jacobian
        call cartesian_to_spherical_2 (x, jacobian = jacobian)
    end function cartesian_to_spherical_j

```

## *K.2 Trigonometric Spherical Coordinates*

```

340c  Declaration of coordinates procedures 337a+≡
    public :: spherical_cos_to_cartesian_2, &
           spherical_cos_to_cartesian, spherical_cos_to_cartesian_j

```

Using the cosine, we have to drop  $P_1$  from the Jacobian

```

340d  Implementation of coordinates procedures 337b+≡
    pure subroutine spherical_cos_to_cartesian_2 (r, phi, cos_theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: cos_theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(cos_theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (cos_theta) + 2
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
            product_sin_theta(i) = &
                product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do
        if (present (x)) then
            x(1) = r * product_sin_theta(1) * sin (phi)
            x(2) = r * product_sin_theta(1) * cos (phi)
            x(3:) = r * product_sin_theta(2:n-1) * cos_theta
        end if
    end subroutine spherical_cos_to_cartesian_2

```

```

        end if
        if (present (jacobian)) then
            jacobian = r**(n-1) * product (product_sin_theta(2:))
        end if
    end subroutine spherical_cos_to_cartesian_2
341a  <Implementation of coordinates procedures 337b>+≡
    pure function spherical_cos_to_cartesian (r, phi, theta) result (x)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(size(theta)+2) :: x
        call spherical_cos_to_cartesian_2 (r, phi, theta, x = x)
    end function spherical_cos_to_cartesian
341b  <Implementation of coordinates procedures 337b>+≡
    pure function spherical_cos_to_cartesian_j (r, phi, theta) &
        result (jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default) :: jacobian
        call spherical_cos_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
    end function spherical_cos_to_cartesian_j
341c  <Declaration of coordinates procedures 337a>+≡
    public :: cartesian_to_spherical_cos_2, &
        cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
341d  <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))
        if (local_r == 0) then
            if (present (r)) then
                r = 0
            end if
            if (present (phi)) then
                phi = 0
            end if

```

```

    if (present (cos_theta)) then
        cos_theta = 0
    end if
    if (present (jacobian)) then
        jacobian = 1
    end if
else
    product_sin_theta(n-1) = 1
    do i = n, 3, -1
        if (product_sin_theta(i-1) == 0) then
            local_cos_theta(i-2) = 0
        else
            local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
        end if
        product_sin_theta(i-2) = &
            product_sin_theta(i-1) * sqrt (1 - local_cos_theta(i-2)**2)
    end do
    if (present (r)) then
        r = local_r
    end if
    if (present (phi)) then
        ! Set phi = 0 for vanishing vector
        if (x(1) == 0 .and. x(2)==0) then
            phi = 0
        else
            phi = atan2 (x(1), x(2))
        end if
    end if
    if (present (cos_theta)) then
        cos_theta = local_cos_theta
    end if
    if (present (jacobian)) then
        jacobian = local_r**(1-n) / product (product_sin_theta(2:))
    end if
end if
end subroutine cartesian_to_spherical_cos_2

```

342 *⟨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

```

343a *⟨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*

343b *⟨Declaration of coordinates procedures 337a⟩+≡*  

```

public :: surface

```

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

343c *⟨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

```
344a <mpi90.f90 344a>≡
    ! mpi90.f90 --
    <Copyleft notice 1>
    module mpi90
        use kinds
        use mpi
        implicit none
        private
        <Declaration of mpi90 procedures 344b>
        <Interfaces of mpi90 procedures 347c>
        <Parameters in mpi90 (never defined)>
        <Variables in mpi90 (never defined)>
        <Declaration of mpi90 types 349b>
        character(len=*), public, parameter :: MPI90_RCS_ID = &
            "$Id: mpi90.nw 314 2010-04-17 20:32:33Z ohl $"
    contains
        <Implementation of mpi90 procedures 345a>
    end module mpi90
```

### *L.1 Basics*

```
344b <Declaration of mpi90 procedures 344b>≡
    public :: mpi90_init
    public :: mpi90_finalize
    public :: mpi90_abort
    public :: mpi90_print_error
    public :: mpi90_size
    public :: mpi90_rank
```

```

345a  <Implementation of mpi90 procedures 345a>≡
      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) 345b>
      end subroutine mpi90_init

345b  <Handle local_error (no mpi90_abort) 345b>≡
      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

345c  <Handle local_error 345c>≡
      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

345d  <Implementation of mpi90 procedures 345a>+≡
      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 345c>
      end subroutine mpi90_finalize

345e  <Implementation of mpi90 procedures 345a>+≡
      subroutine mpi90_abort (code, domain, error)
        integer, intent(in), optional :: code, domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_abort"

```

```

integer :: local_domain, local_code, local_error
external mpi_abort
if (present (code)) then
    local_code = code
else
    local_code = MPI_ERR_UNKNOWN
end if
<Set default for domain 346b>
call mpi_abort (local_domain, local_code, local_error)
<Handle local_error (no mpi90_abort) 345b>
end subroutine mpi90_abort

```

346a <Implementation of mpi90 procedures 345a>+≡

```

subroutine mpi90_print_error (error, msg)
integer, intent(in) :: error
character(len=*), optional :: msg
character(len=*), parameter :: FN = "mpi90_print_error"
integer :: msg_len, local_error
external mpi_error_string
call mpi_error_string (error, msg, msg_len, local_error)
if (local_error /= MPI_SUCCESS) then
    print *, "PANIC: even MPI_ERROR_STRING() failed!!!"
    call mpi90_abort (local_error)
else if (present (msg)) then
    print *, trim (msg), ": ", trim (msg(msg_len+1:))
else
    print *, "mpi90: ", trim (msg(msg_len+1:))
end if
end subroutine mpi90_print_error

```

346b <Set default for domain 346b>≡

```

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

```

346c <Implementation of mpi90 procedures 345a>+≡

```

subroutine mpi90_size (sz, domain, error)
integer, intent(out) :: sz
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_size"
integer :: local_domain, local_error
external mpi_comm_size

```

```

    <Set default for domain 346b>
    call mpi_comm_size (local_domain, sz, local_error)
    <Handle local_error 345c>
end subroutine mpi90_size

347a <Implementation of mpi90 procedures 345a>+≡
subroutine mpi90_rank (rank, domain, error)
  integer, intent(out) :: rank
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  character(len=*), parameter :: FN = "mpi90_rank"
  integer :: local_domain, local_error
  external mpi_comm_rank
  <Set default for domain 346b>
  call mpi_comm_rank (local_domain, rank, local_error)
  <Handle local_error 345c>
end subroutine mpi90_rank

```

## *L.2 Point to Point*

```

347b <Declaration of mpi90 procedures 344b>+≡
  public :: mpi90_send
  public :: mpi90_receive
  public :: mpi90_receive_pointer

347c <Interfaces of mpi90 procedures 347c>≡
  interface mpi90_send
    module procedure &
      mpi90_send_integer, mpi90_send_double, &
      mpi90_send_integer_array, mpi90_send_double_array, &
      mpi90_send_integer_array2, mpi90_send_double_array2
  end interface

347d <Implementation of mpi90 procedures 345a>+≡
  subroutine mpi90_send_integer (value, target, tag, domain, error)
    integer, intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    call mpi90_send_integer_array ((/ value /), target, tag, domain, error)
  end subroutine mpi90_send_integer

347e <Implementation of mpi90 procedures 345a>+≡
  subroutine mpi90_send_double (value, target, tag, domain, error)

```

```

    real(kind=default), intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    call mpi90_send_double_array (/ value /), target, tag, domain, error)
end subroutine mpi90_send_double

348a  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_send_integer_array (buffer, target, tag, domain, error)
        integer, dimension(:), intent(in) :: buffer
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        ⟨Body of mpi90_send_*_array 348b⟩
    end subroutine mpi90_send_integer_array

348b  ⟨Body of mpi90_send_*_array 348b⟩≡
    integer :: local_domain, local_error
    external mpi_send
    ⟨Set default for domain 346b⟩
    call mpi_send (buffer, size (buffer), datatype, target, tag, &
        local_domain, local_error)
    ⟨Handle local_error 345c⟩

348c  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_send_double_array (buffer, target, tag, domain, error)
        real(kind=default), dimension(:), intent(in) :: buffer
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_double_array"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        ⟨Body of mpi90_send_*_array 348b⟩
    end subroutine mpi90_send_double_array

348d  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_send_integer_array2 (value, target, tag, domain, error)
        integer, dimension(:, :), intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(size(value)) :: buffer
        buffer = reshape (value, shape(buffer))
        call mpi90_send_integer_array (buffer, target, tag, domain, error)

```

```

        end subroutine mpi90_send_integer_array2

349a  <Implementation of mpi90 procedures 345a>+≡
        subroutine mpi90_send_double_array2 (value, target, tag, domain, error)
            real(kind=default), dimension(:,:), intent(in) :: value
            integer, intent(in) :: target, tag
            integer, intent(in), optional :: domain
            integer, intent(out), optional :: error
            real(kind=default), dimension(size(value)) :: buffer
            buffer = reshape (value, shape(buffer))
            call mpi90_send_double_array (buffer, target, tag, domain, error)
        end subroutine mpi90_send_double_array2

349b  <Declaration of mpi90 types 349b>≡
        type, public :: mpi90_status
            integer :: count, source, tag, error
        end type mpi90_status

349c  <Implementation of mpi90 procedures 345a>+≡
        subroutine mpi90_receive_integer (value, source, tag, domain, status, error)
            integer, intent(out) :: value
            integer, intent(in), optional :: source, tag, domain
            type(mpi90_status), intent(out), optional :: status
            integer, intent(out), optional :: error
            integer, dimension(1) :: buffer
            call mpi90_receive_integer_array (buffer, source, tag, domain, status, error)
            value = buffer(1)
        end subroutine mpi90_receive_integer

349d  <Interfaces of mpi90 procedures 347c>+≡
        interface mpi90_receive
            module procedure &
                mpi90_receive_integer, mpi90_receive_double, &
                mpi90_receive_integer_array, mpi90_receive_double_array, &
                mpi90_receive_integer_array2, mpi90_receive_double_array2
        end interface

349e  <Set defaults for source, tag and domain 349e>≡
        if (present (source)) then
            local_source = source
        else
            local_source = MPI_ANY_SOURCE
        end if
        if (present (tag)) then
            local_tag = tag
        else

```

```

        local_tag = MPI_ANY_TAG
    end if
    <Set default for domain 346b>
350a <Implementation of mpi90 procedures 345a>+≡
    subroutine mpi90_receive_double (value, source, tag, domain, status, error)
        real(kind=default), intent(out) :: value
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        call mpi90_receive_double_array (buffer, source, tag, domain, status, error)
        value = buffer(1)
    end subroutine mpi90_receive_double
350b <Implementation of mpi90 procedures 345a>+≡
    subroutine mpi90_receive_integer_array &
        (buffer, source, tag, domain, status, error)
        integer, dimension(:), intent(out) :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_receive_*_array 350c>
    end subroutine mpi90_receive_integer_array
350c <Body of mpi90_receive_*_array 350c>≡
    integer :: local_source, local_tag, local_domain, local_error
    integer, dimension(MPI_STATUS_SIZE) :: local_status
    external mpi_receive, mpi_get_count
    <Set defaults for source, tag and domain 349e>
    call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
        local_domain, local_status, local_error)
    <Handle local_error 345c>
    if (present (status)) then
        call decode_status (status, local_status, datatype)
    end if
350d <Declaration of mpi90 procedures 344b>+≡
    private :: decode_status

```

 Can we ignore ierror???

```

350e <Implementation of mpi90 procedures 345a>+≡
    subroutine decode_status (status, mpi_status, datatype)

```

```

type(mpi90_status), intent(out) :: status
integer, dimension(:), intent(in) :: mpi_status
integer, intent(in), optional :: datatype
integer :: ierror
if (present (datatype)) then
    call mpi_get_count (mpi_status, datatype, status%count, ierror)
else
    status%count = 0
end if
status%source = mpi_status(MPI_SOURCE)
status%tag = mpi_status(MPI_TAG)
status%error = mpi_status(MPI_ERROR)
end subroutine decode_status

```

351a *<Implementation of mpi90 procedures 345a>+≡*

```

subroutine mpi90_receive_double_array &
    (buffer, source, tag, domain, status, error)
    real(kind=default), dimension(:), intent(out) :: buffer
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    character(len=*), parameter :: FN = "mpi90_receive_double_array"
    integer, parameter :: datatype = MPI_DOUBLE_PRECISION
    <Body of mpi90_receive_*_array 350c>
end subroutine mpi90_receive_double_array

```

351b *<Implementation of mpi90 procedures 345a>+≡*

```

subroutine mpi90_receive_integer_array2 &
    (value, source, tag, domain, status, error)
    integer, dimension(:,:), intent(out) :: value
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status
    integer, intent(out), optional :: error
    integer, dimension(size(value)) :: buffer
    call mpi90_receive_integer_array &
        (buffer, source, tag, domain, status, error)
    value = reshape (buffer, shape(value))
end subroutine mpi90_receive_integer_array2

```

351c *<Implementation of mpi90 procedures 345a>+≡*

```

subroutine mpi90_receive_double_array2 &
    (value, source, tag, domain, status, error)
    real(kind=default), dimension(:,:), intent(out) :: value
    integer, intent(in), optional :: source, tag, domain
    type(mpi90_status), intent(out), optional :: status

```



```

integer, intent(out), optional :: error
real(kind=default), dimension(size(value)) :: buffer
call mpi90_receive_double_array &
    (buffer, source, tag, domain, status, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_receive_double_array2

```

352a *<Interfaces of mpi90 procedures 347c>+≡*

```

interface mpi90_receive_pointer
    module procedure &
        mpi90_receive_integer_pointer, mpi90_receive_double_pointer
end interface

```

352b *<Implementation of mpi90 procedures 345a>+≡*

```

subroutine mpi90_receive_integer_pointer &
    (buffer, source, tag, domain, status, error)
integer, dimension(:), pointer :: buffer
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_receive_integer_pointer"
integer, parameter :: datatype = MPI_INTEGER
<Body of mpi90_receive_*_pointer 352c>
end subroutine mpi90_receive_integer_pointer

```

352c *<Body of mpi90\_receive\_\*\_pointer 352c>≡*

```

integer :: local_source, local_tag, local_domain, local_error, buffer_size
integer, dimension(MPI_STATUS_SIZE) :: local_status
integer :: ierror
external mpi_receive, mpi_get_count
<Set defaults for source, tag and domain 349e>

```

352d *<Body of mpi90\_receive\_\*\_pointer 352c>+≡*

```

call mpi_probe (local_source, local_tag, local_domain, &
    local_status, local_error)
<Handle local_error 345c>

```

 Can we ignore ierror???

352e *<Body of mpi90\_receive\_\*\_pointer 352c>+≡*

```

call mpi_get_count (local_status, datatype, buffer_size, ierror)
if (associated (buffer)) then
    if (size (buffer) /= buffer_size) then
        deallocate (buffer)
        allocate (buffer(buffer_size))
    end if

```

```

else
    allocate (buffer(buffer_size))
end if

353a  <Body of mpi90_receive_*_pointer 352c>+≡
      call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
                    local_domain, local_status, local_error)

353b  <Body of mpi90_receive_*_pointer 352c>+≡
      <Handle local_error 345c>
      if (present (status)) then
        call decode_status (status, local_status, datatype)
      end if

353c  <Implementation of mpi90 procedures 345a>+≡
      subroutine mpi90_receive_double_pointer &
        (buffer, source, tag, domain, status, error)
        real(kind=default), dimension(:), pointer :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_double_pointer"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        <Body of mpi90_receive_*_pointer 352c>
      end subroutine mpi90_receive_double_pointer

```

### *L.3 Collective Communication*

```

353d  <Declaration of mpi90 procedures 344b>+≡
      public :: mpi90_broadcast

353e  <Interfaces of mpi90 procedures 347c>+≡
      interface mpi90_broadcast
        module procedure &
          mpi90_broadcast_integer, mpi90_broadcast_integer_array, &
          mpi90_broadcast_integer_array2, mpi90_broadcast_integer_array3, &
          mpi90_broadcast_double, mpi90_broadcast_double_array, &
          mpi90_broadcast_double_array2, mpi90_broadcast_double_array3, &
          mpi90_broadcast_logical, mpi90_broadcast_logical_array, &
          mpi90_broadcast_logical_array2, mpi90_broadcast_logical_array3
      end interface

353f  <Set default for domain 346b>+≡
      if (present (domain)) then
        local_domain = domain
      end if

```

```

else
    local_domain = MPI_COMM_WORLD
end if

354a  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_broadcast_integer (value, root, domain, error)
        integer, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_integer_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_integer

354b  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_broadcast_double (value, root, domain, error)
        real(kind=default), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_double_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_double

354c  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_broadcast_logical (value, root, domain, error)
        logical, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        logical, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_logical_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_logical

354d  ⟨Implementation of mpi90 procedures 345a⟩+≡
    subroutine mpi90_broadcast_integer_array (buffer, root, domain, error)
        integer, dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error

```

```

        character(len=*), parameter :: FN = "mpi90_broadcast_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_broadcast_*_array 355a>
    end subroutine mpi90_broadcast_integer_array

355a <Body of mpi90_broadcast_*_array 355a>≡
    integer :: local_domain, local_error
    external mpi_bcast
    <Set default for domain 346b>
    call mpi_bcast (buffer, size (buffer), datatype, root, &
                    local_domain, local_error)
    <Handle local_error 345c>

355b <Implementation of mpi90 procedures 345a>+≡
    subroutine mpi90_broadcast_double_array (buffer, root, domain, error)
        real(kind=default), dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        character(len=*), parameter :: FN = "mpi90_broadcast_double_array"
        <Body of mpi90_broadcast_*_array 355a>
    end subroutine mpi90_broadcast_double_array

355c <Implementation of mpi90 procedures 345a>+≡
    subroutine mpi90_broadcast_logical_array (buffer, root, domain, error)
        logical, dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, parameter :: datatype = MPI_LOGICAL
        character(len=*), parameter :: FN = "mpi90_broadcast_logical_array"
        <Body of mpi90_broadcast_*_array 355a>
    end subroutine mpi90_broadcast_logical_array

355d <Implementation of mpi90 procedures 345a>+≡
    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

```

356a *⟨Implementation of mpi90 procedures 345a⟩*+≡

```

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

```

356b *⟨Implementation of mpi90 procedures 345a⟩*+≡

```

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

```

356c *⟨Implementation of mpi90 procedures 345a⟩*+≡

```

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

```

356d *⟨Implementation of mpi90 procedures 345a⟩*+≡

```

subroutine mpi90_broadcast_double_array3 (value, root, domain, error)
  real(kind=default), dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  real(kind=default), dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_double_array (buffer, root, domain, error)

```

```

    value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_double_array3

```

357 *⟨Implementation of mpi90 procedures 345a⟩+≡*

```

subroutine mpi90_broadcast_logical_array3 (value, root, domain, error)
  logical, dimension(:,:,:), intent(inout) :: value
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  logical, dimension(size(value)) :: buffer
  buffer = reshape (value, shape(buffer))
  call mpi90_broadcast_logical_array (buffer, root, domain, error)
  value = reshape (buffer, shape(value))
end subroutine mpi90_broadcast_logical_array3

```

# —M— IDEAS

## *M.1 Toolbox for Interactive Optimization*

*Idea:* Provide a OpenGL interface to visualize the grid optimization.

*Motivation:* Would help multi channel developers.

*Implementation:* Coding is straightforward, but interface design is hard.

## *M.2 Partially Non-Factorized Importance Sampling*

*Idea:* Allow non-factorized grid optimization in two- or three-dimensional subspaces.

*Motivation:* Handle nastiest subspaces. Non-factorized approaches are impossible in higher than three dimensions (and probably only realistic in two dimensions), but there are cases that are best handled by including non-factorized optimization in two dimensions.

*Implementation:* The problem is that the present `vamp_sample_grid0` can't accomodate this, because other auxiliary information has to be collected, but a generalization is straightforward. Work has to start from an extended `divisions` module.

## *M.3 Correlated Importance Sampling (?)*

*Idea:* Is it possible to include *some* correlations in a mainly factorized context?

*Motivation:* Would be nice ...

*Implementation:* First, I have to think about the maths ...

## *M.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region)*

*Idea:* Solve **vegas**' nastiest problem by finding the direction(s) along which singularities are aligned.

*Motivation:* Automatically choose proper coordinate system in generator generators and separate wild and smooth directions.

*Implementation:* Diagonalize the covariance matrix  $\text{cov}(x_i x_j)$  to find better axes. Caveats:

- damp rotations (rotate only if eigenvalues are spread out sufficiently).
- be careful about blow up of the integration volume, which is  $V' = V d^{d/2}$  in the worst case for hypercubes and can be even worse for stretched cubes. (An adaptive grid can help, since we will have more smooth directions!)

*Maybe* try non-linear transformations as well.

## *M.5 Automagic Multi Channel*

*Idea:* Find and extract one singularity after the other.

*Motivation:* Obvious.

*Implementation:* Either use multiple of **vegas**'  $p(x)$  for importance sampling. Or find hot region(s) and split the integration region (à la signal/background).



# —N—

## CROSS REFERENCES

### *N.1 Identifiers*

BUFFER\_SIZE: [59b](#), [60a](#), [108b](#), [109a](#), [109b](#), [110](#), [265b](#)  
DEFAULT\_BUFFER\_SIZE: [254a](#), [261c](#), [261e](#), [274b](#), [275a](#)  
DEFAULT\_SEED: [256a](#), [256c](#)  
EXC\_DEFAULT: [247a](#), [247e](#)  
EXC\_ERROR: [90b](#), [246c](#), [247a](#), [247c](#)  
EXC\_FATAL: [50a](#), [50b](#), [51a](#), [91a](#), [97b](#), [246c](#), [247c](#)  
EXC\_INFO: [96b](#), [169](#), [179a](#), [246c](#), [247c](#)  
EXC\_NONE: [246b](#), [246c](#), [247c](#)  
EXC\_WARN: [90b](#), [99a](#), [106b](#), [121](#), [124b](#), [135c](#), [137d](#), [138a](#), [169](#), [176d](#), [177a](#),  
[180b](#), [246c](#), [247c](#)  
K: [253a](#), [253b](#), [253a](#), [254d](#), [254e](#), [253a](#), [254f](#), [255b](#), [255e](#), [256d](#), [257a](#), [257b](#),  
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[235b](#), [235c](#), [236a](#), [236b](#), [236c](#)  
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](#)  
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LIPS3\_unit\_to\_s2\_t1\_angles\_m0: [331f](#), [331g](#), [332b](#)  
M: [241b](#), [253c](#), [254e](#), [254f](#), [256d](#), [257b](#), [257c](#), [258c](#), [258f](#), [259g](#), [260a](#), [274d](#),

276e, 282c, 282d, 283b, 283c, 283d, 283e, 284a  
 MAX\_SEED: [256b](#), [256c](#)  
 MAX\_UNIT: [267d](#), [268a](#), [312b](#), [312c](#)  
 MIN\_NUM\_DIV: [46a](#)  
 MIN\_UNIT: [267d](#), [268a](#), [312b](#), [312c](#)  
 NAME\_LENGTH: [246b](#), [247a](#)  
 NO\_DATA: [77c](#), [195d](#), [197b](#), [198b](#), [211b](#), [212b](#), [213b](#), [214](#)  
 NUM\_DIV\_DEFAULT: [78](#), [79a](#), [79a](#)  
 PI: [191b](#), [193](#), [194a](#), [194b](#), [224b](#), [224c](#), [225a](#), [226c](#), [227f](#), [228b](#), [229](#), [244b](#),  
 286a, [287c](#), [289b](#), [327a](#), [327b](#), [332e](#), [333c](#), [333d](#), [334](#), [336](#), [343c](#)  
 PRIMES: [311b](#), [311c](#)  
 QUAD\_POWER: [93a](#), [93c](#)  
 TAG\_GRID: [177b](#), [177c](#), [178a](#), [178d](#)  
 TAG\_HISTORY: [177c](#), [178a](#), [178d](#)  
 TAG\_INTEGRAL: [177c](#), [178a](#), [178d](#)  
 TAG\_NEXT\_FREE: [178d](#)  
 TAG\_STD\_DEFS: [178d](#)  
 TT: [256b](#), [256f](#)  
 ULP: [259b](#), [259d](#), [259e](#)  
 VAMP\_MAX\_WASTE: [174d](#), [176a](#), [176a](#)  
 VAMP\_ROOT: [167d](#), [168a](#), [168b](#), [168c](#), [169](#), [171a](#), [171e](#), [172a](#), [173a](#), [173b](#),  
 174a, [174b](#), [174d](#), [176c](#), [177a](#), [177b](#), [177c](#), [178e](#), [179a](#), [179c](#), [180b](#), [181d](#),  
 182a, [183d](#), [183e](#), [184a](#), [184b](#), [184f](#), [185a](#), [185b](#), [185c](#)  
 abs\_evec: [128a](#), [128b](#), [128c](#), [128f](#), [129c](#), [130a](#)  
 accuracy: [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [96b](#), [103b](#), [120b](#), [140b](#), [140c](#), [141c](#),  
 169, [174d](#), [179a](#)  
 adaptive\_division: [57a](#), [57f](#)  
 average: [108b](#), [110](#), [133c](#), [291b](#), [291c](#), [292a](#), [292d](#), [292e](#)  
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 108b, [110](#), [120b](#), [123b](#), [124e](#), [140b](#), [140c](#), [141c](#), [160b](#), [162](#), [165b](#), [169](#), [174d](#),  
[178e](#)  
 boost\_many\_momentum: [324b](#), [324c](#), [326b](#)  
 boost\_many\_velocity: [324b](#), [324c](#), [325b](#), [326b](#)  
 boost\_momentum: [227f](#), [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](#), [261c](#), [261e](#), [263f](#), [265b](#), [265c](#), [269c](#), [270b](#), [271a](#),  
 271c, [273c](#), [274c](#), [274d](#), [274e](#), [275a](#), [275b](#), [276b](#), [276c](#), [276e](#), [277a](#), [277b](#),  
 277c, [277d](#), [277e](#), [278a](#), [278b](#), [280g](#), [281a](#)  
 calls: [84a](#), [84a](#), [84a](#), [84a](#), [84a](#), [24d](#), [84a](#), [84a](#), [84a](#), [84a](#), [76b](#), [84a](#), [84b](#), [89a](#),

[98c](#), [100c](#), [106a](#), [106e](#), [107a](#), [107b](#), [108b](#), [110](#), [124e](#), [135a](#), [140b](#), [140c](#), [141c](#),  
[144b](#), [145b](#), [151](#), [152b](#), [157b](#), [159](#), [160b](#), [162](#), [163](#), [165b](#), [238](#), [241a](#), [241b](#),  
[242](#), [243](#)  
calls\_per\_cell: [76b](#), [84a](#), [84b](#), [88a](#), [89d](#), [97b](#), [98c](#), [98d](#), [144b](#), [145b](#), [151](#),  
[152b](#), [157b](#), [159](#), [163](#)  
cartesian\_to\_spherical: [338c](#), [340a](#)  
cartesian\_to\_spherical\_2: [338c](#), [338d](#), [340a](#), [340b](#)  
cartesian\_to\_spherical\_cos: [194a](#), [341c](#), [342](#)  
cartesian\_to\_spherical\_cos\_2: [196b](#), [341c](#), [341d](#), [342](#), [343a](#)  
cartesian\_to\_spherical\_cos\_j: [194b](#), [341c](#), [343a](#)  
cartesian\_to\_spherical\_j: [338c](#), [340b](#)  
cell: [87a](#), [43b](#), [87a](#), [87a](#), [87b](#), [87d](#), [88b](#)  
check\_inverses: [195c](#), [196a](#), [199c](#)  
check\_inverses3: [195c](#), [196b](#), [199c](#)  
check\_jacobians: [195c](#), [195d](#), [199c](#), [210c](#), [210d](#), [218a](#)  
check\_kinematics: [233b](#), [233c](#), [238](#)  
cl: [132a](#), [132b](#), [132c](#), [132d](#)  
clear\_exception: [24a](#), [24b](#), [24c](#), [24d](#), [103b](#), [120b](#), [213b](#), [214](#), [241a](#), [241b](#),  
[242](#), [243](#), [247d](#), [248a](#), [249](#)  
clear\_integral\_and\_variance: [44c](#), [45c](#), [84a](#), [87b](#)  
cl\_num: [132a](#), [132b](#), [132c](#), [132d](#)  
cl\_pos: [132a](#), [132b](#), [132c](#), [132d](#)  
collect: [54b](#), [54c](#), [55c](#)  
constants: [191b](#), [221a](#), [244b](#), [286a](#), [288b](#), [324a](#), [329d](#), [333d](#), [334](#), [336](#)  
coordinates: [191b](#), [195b](#), [199c](#), [201b](#), [201c](#), [336](#)  
copy\_array\_pointer: [52b](#), [54a](#), [60d](#), [60e](#), [60f](#), [60g](#), [69](#), [97c](#), [159](#), [163](#), [164b](#),  
[306d](#), [306e](#)  
copy\_division: [38a](#), [51a](#), [69](#), [69](#), [99b](#), [163](#)  
copy\_history: [58b](#), [70b](#), [107b](#), [108b](#), [110](#), [165b](#)  
copy\_integer\_array2\_pointer: [306d](#), [306e](#), [307c](#)  
copy\_integer\_array\_pointer: [306d](#), [306e](#), [307a](#)  
copy\_raw\_state: [262c](#), [263e](#), [263f](#), [263g](#), [264a](#), [264b](#)  
copy\_raw\_state\_to\_state: [263e](#), [264a](#)  
copy\_real\_array2\_pointer: [306d](#), [306e](#), [307d](#)  
copy\_real\_array\_pointer: [306d](#), [306e](#), [307b](#)  
copy\_state: [263e](#), [263f](#)  
copy\_state\_to\_raw\_state: [262b](#), [263e](#), [264b](#)  
cos\_theta: [128d](#), [128e](#), [128f](#), [196b](#), [327a](#), [327b](#), [328c](#), [328d](#), [329b](#), [332d](#),  
[332e](#), [337b](#), [338d](#), [340d](#), [341d](#), [342](#)  
create\_array\_pointer: [97c](#), [145b](#), [152b](#), [304b](#), [304c](#)  
create\_division: [38a](#), [38b](#), [78](#)

create\_empty\_division: 38a, [39a](#), [99c](#), [147a](#)  
 create\_histogram: [213b](#), [214](#), [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: [261b](#), [261d](#), [261e](#), [262c](#)  
 create\_raw\_state\_from\_seed: [261b](#), [261c](#), [262a](#)  
 create\_raw\_state\_from\_state: [261b](#), [262b](#)  
 create\_real\_array2\_pointer: [304b](#), [304c](#), [306c](#), [307d](#)  
 create\_real\_array\_pointer: [304b](#), [304c](#), [306a](#), [307b](#)  
 create\_sample: [204](#), [206c](#), [218f](#)  
 create\_state\_from\_raw\_state: [261b](#), [261e](#)  
 create\_state\_from\_seed: [261b](#), [261c](#)  
 create\_state\_from\_state: [261b](#), [261d](#)  
 ctest: [133c](#)  
 debug\_division: [56a](#), [56b](#)  
 decode\_status: [350c](#), [350d](#), [350e](#), [353b](#)  
 delete\_division: [38a](#), [70a](#), [147a](#), [163](#), [164a](#)  
 delete\_histogram: [213b](#), [214](#), [295b](#), [295c](#)  
 delete\_histogram1: [295c](#), [295d](#), [297c](#)  
 delete\_histogram2: [295c](#), [295d](#), [298a](#)  
 delete\_sample: [204](#), [206b](#), [219a](#)  
 delta: [47c](#), [47c](#), [47c](#), [48b](#), [48c](#), [115](#), [195d](#), [289b](#)  
 descr\_fmt: [61c](#), [62a](#), [62b](#), [144b](#), [145a](#), [145b](#), [148d](#), [149](#)  
 destroy\_raw\_state: [262d](#), [262e](#), [263a](#)  
 destroy\_state: [262d](#), [262e](#), [262f](#)  
 determinant: [114b](#), [116b](#), [316a](#), [316b](#), [321d](#)  
 diag: [317b](#), [321b](#), [321c](#)  
 diagonalize\_real\_symmetric: [317b](#), [128f](#), [129b](#), [129c](#), [130e](#), [141c](#), [317a](#),  
[317b](#), [321d](#)  
 distribute: [15](#), [16](#), [54a](#), [54c](#), [55b](#), [103b](#)  
 div\_history: [58a](#), [58c](#), [59a](#), [59b](#), [68b](#), [68c](#), [68d](#), [70b](#), [106a](#), [108b](#), [110](#)  
 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](#), [97a](#), [99d](#)  
 division\_variance: [60c](#), [60f](#)  
 division\_x: [60c](#), [60d](#)

domain: 78, 78, 23c, 24a, 24d, 78, 78, 78, 78, 78, 117a, 167d, 173a, 186a,  
 186b, 187a, 187b, 188b, 188c, 189a, 189c, 190, 345e, 346b, 346c, 347a,  
 347d, 347e, 348a, 348c, 348d, 349a, 349c, 350a, 350b, 351a, 351b, 351c,  
 352b, 353c, 353f, 354a, 354b, 354c, 354d, 355b, 355c, 355d, 356a, 356b,  
 356c, 356d, 357  
 double\_array2\_fmt: 144b, 145a, 145b  
 double\_array\_fmt: 61c, 62a, 62b, 144b, 145a, 145b, 148d, 149  
 double\_fmt: 61c, 62a, 62b, 144b, 145a, 145b, 148d, 149  
 dump\_division: 56a, 56c, 214  
 dv2g: 76b, 84b, 84b, 90a, 98c, 144b, 145b, 151, 152b, 157b, 159, 163  
 dx: 37b, 38b, 43b, 44a, 48e, 52b, 54a, 57d, 61c, 62b, 64b, 65b, 66d, 67b,  
 69, 78, 114b, 116b, 196a, 196b  
 exception: 23c, 246b, 246b, 50a, 50b, 78, 80c, 82a, 83, 86c, 93a, 94, 97a,  
 99d, 101b, 102c, 103b, 117a, 118b, 118d, 119b, 120b, 134d, 136, 138c,  
 139a, 140b, 140c, 141c, 167d, 168b, 168c, 169, 173a, 173b, 174a, 174d,  
 181d, 182a, 182b, 182c, 213b, 214, 238, 246b, 247c, 247e, 248a, 248b  
 exceptions: 246a, 23b, 246a, 37a, 75b, 166c, 195b, 201b, 210b, 238, 246a  
 f: 22, 44d, 59b, 88c, 88c, 89a, 89b, 89c, 125b, 134d, 135a, 135b, 135c,  
 191b, 192a, 192b, 192c, 195a, 197b, 204, 206a, 209b, 211b, 213b, 214,  
 287a, 287b, 287c  
 f0: 204, 205a, 206a  
 f2: 89b, 89c  
 factorize: 104b, 310d, 311b  
 fill\_histogram: 213b, 214, 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, 148b, 148c, 150a, 150b, 154a, 154b,  
 156a, 156b, 267d, 268b, 268c, 268d, 268e, 268f, 294a, 298b, 301, 312a,  
312c  
 f\_max: 76b, 84e, 89a, 89b, 98c, 100c, 106a, 107b, 108b, 110, 124e, 135a,  
 135c, 137a, 137d, 138a, 84e, 144b, 145b, 151, 152b, 157b, 159, 160b, 162,  
 163, 165b  
 f\_min: 76b, 84e, 89a, 98c, 100c, 106a, 107b, 124e, 84e, 144b, 145b, 151,  
 152b, 157b, 159, 160b, 162, 163, 165b  
 f\_norm: 204, 205a, 205b  
 fork\_division: 49c, 50a, 50a, 98d  
 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, 86c, 22, 22, 22, 22, 22, 88c, 94, 103b, 113a,  
 113b, 115, 120b, 121, 125b, 134d, 136, 138c, 139a, 140b, 140c, 141c, 169,  
 174d, 176d, 180b, 181d, 182a, 182b, 182c



histogram2: [295a](#), [295a](#), [296a](#), [297a](#), [297b](#), [298a](#), [300e](#), [301](#)  
 histograms: [195b](#), [201b](#), [210b](#), [294a](#)  
 i: [15](#), [16](#), [17](#), [128a](#), [128a](#), [128a](#), [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](#), [75a](#), [91d](#), [97a](#), [97c](#), [98c](#), [98d](#), [128a](#), [99b](#), [99c](#), [99d](#),  
[100a](#), [100b](#), [100c](#), [101b](#), [102b](#), [102c](#), [103b](#), [104b](#), [105b](#), [108b](#), [109b](#), [110](#),  
[113a](#), [113b](#), [115](#), [128a](#), [128b](#), [128c](#), [128d](#), [128e](#), [128f](#), [129c](#), [130a](#), [130e](#),  
[132a](#), [132d](#), [133b](#), [133c](#), [144b](#), [145b](#), [148d](#), [149](#), [151](#), [152b](#), [154c](#), [155b](#),  
[157b](#), [158](#), [159](#), [161](#), [169](#), [188c](#), [192c](#), [196a](#), [196b](#), [205a](#), [206a](#), [213b](#), [214](#),  
[218e](#), [218f](#), [238](#), [242](#), [248b](#), [266b](#), [266d](#), [266f](#), [267b](#), [267d](#), [282b](#), [282d](#), [283b](#),  
[283c](#), [283d](#), [283e](#), [284a](#), [284b](#), [287a](#), [287b](#), [287c](#), [289c](#), [296b](#), [297b](#), [298b](#),  
[299b](#), [308d](#), [309a](#), [309b](#), [309c](#), [128a](#), [311b](#), [312c](#), [316b](#), [321a](#), [321b](#), [321d](#),  
[325b](#), [333d](#), [334](#), [337b](#), [338d](#), [340d](#), [341d](#)  
 ia: [88b](#), [89b](#), [89c](#), [89d](#), [134d](#), [135a](#)  
 ihp: [31b](#), [31b](#), [113a](#), [191b](#), [194a](#), [195a](#), [196a](#)  
 inject\_division: [43a](#), [43b](#), [88b](#)  
 inject\_division\_short: [43a](#), [44b](#), [135a](#)  
 inside\_division: [57a](#), [57b](#), [88c](#)  
 integer\_array\_fmt: [144b](#), [145a](#), [145b](#), [148d](#), [149](#)  
 integer\_array\_state: [277e](#), [279f](#)  
 integer\_array\_stateless: [275b](#), [277e](#), [279b](#), [280a](#)  
 integer\_array\_static: [279b](#), [279f](#)  
 integer\_fmt: [61c](#), [62a](#), [62b](#), [144b](#), [145a](#), [145b](#), [148d](#), [149](#)  
 integer\_state: [277b](#), [279f](#)  
 integer\_stateless: [273c](#), [277b](#), [278d](#), [280a](#)  
 integer\_static: [278d](#), [279f](#)  
 integral: [94](#), [94](#), [94](#), [94](#), [23c](#), [24c](#), [24d](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [37b](#), [38b](#),  
[39a](#), [40b](#), [44d](#), [45c](#), [52b](#), [94](#), [52c](#), [54a](#), [54b](#), [55d](#), [56b](#), [56c](#), [58c](#), [60e](#), [94](#), [61c](#),  
[62b](#), [63a](#), [64b](#), [65b](#), [66d](#), [67b](#), [69](#), [70a](#), [90b](#), [94](#), [95a](#), [96a](#), [103b](#), [106a](#), [107b](#),  
[108b](#), [110](#), [120b](#), [123b](#), [124e](#), [140b](#), [140c](#), [141c](#), [160b](#), [162](#), [165b](#), [169](#), [174d](#),  
[178e](#), [197b](#), [198a](#), [198b](#), [199b](#), [211b](#), [212b](#), [213b](#), [214](#), [238](#), [241a](#), [241b](#), [242](#),  
[243](#)  
 invariants\_from\_p: [227e](#), [227f](#), [233c](#), [234b](#), [234c](#), [235c](#), [236a](#)  
 invariants\_from\_x: [227e](#), [228b](#), [233c](#), [234b](#), [234c](#), [235a](#), [235b](#), [235c](#), [236a](#),  
[236b](#), [236c](#)  
 invariants\_to\_p: [227e](#), [228a](#), [233c](#), [234b](#), [234c](#), [235a](#), [235b](#), [235c](#), [236a](#),  
[236b](#), [236c](#)  
 invariants\_to\_x: [227e](#), [229](#), [233c](#), [234b](#), [234c](#), [235c](#), [236a](#)  
 iteration: [14](#), [15](#), [17](#), [94](#), [94](#), [94](#), [95a](#), [103b](#), [106b](#), [120b](#), [121](#), [123b](#), [124b](#),  
[169](#), [174d](#), [176d](#), [177a](#), [177c](#), [178a](#), [180b](#)  
 iterations: [14](#), [15](#), [17](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [59b](#), [94](#), [103b](#),

108b, 110, 120b, 138c, 139a, 169, 174d, 182b, 182c, 197b, 198a, 198b,  
 199c, 201c, 211b, 212a, 212b, 213b, 214, 217a, 217b, 217c, 217d, 218e,  
 218f, 238, 241a, 241b, 242, 243  
 iv: [126b](#), 128a, 128b, 128c, 128d, 128f, 129c, 130a  
 j: 31c, 50a, 50b, 52a, 53, 79c, 87a, [87d](#), 97a, 98d, 87d, 87d, 99b, 99d, 100a,  
 100b, 104b, 105a, 105b, 108b, 110, 114b, 116b, 130e, 144b, 145b, 151,  
 152b, 160b, 162, 191b, 194b, 195a, 195d, 196b, 205a, 206a, 208b, 208c,  
 209a, 214, 218e, 218f, 254b, 254e, 254f, 255e, 256d, 257b, 257f, 258e, 258f,  
 259c, 259d, 259g, 308d, 309a, 309b, 309c, 314, 315d, 317b  
 jacobi: 76b, 84b, [84b](#), 88b, 98c, 100c, 135a, 144b, 145b, 151, 152b, 157b,  
 159, 163  
 jacobian: [31c](#), 31c, 31c, 113a, 113b, 114b, 116b, 225a, 226b, [226c](#), 227c,  
 227d, 227f, 228a, 228b, 229, 230b, 231a, 231c, 233c, 233d, 235c, 236a,  
 236b, 236c, 326g, [327a](#), [327b](#), 330a, 330b, 330c, 330d, 330e, 331a, 331d,  
 331e, 333d, 337b, 338b, 338d, 340b, 340d, 341b, 341d, 343a  
 jacobi\_rotation: 320a, [320b](#), 320c, 320d  
 join\_division: 49c, [50b](#), 100a  
 k: [47c](#), [48b](#), 48c, [87d](#), 88a, 230b, 231a, 231c, 232, 237b, 289b, 332d, 47c,  
 332e, 333a  
 kinematics: 221a, 238, [324a](#), 329d, 333d, 334  
 lambda: 224b, 226c, 227f, 228b, 229, 321d, [326c](#), 326d, 327a, 328c, 333d  
 last: 255d, 260c, 260e, 263f, 264c, 265b, 265c, 269c, 270b, 271a, 271c,  
 273c, 274a, 275a, 275a, 274c, 274d, 274e, [275a](#), 275b, 275c, 275a, 276b,  
 276c, 276d, 276e, 277a, 277b, 277c, 277d, 277e, 278a, 278b, 280g, 281a  
 lcm: 53, 310d, [311a](#)  
 linalg: 75b, 238, [313a](#), 317b, 321d  
 local\_avg\_chi2: [94](#), [96a](#), 103b, 106b, 120b, 121, 124b, 169, 174d, 176d,  
 177a, 178e, 180b  
 local\_integral: [94](#), [96a](#), 96b, 103b, 106b, 120b, 124b, 169, 174d, 177a,  
 178e, 179a, 180b  
 local\_std\_dev: [94](#), [96a](#), 96b, 103b, 106b, 120b, 124b, 169, 174d, 177a,  
 178e, 179a, 180b  
 logical\_fmt: 61c, [62a](#), 62b, 144b, [145a](#), 145b  
 lorentzian: 191b, [192b](#), 192c  
 lorentzian\_normalized: 191b, [192a](#), 192b  
 lu\_decompose: 313b, [314](#), 316b, 321d  
 luxury\_state: [280h](#), 282a  
 luxury\_state\_integer: 280h, [281a](#), 281b, 282a  
 luxury\_stateless: [280g](#), 281a, 281d, 281g  
 luxury\_state\_real: [281b](#), 282a  
 luxury\_static: [281c](#), 282a



luxury\_static\_integer: [281c](#), [281d](#), [281e](#), [282a](#)  
luxury\_static\_real: [281e](#), [282a](#)  
m: [39c](#), [40a](#), [46b](#), [47b](#), [40a](#), [47c](#), [48b](#), [48c](#), [58c](#), [59b](#), [310e](#), [310f](#), [40a](#), [311a](#),  
[329c](#), [334](#)  
map\_domain: [78](#), [79b](#), [79c](#)  
marshal\_div\_history: [68a](#), [68b](#), [160b](#)  
marshal\_div\_history\_size: [68a](#), [68c](#), [160b](#), [161](#)  
marshal\_division: [66c](#), [66d](#), [157b](#)  
marshal\_division\_size: [66c](#), [67a](#), [157b](#), [158](#)  
marshal\_raw\_state: [269a](#), [269b](#), [269c](#), [270c](#), [270e](#), [271a](#), [271d](#)  
marshal\_raw\_state\_size: [269a](#), [269b](#), [270a](#), [270d](#), [271b](#), [272a](#)  
marshal\_state: [269a](#), [269b](#), [269c](#), [270b](#), [271a](#)  
marshal\_state\_size: [269a](#), [269b](#), [270a](#), [271b](#)  
massless\_isotropic\_decay: [232](#), [332c](#), [332d](#)  
midpoint: [298b](#), [299b](#), [300a](#), [300b](#), [301](#)  
midpoint1: [300b](#), [300c](#), [300d](#)  
midpoint2: [300b](#), [300c](#), [300e](#)  
more\_pancake\_than\_cigar: [126b](#), [127a](#), [127b](#)  
mpi90: [166c](#), [201c](#), [219b](#), [219c](#), [238](#), [344a](#), [346a](#)  
mpi90\_abort: [344b](#), [345c](#), [345e](#), [346a](#)  
mpi90\_broadcast: [17](#), [169](#), [174d](#), [178e](#), [179a](#), [188b](#), [189a](#), [201c](#), [219c](#), [238](#),  
[242](#), [353d](#), [353e](#)  
mpi90\_broadcast\_double: [353e](#), [354b](#)  
mpi90\_broadcast\_double\_array: [353e](#), [354b](#), [355b](#), [356a](#), [356d](#)  
mpi90\_broadcast\_double\_array2: [353e](#), [356a](#)  
mpi90\_broadcast\_double\_array3: [353e](#), [356d](#)  
mpi90\_broadcast\_integer: [353e](#), [354a](#)  
mpi90\_broadcast\_integer\_array: [353e](#), [354a](#), [354d](#), [355d](#), [356c](#)  
mpi90\_broadcast\_integer\_array2: [353e](#), [355d](#)  
mpi90\_broadcast\_integer\_array3: [353e](#), [356c](#)  
mpi90\_broadcast\_logical: [353e](#), [354c](#)  
mpi90\_broadcast\_logical\_array: [353e](#), [354c](#), [355c](#), [356b](#), [357](#)  
mpi90\_broadcast\_logical\_array2: [353e](#), [356b](#)  
mpi90\_broadcast\_logical\_array3: [353e](#), [357](#)  
mpi90\_finalize: [201c](#), [219c](#), [238](#), [344b](#), [345d](#)  
mpi90\_init: [201c](#), [219c](#), [238](#), [344b](#), [345a](#)  
mpi90\_print\_error: [344b](#), [345b](#), [345c](#), [346a](#)  
mpi90\_rank: [17](#), [167d](#), [168b](#), [168c](#), [169](#), [171a](#), [171e](#), [172a](#), [173a](#), [173b](#), [174a](#),  
[174b](#), [174d](#), [181d](#), [182a](#), [183d](#), [183e](#), [184a](#), [184b](#), [184f](#), [185a](#), [185b](#), [185c](#),  
[188b](#), [189a](#), [201c](#), [219c](#), [238](#), [344b](#), [347a](#)  
mpi90\_receive: [178a](#), [186b](#), [190](#), [347b](#), [349d](#)

mpi90\_receive\_double: [349d](#), [350a](#)  
 mpi90\_receive\_double\_array: [349d](#), [350a](#), [351a](#), [351c](#)  
 mpi90\_receive\_double\_array2: [349d](#), [351c](#)  
 mpi90\_receive\_double\_pointer: [352a](#), [353c](#)  
 mpi90\_receive\_integer: [349c](#), [349d](#)  
 mpi90\_receive\_integer\_array: [349c](#), [349d](#), [350b](#), [351b](#)  
 mpi90\_receive\_integer\_array2: [349d](#), [351b](#)  
 mpi90\_receive\_integer\_pointer: [352a](#), [352b](#)  
 mpi90\_receive\_pointer: [352a](#), [352a](#), [352a](#), [187b](#), [347b](#), [352a](#)  
 mpi90\_send: [177c](#), [186a](#), [187a](#), [189c](#), [347b](#), [347c](#)  
 mpi90\_send\_double: [347c](#), [347e](#)  
 mpi90\_send\_double\_array: [347c](#), [347e](#), [348c](#), [349a](#)  
 mpi90\_send\_double\_array2: [347c](#), [349a](#)  
 mpi90\_send\_integer: [347c](#), [347d](#)  
 mpi90\_send\_integer\_array: [347c](#), [347d](#), [348a](#), [348d](#)  
 mpi90\_send\_integer\_array2: [347c](#), [348d](#)  
 mpi90\_size: [17](#), [169](#), [174d](#), [201c](#), [219c](#), [238](#), [344b](#), [346c](#)  
 mpi90\_status: [186b](#), [187b](#), [190](#), [349b](#), [349c](#), [350a](#), [350b](#), [350e](#), [351a](#), [351b](#),  
     [351c](#), [352b](#), [353c](#)  
 multi\_channel: [197a](#), [198a](#), [199c](#), [211a](#), [212a](#), [217c](#)  
 multi\_channel\_generator: [213a](#), [214](#), [217d](#)  
 ndim: [78](#), [79c](#), [82a](#), [84a](#), [86c](#), [87a](#), [93a](#), [94](#), [97a](#), [97c](#), [106e](#), [129c](#), [130a](#), [145b](#),  
     [147a](#), [152b](#), [157b](#), [158](#), [159](#), [160b](#), [161](#), [162](#), [163](#), [317b](#), [78](#), [78](#), [320a](#)  
 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](#), [82a](#), [42](#), [84a](#),  
     [85b](#), [104b](#), [105b](#)  
 norm: [128d](#), [128f](#), [205a](#), [205b](#)  
 num\_calls: [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [24a](#), [24c](#), [81b](#), [81b](#), [81b](#), [81b](#),  
     [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [50a](#), [51a](#), [52b](#), [54a](#), [76b](#), [78](#), [80c](#),  
     [81b](#), [82a](#), [83](#), [84a](#), [98c](#), [112a](#), [117a](#), [117b](#), [118b](#), [118d](#), [119b](#), [81b](#), [81b](#), [120b](#),  
     [122b](#), [139a](#), [144b](#), [145b](#), [148d](#), [149](#), [151](#), [152b](#), [154c](#), [155b](#), [157b](#), [159](#), [163](#),  
     [164b](#), [165a](#), [167d](#), [168b](#), [168c](#), [173a](#), [173b](#), [174a](#), [174d](#), [182c](#), [189a](#)  
 num\_cells: [82a](#), [84a](#), [84b](#), [97a](#), [98c](#)  
 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](#), [78](#),  
     [80a](#), [80c](#), [81b](#), [82a](#), [83](#), [84a](#), [93a](#), [42](#), [97a](#), [97c](#), [99c](#), [117a](#), [118b](#), [118d](#), [119b](#),  
     [140b](#), [140c](#), [141c](#), [144b](#), [145b](#), [151](#), [152b](#), [157b](#), [159](#), [163](#), [164a](#), [167d](#), [168b](#),  
     [168c](#), [173a](#), [173b](#), [174a](#)  
 numeric\_jacobian: [116a](#), [116b](#)  
 object: [177b](#), [177c](#), [178a](#), [178b](#), [178c](#)  
 one\_to\_two\_massive: [328a](#), [328b](#), [328c](#)

one\_to\_two\_massless: [328a](#), [328b](#), [328d](#)  
on\_shell: [327a](#), [327b](#), [328c](#), [329a](#), [329c](#)  
outer\_product: [85c](#), [89b](#), [89d](#), [310b](#), [310c](#), [314](#)  
phase\_space: [225b](#), [227a](#), [230b](#), [231c](#), [233c](#), [329d](#)  
phase\_space\_volume: [223b](#), [232](#), [238](#), [333b](#), [333c](#)  
phi: [31a](#), [31a](#), [31a](#), [113a](#), [113b](#), [114b](#), [115](#), [116b](#), [136](#), [182a](#), [191b](#), [193](#),  
[194a](#), [195a](#), [195d](#), [196a](#), [196b](#), [204](#), [208c](#), [209b](#), [210d](#), [214](#), [224b](#), [224c](#),  
[225b](#), [227b](#), [227c](#), [227f](#), [228a](#), [228b](#), [229](#), [233d](#), [327a](#), [327b](#), [328c](#), [328d](#),  
[329b](#), [330c](#), [330d](#), [332d](#), [332e](#), [333d](#), [337b](#), [338a](#), [338b](#), [338d](#), [340a](#), [340d](#),  
[341a](#), [341b](#), [341d](#), [342](#)  
phi1: [234a](#), [235a](#), [237b](#)  
phi12: [234a](#), [234b](#), [237b](#), [238](#)  
phi2: [233d](#), [234a](#), [235b](#), [237b](#)  
phi21: [234a](#), [234c](#), [237b](#), [238](#)  
print\_LIPS3\_m5i2a3: [233b](#), [233d](#)  
print\_history: [59a](#), [59b](#), [60b](#), [108b](#)  
print\_history,: [60b](#)  
print\_results: [199a](#), [199b](#), [199c](#)  
probabilities: [58c](#), [58d](#), [58e](#)  
probability: [48d](#), [48e](#), [91c](#)  
psi: [204](#), [207](#), [208c](#)  
quadrupole: [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [76b](#), [78](#), [80c](#), [81b](#), [82a](#), [83](#), [93a](#), [98b](#),  
[117a](#), [118b](#), [118d](#), [119b](#), [140b](#), [140c](#), [141c](#), [144b](#), [145b](#), [151](#), [152b](#), [157b](#),  
[159](#), [163](#), [167d](#), [168b](#), [168c](#), [173a](#), [173b](#), [174a](#)  
quadrupole\_division: [49a](#), [49b](#), [93a](#)  
r: [43b](#), [44b](#), [88b](#), [89c](#), [115](#), [128e](#), [128f](#), [129b](#), [129c](#), [134d](#), [135a](#), [136](#), [137b](#),  
[137d](#), [138a](#), [192b](#), [193](#), [194a](#), [196b](#), [250](#), [252g](#), [273c](#), [274a](#), [274d](#), [274e](#),  
[277b](#), [277c](#), [277d](#), [278d](#), [278e](#), [279a](#), [332d](#), [333a](#), [333d](#), [337b](#), [338a](#), [338b](#),  
[338d](#), [340a](#), [340d](#), [341a](#), [341b](#), [341d](#), [342](#)  
raise\_exception: [50a](#), [50b](#), [51a](#), [90b](#), [91a](#), [96b](#), [97b](#), [106b](#), [121](#), [124b](#),  
[135c](#), [137d](#), [138a](#), [169](#), [176d](#), [177a](#), [179a](#), [180b](#), [247d](#), [247e](#), [248b](#)  
random\_LIPS3: [331b](#), [331c](#)  
random\_LIPS3\_unit: [331b](#), [331c](#), [331d](#)  
random\_LIPS3\_unit\_massless: [331b](#), [331c](#), [331e](#)  
read\_division: [61a](#), [61b](#), [145b](#)  
read\_division\_name: [61a](#), [61b](#), [64a](#)  
read\_division\_raw: [61a](#), [61b](#), [152b](#)  
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: [143a](#), [143c](#), [148c](#), [183a](#), [183c](#), [184b](#)

read\_grid\_raw\_name: [143b](#), [144a](#), [154b](#)  
 read\_grid\_raw\_unit: [143b](#), [144a](#), [152b](#), [154b](#), [155b](#)  
 read\_grids\_name: [143a](#), [143c](#), [150b](#), [184c](#), [184e](#), [185c](#)  
 read\_grids\_raw\_name: [143b](#), [144a](#), [156b](#)  
 read\_grids\_raw\_unit: [143b](#), [144a](#), [155b](#), [156b](#)  
 read\_grids\_unit: [143a](#), [143c](#), [149](#), [150b](#), [184c](#), [184e](#), [185a](#)  
 read\_grid\_unit: [143a](#), [143c](#), [145b](#), [148c](#), [149](#), [183a](#), [183c](#), [183e](#)  
 read\_raw\_state\_name: [264f](#), [265a](#), [268f](#)  
 read\_raw\_state\_unit: [264f](#), [265a](#), [265c](#), [266a](#), [268f](#)  
 read\_state\_array: [265c](#), [266a](#), [266d](#), [266e](#), [267b](#), [267c](#)  
 read\_state\_name: [264f](#), [265a](#), [268e](#)  
 read\_state\_unit: [264f](#), [265a](#), [265c](#), [268e](#)  
 real\_array\_state: [278a](#), [278b](#), [279f](#), [280d](#)  
 real\_array\_stateless: [276e](#), [277a](#), [278a](#), [278b](#), [279c](#), [279d](#), [280a](#), [280e](#)  
 real\_array\_static: [279c](#), [279d](#), [279f](#), [280d](#)  
 real\_state: [277c](#), [277d](#), [279f](#), [280d](#)  
 real\_stateless: [274d](#), [274e](#), [277c](#), [277d](#), [278e](#), [279a](#), [280a](#), [280e](#)  
 real\_static: [278e](#), [279a](#), [279f](#), [280d](#)  
 rebin: [39c](#), [45e](#), [47c](#), [48a](#)  
 rebinning\_weights: [40a](#), [45e](#), [46b](#), [47a](#), [49b](#), [58c](#)  
 record\_efficiency: [44c](#), [45b](#), [89b](#), [135a](#)  
 record\_integral: [44c](#), [44d](#), [89b](#)  
 record\_variance: [44c](#), [45a](#), [89d](#)  
 refine\_division: [45d](#), [45e](#), [93a](#), [93b](#)  
 reshape\_division: [38a](#), [39c](#), [84a](#)  
 rigid\_division: [57a](#), [57e](#), [84a](#), [85b](#), [87a](#), [98c](#)  
 s\_buffer: [255a](#), [274b](#), [275a](#), [278d](#), [278e](#), [279a](#), [279b](#), [279c](#), [279d](#), [281c](#),  
[281d](#), [281e](#)  
 s\_buffer\_end: [274b](#), [275a](#), [278d](#), [278e](#), [279a](#), [279b](#), [279c](#), [279d](#), [281d](#)  
 schedule: [174d](#), [179b](#), [179c](#)  
 seed\_raw\_state: [255c](#), [255d](#), [258b](#), [262a](#)  
 seed\_state: [255d](#), [258b](#)  
 seed\_stateless: [255a](#), [255c](#), [255e](#), [258g](#), [259a](#)  
 seed\_static: [255a](#), [258b](#)  
 seed\_value: [255e](#), [256c](#), [256d](#), [256f](#), [259c](#), [259d](#)  
 select\_rotation\_axis: [126a](#), [128f](#), [141c](#)  
 select\_rotation\_subspace: [126a](#), [130b](#)  
 select\_subspace\_explicit: [129b](#), [129c](#), [130b](#), [130c](#)  
 select\_subspace\_guess: [129c](#), [130b](#), [130c](#)  
 set\_grid\_options: [80c](#), [81a](#), [81b](#), [82a](#)  
 set\_rigid\_division: [38a](#), [39b](#)

`sigma_raw`: [230a](#), [230c](#), [231c](#), [237b](#)

`single_channel`: [197a](#), [197b](#), [199c](#), [211a](#), [211b](#), [217a](#)

`single_channel_generator`: [213a](#), [213b](#), [217b](#)

`sin_theta`: [128d](#), [128e](#), [128f](#), [329b](#), [332d](#), [332e](#)

`s_last`: [255a](#), [274b](#), [275a](#), [278d](#), [278e](#), [279a](#), [279b](#), [279c](#), [279d](#), [281d](#)

`sort`: [127a](#), [130e](#), [133c](#), [141c](#), [179c](#), [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](#)

`spherical_cos_to_cartesian`: [193](#), [340c](#), [341a](#)

`spherical_cos_to_cartesian_2`: [196b](#), [340c](#), [340d](#), [341a](#), [341b](#)

`spherical_cos_to_cartesian_j`: [340c](#), [341b](#)

`spherical_to_cartesian`: [337a](#), [338a](#)

`spherical_to_cartesian_2`: [337a](#), [337b](#), [338a](#), [338b](#)

`spherical_to_cartesian_j`: [337a](#), [338b](#)

`s_state`: [255a](#), [255b](#), [258d](#), [278d](#), [278e](#), [279a](#), [279b](#), [279c](#), [279d](#)

`standard_deviation`: [133b](#), [133c](#), [291b](#), [292a](#), [292d](#)

`standard_deviation_percent`: [49b](#), [58c](#), [292c](#), [292d](#)

`std_dev`: [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [94](#), [95a](#), [96a](#), [103b](#), [106a](#),  
[107b](#), [108b](#), [110](#), [120b](#), [123b](#), [124e](#), [140b](#), [140c](#), [141c](#), [160b](#), [162](#), [165b](#), [169](#),  
[174d](#), [178e](#), [199b](#)

`stest`: [288b](#), [289c](#)

`stest_functions`: [288b](#), [289c](#)

`stratified`: [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [81b](#), [37b](#), [38b](#), [39b](#),  
[39c](#), [81b](#), [42](#), [44d](#), [45a](#), [51a](#), [81b](#), [52b](#), [54a](#), [57c](#), [58a](#), [58c](#), [59b](#), [61c](#), [62b](#),  
[64b](#), [65b](#), [66d](#), [67b](#), [68b](#), [68d](#), [69](#), [70b](#), [76b](#), [78](#), [80c](#), [81b](#), [82a](#), [83](#), [81b](#), [84a](#),  
[98b](#), [106a](#), [107b](#), [108b](#), [110](#), [117a](#), [118b](#), [118d](#), [119b](#), [124e](#), [140b](#), [140c](#),  
[141c](#), [144b](#), [145b](#), [151](#), [152b](#), [157b](#), [159](#), [160b](#), [162](#), [163](#), [165b](#), [167d](#), [168b](#),  
[168c](#), [173a](#), [173b](#), [174a](#)

`stratified_division`: [57a](#), [57c](#), [82a](#), [97b](#)

`subdivide`: [54a](#), [54c](#), [55a](#)

`subroutine`: [14](#), [15](#), [17](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#), [331d](#),  
[331d](#), [331d](#), [3](#)

84e, 85d, 86a, 86c, 91d, 93a, 93b, 94, 95a, 97a, 99d, 101b, 102c, 103b,  
 104b, 106e, 107a, 107b, 108b, 109b, 110, 114b, 115, 116b, 117a, 117b,  
 118b, 118d, 119b, 120b, 122b, 123b, 124a, 124e, 127a, 128f, 129b, 129c,  
 130e, 132d, 134d, 136, 138c, 139a, 140b, 140c, 141c, 144b, 145b, 148b,  
 148c, 148d, 149, 150a, 150b, 151, 152b, 154a, 154b, 154c, 155b, 156a,  
 156b, 157b, 158, 159, 160b, 161, 162, 163, 164a, 164b, 165a, 165b, 166a,  
 167d, 168b, 168c, 169, 171a, 171e, 172a, 173a, 173b, 174a, 174b, 174c,  
 174d, 179c, 181d, 182a, 182b, 182c, 183d, 183e, 184a, 184b, 184f, 185a,  
 185b, 185c, 186a, 186b, 187a, 187b, 188b, 188c, 189a, 189c, 190, 195d,  
 196a, 196b, 197b, 198a, 199b, 206b, 206c, 210d, 211b, 212a, 213b, 214,  
 233c, 233d, 247c, 247e, 248a, 248b, 252f, 254b, 255a, 255c, 255d, 255e,  
 258e, 258g, 261c, 261d, 261e, 262a, 262b, 262c, 262f, 263a, 263f, 263g,  
 264a, 264b, 264c, 265b, 265c, 265d, 266a, 266b, 266d, 266f, 267b, 267d,  
 268c, 268d, 268e, 268f, 269c, 270a, 270b, 270c, 270d, 270e, 271a, 271b,  
 271c, 271d, 272a, 272b, 273c, 274d, 274e, 275b, 276e, 277a, 277b, 277c,  
 277d, 277e, 278a, 278b, 278d, 278e, 279a, 279b, 279c, 279d, 280g, 280h,  
 281a, 281b, 281c, 281d, 281e, 282b, 284b, 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, 340a, 340d, 341d, 342, 345a,  
 345d, 345e, 346a, 346c, 347a, 347d, 347e, 348a, 348c, 348d, 349a, 349c,  
 350a, 350b, 350e, 351a, 351b, 351c, 352b, 353c, 354a, 354b, 354c, 354d,  
 355b, 355c, 355d, 356a, 356b, 356c, 356d, 357  
 sum\_chi2: 76b, 80c, 90b, 95a, 98a, 100c, 112a, 117a, 118b, 122b, 123b,  
 144b, 145b, 148d, 149, 151, 152b, 154c, 155b, 157b, 159, 163, 164b, 189a  
 sum\_division: 49c, 51b, 55d, 100b  
 sum\_f: 88a, 89b, 89c, 89d  
 sum\_f2: 88a, 89b, 89c, 89d  
 sum\_integral: 76b, 80c, 90b, 95a, 98a, 100c, 112a, 117a, 118b, 122b, 123b,  
 144b, 145b, 148d, 149, 151, 152b, 154c, 155b, 157b, 159, 163, 164b, 189a  
 summarize\_division: 58b, 58c, 107b  
 sum\_weights: 76b, 80c, 85c, 85e, 90b, 95a, 98a, 100c, 112a, 117a, 118b,  
 122b, 123b, 144b, 145b, 148d, 149, 151, 152b, 154c, 155b, 157b, 159, 163,  
 164b, 189a  
 sum\_x: 89d  
 sum\_xx: 89d  
 surface: 192b, 343b, 343c  
 s\_virginal: 255a, 255b, 258d, 278c  
 swap: 226a, 307e, 308a, 308d, 309b, 309c, 314, 315d  
 swap\_integer: 307e, 308a, 308b  
 swap\_real: 307e, 308a, 308c

tao\_random\_copy: 252b, 261d, 263b, 273b  
 tao\_random\_create: 16, 24a, 199c, 201c, 216, 219c, 238, 260f, 251g, 251h, 252f, 252g, 260f, 273b, 283c  
 tao\_random\_destroy: 252a, 262d, 273b  
 tao\_random\_flush: 252c, 261c, 261e, 264a, 264c, 273b  
 tao\_random\_luxury: 251d, 251e, 251f, 281f, 273b, 280g, 281f, 282d  
 tao\_random\_marshall: 269a, 269b, 284a  
 tao\_random\_marshall\_size: 269a, 269b, 284a  
 tao\_random\_number: 279e, 88b, 115, 133c, 135a, 135c, 137b, 137d, 138a, 196a, 196b, 218f, 233c, 238, 250, 251b, 252f, 252g, 273b, 279e, 280c, 282d, 283b, 283c, 283d, 283e, 284a, 321d, 331d, 331e, 333d, 334  
 tao52\_random\_numbers: 273a, 285  
 tao\_random\_numbers: 272c, 23b, 75b, 272c, 272c, 133c, 166c, 195b, 199c, 201b, 201c, 210b, 218d, 221a, 238, 272c, 273a, 282b, 284b, 285, 321d, 329d, 333d, 334  
 tao\_random\_raw\_state: 251a, 260b, 260b, 260b, 252f, 252g, 260b, 255c, 260b, 260c, 260d, 260e, 261e, 262a, 262b, 262c, 263a, 263g, 264a, 264b, 265d, 266a, 268d, 268f, 270c, 270d, 270e, 271d, 272a, 272b  
 tao\_random\_read: 252d, 264f, 273b, 283e  
 tao\_random\_seed: 199c, 201c, 216, 219c, 238, 257g, 251c, 257g, 273b, 257g, 278c, 282d, 283b, 283e, 284a, 321d  
 tao\_random\_state: 14, 15, 16, 17, 260c, 23c, 260c, 260c, 86c, 260c, 94, 103b, 115, 120b, 134d, 136, 138c, 139a, 140b, 140c, 141c, 169, 174d, 181d, 182a, 182b, 182c, 195d, 196a, 196b, 197b, 198a, 199c, 201c, 210d, 211b, 212a, 213b, 214, 218e, 233c, 238, 260c, 260c, 251a, 260c, 260c, 260c, 252f, 252g, 255d, 260c, 260e, 260c, 261c, 261d, 261e, 262b, 262f, 263f, 264a, 264b, 264c, 265b, 265c, 268c, 268e, 269c, 270a, 270b, 271a, 271b, 271c, 277b, 277c, 277d, 277e, 278a, 278b, 280h, 281a, 281b, 282b, 284b, 331d, 331e  
 tao\_random\_test: 252e, 273b, 282b, 284b, 285  
 tao\_random\_unmarshal: 269a, 269b, 284a  
 tao\_random\_write: 252d, 264d, 273b, 283e  
 tao\_test: 285  
 two\_to\_three\_massless: 326e, 326f, 327b  
 unit: 61c, 62b, 63b, 64a, 64b, 65b, 66a, 66b, 73d, 73f, 108b, 109b, 110, 128e, 129b, 144b, 145b, 148b, 148c, 148d, 149, 150a, 150b, 151, 152b, 154a, 154b, 154c, 155b, 156a, 156b, 183d, 183e, 184f, 185a, 252d, 265b, 265c, 265d, 266a, 266b, 266d, 266f, 267b, 267d, 268c, 268d, 268e, 268f, 298b, 299b, 301, 312c, 317b, 321a, 321c, 321d, 332a, 332b  
 unmarshal\_div\_history: 68a, 68d, 162  
 unmarshal\_division: 66c, 67b, 159

unmarshal\_raw\_state: 269a, 269b, 270b, 270e, 271c, 272b  
 unmarshal\_state: 269a, 269b, 270b, 271c  
 utils: 37a, 75b, 133c, 166c, 221a, 238, 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, 75b, 76a, 90b, 108b, 110,  
 133c, 76a, 76a, 166b, 76a, 76a, 76a, 191b, 195b, 199c, 201c, 204, 210a,  
 218d, 221a, 247e  
 vamp\_apply\_equivalences: 91d, 91d, 120b  
 vamp\_average\_iterations: 95b, 94, 95b, 95c, 103b, 120b, 121, 123d, 169,  
 176d, 177a, 180b  
 vamp\_average\_iterations\_grid: 95a, 95b, 95c  
 vamp\_average\_iterations\_grids: 123b, 123c, 123d  
 vamp\_broadcast\_grids: 185d, 189a  
 vamp\_broadcast\_many\_grids: 188a, 188c  
 vamp\_broadcast\_one\_grid: 188a, 188b, 188c  
 vamp\_check\_jacobian: 115, 114a, 115, 195d, 210d  
 vamp\_copy\_grid: 163, 77a, 163, 164b  
 vamp\_copy\_grids: 164b, 116c, 164b  
 vamp\_copy\_history: 165b, 106c, 165b  
 vamp\_create\_empty\_grid: 15, 17, 77d, 77d, 80a, 101b, 103b, 149, 155b,  
 164b, 167d, 169, 173a, 189a  
 vamp\_create\_grid: 77d, 24a, 77d, 77d, 77d, 78, 77d, 117a, 140c, 141c,  
 167b, 167c, 167d, 197b, 211b, 213b, 241a, 241b, 243  
 vamp\_create\_grids: 173a, 116c, 117a, 172d, 172e, 173a, 173a, 198b, 212b,  
 214, 242  
 vamp\_create\_history: 106e, 106c, 106e, 197b, 198b, 211b, 212b, 214, 238  
 vamp\_data\_t: 22, 31c, 77b, 77b, 77c, 86c, 94, 103b, 113a, 113b, 115, 120b,  
 125b, 134d, 136, 138c, 139a, 140b, 140c, 141c, 191b, 192c, 194b, 195a,  
 204, 206a, 209a, 209b  
 vamp\_delete\_grid: 15, 17, 164a, 164a, 164a, 77a, 164a, 102c, 103b, 140c,  
 141c, 149, 155b, 164a, 165a, 167b, 167c, 171a, 197b, 211b, 213b, 241a,  
 241b, 243  
 vamp\_delete\_grids: 165a, 116c, 165a, 172d, 172e, 174c, 198b, 212b, 214,  
 242  
 vamp\_delete\_history: 166a, 106c, 166a, 197b, 198b, 211b, 212b, 213b,  
 214  
 vamp\_discard\_integral: 80c, 24c, 80c, 78, 80b, 80c, 118b, 120b, 140b,  
 167b, 167c, 168b, 180b, 197b, 211b, 213b, 241a, 241b, 243  
 vamp\_discard\_integrals: 118b, 118a, 118b, 118d, 172d, 172e, 173b,  
 198b, 212b, 214, 242



[illegible]

vamp\_integratex\_region: [141a](#), [141b](#), [141c](#)  
 vampi\_tests: [201b](#), [201c](#)  
 vamp\_join\_grid: [96c](#), [15](#), [17](#), [96c](#), [96c](#), [96d](#), [101a](#), [103b](#), [169](#)  
 vamp\_join\_grid\_multi: [96c](#), [96d](#), [102c](#)  
 vamp\_join\_grid\_single: [96c](#), [96d](#), [99d](#), [102c](#)  
 vamp\_marshall\_grid: [157b](#), [29](#), [157a](#), [157b](#), [186a](#), [187a](#), [188b](#)  
 vamp\_marshall\_grid\_size: [158](#), [158](#), [29](#), [157a](#), [158](#), [186a](#), [187a](#), [188b](#)  
 vamp\_marshall\_history: [160b](#), [160a](#), [160b](#), [189c](#)  
 vamp\_marshall\_history\_size: [161](#), [160a](#), [161](#), [189c](#)  
 vamp\_multi\_channel: [113a](#), [112b](#), [113a](#), [191b](#), [195a](#)  
 vamp\_multi\_channel0: [113b](#), [112b](#), [113b](#), [204](#), [209b](#)  
 vamp\_next\_event\_multi: [134b](#), [134c](#), [136](#), [181a](#), [181c](#), [182a](#)  
 vamp\_next\_event\_single: [134b](#), [134c](#), [134d](#), [136](#), [181a](#), [181c](#), [181d](#)  
 vamp\_nullify\_covariance: [85d](#), [85a](#), [85d](#), [120b](#), [176b](#), [180b](#)  
 vamp\_nullify\_f\_limits: [84c](#), [84d](#), [84e](#), [93a](#), [93b](#)  
 vamp\_nullify\_variance: [86a](#), [85a](#), [86a](#), [120b](#), [176b](#), [180b](#)  
 vamp\_parallel\_mpi: [166c](#), [166c](#), [166c](#), [166c](#), [167a](#)  
 vamp\_print\_covariance: [130d](#), [130e](#)  
 vamp\_print\_histories: [107d](#), [108a](#), [109b](#), [171b](#), [171d](#), [172a](#)  
 vamp\_print\_history: [107d](#), [107d](#), [108a](#), [171b](#), [171c](#), [171d](#), [197b](#), [198b](#),  
[211b](#), [212b](#), [213b](#), [214](#), [241a](#), [241b](#), [242](#), [243](#)  
 vamp\_print\_one\_history: [107d](#), [108a](#), [108b](#), [109b](#), [171b](#), [171d](#), [171e](#)  
 vamp\_probability: [91b](#), [91c](#), [113a](#), [221a](#), [237b](#)  
 vamp\_read\_grid: [143c](#), [143a](#), [143c](#), [145b](#), [183a](#), [183b](#), [183c](#)  
 vamp\_read\_grid\_raw: [143b](#), [144a](#)  
 vamp\_read\_grids: [143c](#), [143a](#), [143c](#), [149](#), [184c](#), [184d](#), [184e](#)  
 vamp\_read\_grids\_raw: [143b](#), [144a](#), [155b](#)  
 vamp\_receive\_grid: [17](#), [186b](#), [30](#), [169](#), [177b](#), [178a](#), [185d](#), [186b](#), [187b](#)  
 vamp\_receive\_history: [178a](#), [189b](#), [190](#)  
 vamp\_reduce\_channels: [122b](#), [120b](#), [122a](#), [122b](#), [177a](#), [180b](#)  
 vamp\_refine\_grid: [14](#), [15](#), [17](#), [93a](#), [86b](#), [93a](#), [94](#), [103b](#), [120b](#), [169](#), [176c](#)  
 vamp\_refine\_grids: [86b](#), [93b](#)  
 vamp\_refine\_weights: [124a](#), [123a](#), [124a](#), [172d](#), [172e](#), [174b](#), [198b](#), [212b](#),  
[214](#), [242](#)  
 vamp\_reshape\_grid: [83](#), [83](#), [80c](#), [82b](#), [83](#), [119b](#), [167b](#), [167c](#), [168c](#)  
 vamp\_reshape\_grid\_internal: [82a](#), [82b](#), [83](#), [93a](#)  
 vamp\_reshape\_grids: [119b](#), [118b](#), [119a](#), [119b](#)  
 vamp\_rest: [75b](#), [76a](#)  
 vamp\_rigid\_divisions: [15](#), [17](#), [85b](#), [85a](#), [85b](#), [103b](#), [169](#)  
 vamp\_sample\_grid: [94](#), [14](#), [94](#), [94](#), [94](#), [94](#), [94](#), [24b](#), [24c](#), [94](#), [94](#), [94](#), [94](#), [86b](#),  
[94](#), [94](#), [94](#), [94](#), [138c](#), [140b](#), [167b](#), [167c](#), [169](#), [180b](#), [182b](#), [197b](#), [211b](#),

[213b](#), [241a](#), [241b](#), [243](#)  
vamp\_sample\_grid0: [14](#), [15](#), [86c](#), [17](#), [86c](#), [86b](#), [86c](#), [94](#), [103b](#), [86c](#), [121](#), [86c](#),  
[138c](#), [139a](#), [169](#), [86c](#), [176d](#), [182b](#), [182c](#), [86c](#)  
vamp\_sample\_grid\_parallel: [103b](#), [103b](#), [103a](#), [103b](#)  
vamp\_sample\_grids: [120b](#), [120a](#), [120b](#), [139a](#), [172d](#), [172e](#), [120b](#), [174d](#),  
[198b](#), [212b](#), [214](#), [242](#)  
vamp\_send\_grid: [17](#), [186a](#), [30](#), [169](#), [177b](#), [177c](#), [185d](#), [186a](#), [186a](#),  
[187a](#)  
vamp\_send\_history: [177c](#), [189b](#), [189c](#)  
vamp\_serial\_mpi: [166b](#), [166b](#), [166b](#), [166c](#), [167a](#)  
vamp\_stat: [37a](#), [75b](#), [133c](#), [291a](#)  
vamp\_sum\_channels: [125b](#), [125a](#), [125b](#)  
vamp\_terminate\_history: [107a](#), [106b](#), [106c](#), [107a](#), [121](#), [124b](#), [169](#), [176d](#),  
[177a](#), [180b](#)  
vamp\_test0: [203b](#), [211b](#), [212b](#), [216](#)  
vamp\_test0\_functions: [204](#), [210b](#), [218d](#)  
vamp\_tests: [195b](#), [199c](#), [195b](#)  
vamp\_tests0: [210a](#), [218d](#), [219b](#)  
vamp\_unmarshal\_grid: [159](#), [29](#), [157a](#), [159](#), [186b](#), [187b](#), [188b](#)  
vamp\_unmarshal\_history: [162](#), [160a](#), [162](#), [190](#)  
vamp\_update\_weights: [118d](#), [118c](#), [118d](#), [124a](#), [172d](#), [172e](#), [174a](#)  
vamp\_warmup\_grid: [138c](#), [138c](#), [138b](#), [138c](#), [181a](#), [181b](#), [182b](#), [213b](#)  
vamp\_warmup\_grids: [139a](#), [138b](#), [139a](#), [181a](#), [181b](#), [182c](#), [214](#)  
vamp\_write\_grid: [143c](#), [143a](#), [143c](#), [183a](#), [183b](#), [183c](#), [197b](#), [211b](#), [241a](#),  
[241b](#)  
vamp\_write\_grid\_raw: [143b](#), [144a](#)  
vamp\_write\_grids: [143c](#), [143a](#), [143c](#), [184c](#), [184d](#), [184e](#), [198b](#), [212b](#), [242](#)  
vamp\_write\_grids\_raw: [143b](#), [144a](#)  
vamp\_write\_histories: [107d](#)  
vamp\_write\_history: [107d](#), [108a](#)  
vamp\_write\_one\_history: [107d](#)  
var\_f: [45a](#), [89c](#), [89c](#), [89d](#)  
volume\_division: [57a](#), [57d](#), [84b](#), [98c](#)  
w: [51a](#), [97b](#), [191b](#), [195a](#), [198b](#), [204](#), [209b](#), [212b](#), [214](#), [231b](#), [231c](#)  
wgt: [43b](#), [44a](#), [44b](#), [88b](#), [88b](#), [88b](#), [88b](#), [88c](#), [89c](#), [89c](#), [134d](#), [135a](#), [136](#),  
[137c](#), [137d](#), [138a](#)  
wgt0: [132b](#), [132d](#)  
wgt1: [132b](#), [132d](#)  
wgts: [88b](#), [89c](#), [115](#), [134d](#), [135a](#)  
write\_division: [61a](#), [61b](#), [144b](#)  
write\_division\_name: [61a](#), [61b](#), [63b](#)

write\_division\_raw: 61a, 61b, 151  
 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: 143a, 143c, 148b, 183a, 183c, 184a  
 write\_grid\_raw\_name: 143b, 144a, 154a  
 write\_grid\_raw\_unit: 143b, 144a, 151, 154a, 154c  
 write\_grids\_name: 143a, 143c, 150a, 184c, 184e, 185b  
 write\_grids\_raw\_name: 143b, 144a, 156a  
 write\_grids\_raw\_unit: 143b, 144a, 154c, 156a  
 write\_grids\_unit: 143a, 143c, 148d, 150a, 184c, 184e, 184f  
 write\_grid\_unit: 143a, 143c, 144b, 148b, 148d, 183a, 183c, 183d  
 write\_histogram: 213b, 214, 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, 110  
 write\_raw\_state\_name: 264d, 264e, 268d  
 write\_raw\_state\_unit: 264d, 264e, 265b, 265d, 268d  
 write\_state\_array: 265b, 265d, 266b, 266c, 266f, 267a  
 write\_state\_name: 264d, 264e, 268c  
 write\_state\_unit: 264d, 264e, 265b, 268c  
 wx: 237a, 237b, 242  
 x: 23a, 31a, 31b, 31c, 88b, 88b, 88b, 88b, 88b, 88b, 37b, 38b, 39a, 39b, 39c, 40b, 43b, 44a, 44b, 45e, 88b, 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, 88b, 88b, 88c, 89b, 89c, 91c, 113a, 113b, 114b, 115, 116b, 125b, 132a, 132d, 134d, 135a, 136, 181d, 182a, 192a, 192b, 192c, 193, 194a, 194b, 195a, 195d, 196a, 196b, 205a, 206a, 207, 208a, 208b, 208c, 209a, 209b, 210d, 213b, 214, 224b, 224c, 225b, 227b, 227d, 228b, 229, 230b, 231a, 231c, 232, 233c, 234b, 234c, 237b, 238, 249, 251f, 255c, 255e, 256d, 256e, 257a, 257b, 257c, 257e, 257f, 259c, 259d, 259e, 259f, 259g, 260a, 260b, 260d, 263g, 265d, 266a, 267b, 270c, 270d, 270e, 271d, 272a, 272b, 277b, 277c, 277d, 277e, 278a, 278b, 287c, 289b, 289c, 291c, 292a, 292b, 292d, 292e, 296b, 297b, 300d, 300e, 310c, 330a, 330b, 331d, 331e, 332d, 333a, 337b, 338a, 338d, 340a, 340b, 340d, 341a, 341d, 342, 343a  
 x5: 227d, 229, 233c, 234b, 234c, 235c, 236a  
 x\_mid: 43b, 88b, 89c, 89d  
 x\_new: 47c, 48c

## N.2 Refinements

*⟨API documentation 250⟩*  
*⟨Accept distribution among  $n$  workers 105a⟩*  
*⟨Adjust Jacobian 225a⟩*  
*⟨Adjust grid and other state for new num\_calls 84a⟩*  
*⟨Adjust  $h\%div$  iff necessary 107c⟩*  
*⟨Allocate or resize the divisions 99c⟩*  
*⟨Alternative to basic.f90 24d⟩*  
*⟨Application in Rambo mode 243⟩*  
*⟨Application in massless single channel mode 241b⟩*  
*⟨Application in multi channel mode 242⟩*  
*⟨Application in single channel mode 241a⟩*  
*⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  319c⟩*  
*⟨Bail out if any (d == NaN) 47b⟩*  
*⟨Bail out if exception exc raised 99a⟩*  
*⟨Body of create\_\*\_array2\_pointer 305b⟩*  
*⟨Body of create\_\*\_array\_pointer 305a⟩*  
*⟨Body of mpi90\_broadcast\_\*\_array 355a⟩*  
*⟨Body of mpi90\_receive\_\*\_array 350c⟩*  
*⟨Body of mpi90\_receive\_\*\_pointer 352c⟩*  
*⟨Body of mpi90\_send\_\*\_array 348b⟩*  
*⟨Body of multi\_channel 198b⟩*  
*⟨Body of tao\_random\_\* 274a⟩*  
*⟨Body of tao\_random\_\*\_array 275c⟩*  
*⟨Boost and rescale the vectors 333a⟩*  
*⟨Bootstrap the 52-bit x buffer 259d⟩*  
*⟨Bootstrap the x buffer 256d⟩*  
*⟨Check optional arguments in vamp\_sample\_grid0 91a⟩*  
*⟨Choose a x and calculate  $f(x)$  135a⟩*  
*⟨Cleanup in vamp\_test0 219a⟩*  
*⟨Clenshaw's recurrence formula 287b⟩*  
*⟨Collect integration and grid optimization data for current cell 89d⟩*  
*⟨Collect integration and grid optimization data for x from f 89a⟩*  
*⟨Collect results of vamp\_sample\_grid0 90a⟩*  
*⟨Combine the rest of gs onto g 100c⟩*  
*⟨Constants in divisions 65a⟩*  
*⟨Constants in vamp 152a⟩*  
*⟨Constants in vamp\_equivalences 72b⟩*  
*⟨Construct  $\hat{R}(\theta; i, j)$  128e⟩*

<Copy results of `vamp_sample_grid` to dummy variables 96a>  
 <Copy results of `vamp_sample_grids` to dummy variables 178e>  
 <Copy the rest of `g` to the `gs` 97c>  
 <Copyleft notice 1>  
 <Count up cell, exit if done 87a>  
 <Declaration of 30-bit `tao_random_numbers` 266c>  
 <Declaration of 52-bit `tao_random_numbers` 267a>  
 <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 222d>  
 <Declaration of divisions procedures 38a>  
 <Declaration of divisions procedures (removed from WHIZARD) 60c>  
 <Declaration of divisions types 37b>  
 <Declaration of exceptions procedures 247b>  
 <Declaration of exceptions types 246b>  
 <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 344b>  
 <Declaration of mpi90 types 349b>  
 <Declaration of phase\_space procedures 331b>  
 <Declaration of phase\_space types 330a>  
 <Declaration of procedures in `vamp_tests0` 211a>  
 <Declaration of procedures in `vamp_tests` 195c>  
 <Declaration of procedures in `vamp_tests0` (broken?) 210c>  
 <Declaration of `specfun` procedures 286b>  
 <Declaration of `stest_functions` procedures 289a>  
 <Declaration of `tao_random_numbers` 254c>  
 <Declaration of `tao_random_numbers` (unused luxury) 281g>  
 <Declaration of `utils` procedures 304b>  
 <Declaration of `vamp` procedures 77a>  
 <Declaration of `vamp` procedures (removed from WHIZARD) 116a>  
 <Declaration of `vamp` types 77b>  
 <Declaration of `vamp_equivalences` procedures 72d>  
 <Declaration of `vamp_equivalences` types 71c>  
 <Declaration of `vamp_grid_type` types 76b>  
 <Declaration of `vampi` procedures 167b>  
 <Declaration of `vampi` types 172b>

<Declaration of `vamp_stat` procedures 291b>  
 <Decode `channel` into `ch` and `p(:)` 208b>  
 <Determine  $\phi$  for the Jacobi rotation  $P(\phi; p, q)$  with  $A'_{pq} = 0$  319a>  
 <Distribute complete grids among processes 176b>  
 <Distribute each grid among processes 180b>  
 <Estimate `waste` of processor time 180a>  
 <Execute `command` 218c>  
 <Execute `command` in `vamp_test` (never defined)>  
 <Execute tests in `vamp_test0` 217a>  
 <Exit `iterate` if accuracy has been reached 96b>  
 <Exit `iterate` if accuracy has been reached (MPI) 179a>  
 <Fill state from `x` 257e>  
 <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` 104a>  
 <Generate isotropic null vectors 332e>  
 <Get  $\cos\theta$  and  $\sin\theta$  from `evects` 128d>  
 <Get `x` in the current cell 88b>  
 <Handle `g%calls_per_cell` for `d == 0` 97b>  
 <Handle `local_error` 345c>  
 <Handle `local_error` (no `mpi90_abort`) 345b>  
 <Handle optional `pancake` and `cigar` 129a>  
 <Idioms 101a>  
 <Implementation of 30-bit `tao_random_numbers` 254b>  
 <Implementation of 52-bit `tao_random_numbers` 258e>  
 <Implementation of `coordinates` procedures 337b>  
 <Implementation of `cross_section` procedures 223a>  
 <Implementation of `divisions` procedures 38b>  
 <Implementation of `divisions` procedures (removed from WHIZARD) 45b>  
 <Implementation of `exceptions` procedures 247c>  
 <Implementation of `histograms` procedures 295f>  
 <Implementation of `kinematics` procedures 325a>  
 <Implementation of `linalg` procedures 314>  
 <Implementation of `mpi90` procedures 345a>  
 <Implementation of `phase_space` procedures 331d>  
 <Implementation of procedures in `vamp_tests0` 211b>  
 <Implementation of procedures in `vamp_tests` 196a>  
 <Implementation of procedures in `vamp_tests` (broken?) 195d>  
 <Implementation of procedures in `vamp_tests0` (broken?) 210d>  
 <Implementation of `specfun` procedures 287c>

<Implementation of `stest_functions` procedures 289b>  
 <Implementation of `tao_random_numbers` 255a>  
 <Implementation of `utils` procedures 305c>  
 <Implementation of `vamp` procedures 78>  
 <Implementation of `vamp` procedures (removed from *WHIZARD*) 116b>  
 <Implementation of `vamp_equivalences` procedures 72c>  
 <Implementation of `vampi` procedures 167d>  
 <Implementation of `vampi` procedures (doesn't work with *MPICH* yet) 187a>  
 <Implementation of `vamp_stat` procedures 291c>  
 <Implementation of `vamp_test0_functions` procedures 205a>  
 <Implementation of `vamp_test_functions` procedures 192a>  
 <Increment  $k$  until  $\sum m_k \geq \Delta$  and keep the surplus in  $\delta$  48b>  
 <Initialize a virginal random number generator 278c>  
 <Initialize clusters 132a>  
 <Initialize `num_rot` 320e>  
 <Initialize stratified sampling 42>  
 <Insure that associated (`g%map`) == `.false.` 147b>  
 <Insure that associated (`g%mu_x`) == `.false.` 148a>  
 <Insure that size (`g%div`) == `ndim` 147a>  
 <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` 279e>  
 <Interfaces of 52-bit `tao_random_numbers` 280c>  
 <Interfaces of divisions procedures 61b>  
 <Interfaces of exceptions procedures (never defined)>  
 <Interfaces of histograms procedures 295c>  
 <Interfaces of kinematics procedures 324c>  
 <Interfaces of `mpi90` procedures 347c>  
 <Interfaces of `phase_space` procedures 331c>  
 <Interfaces of `tao_random_numbers` 257g>  
 <Interfaces of `tao_random_numbers` (unused luxury) 281f>  
 <Interfaces of `utils` procedures 304c>  
 <Interfaces of `vamp` procedures 95c>  
 <Interfaces of `vampi` procedures 171d>  
 <Interpolate the new  $x_i$  from  $x_k$  and  $\delta$  48c>  
 <Join closest clusters 132b>  
 <Join importance sampling divisions 51b>  
 <Join pseudo stratified sampling divisions 54b>



<Join pure stratified sampling divisions 52c>  
 <Load a and refresh state 254d>  
 <Load 52-bit a and refresh state 258f>  
 <Local variables in vamp\_sample\_grid0 87c>  
 <MPI communication example 29>  
 <MPI communication example' 30>  
 <Maybe accept unweighted event 135c>  
 <Maybe accept unweighted multi channel event 137d>  
 <Maybe accept unweighted multi channel event (old version) 138a>  
 <Module vamp\_test0\_functions 204>  
 <Module vamp\_test\_functions 191b>  
 <Module vamp\_tests 195b>  
 <Modules used by vamp\_test0 218d>  
 <Modules used by vamp\_tests0 210b>  
 <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 253a>  
 <Parameters in tao\_random\_numbers (alternatives) 253b>  
 <Parameters in tao\_random\_test 282c>  
 <Parameters in utils 311c>  
 <Parameters in vampi 168a>  
 <Parameters local to tao\_random\_seed 256a>  
 <Parse the commandline in vamp\_test and set command (never defined)>  
 <Perform more tests of tao\_random\_numbers 283c>  
 <Perform simple tests of tao\_random\_numbers 282d>  
 <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 178a>  
 <Reload buffer or exit 276d>  
 <Reset counters in vamp\_sample\_grid0 87b>  
 <Resize arrays, iff necessary 40b>  
 <Return optional arguments in lu\_decompose 315d>  
 <Sample calls\_per\_cell points in the current cell 88a>  
 <Sample g%g0%grids(ch) 176d>  
 <Sample the grid g%grids(ch) 121>  
 <Select channel from weights 137b>  
 <Serial implementation of  $S_n = S_0(rS_0)^n$  14>

<Set default for domain 346b>  
 <Set defaults for source, tag and domain 349e>  
 <Set i, delta\_x, x, and wgt from xi 44a>  
 <Set i(1), i(2) to the axes of the optimal plane 128a>  
 <Set i(1), i(2) to the axes of the optimal plane (broken!) 128b>  
 <Set iv to the index of the optimal eigenvector 126b>  
 <Set j to minloc(key) 309a>  
 <Set m to (1,1,...) 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<sub>2</sub>, t<sub>1</sub>,  $\phi$ , cos  $\theta_3$ ,  $\phi_3$ ) from (x<sub>1</sub>, ..., x<sub>5</sub>) 224b>  
 <Set (s<sub>2</sub>, t<sub>1</sub>,  $\phi$ , cos  $\theta_3$ ,  $\phi_3$ ) from (x<sub>1</sub>, ..., x<sub>5</sub>) (massless case) 224c>  
 <Set subspace to the axes of the optimal plane 130a>  
 <Set up integrand and region in vamp\_test0 218f>  
 <Set up s and t 256f>  
 <Set up seed\_value from seed or DEFAULT\_SEED 256c>  
 <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 257d>  
 <Ship g%g0%grids from the root to the assigned processor 177b>  
 <Ship the result for channel #ch back to the root 177c>  
 <Specific procedures for 30-bit tao\_random\_number 279f>  
 <Specific procedures for 52-bit tao\_random\_number 280d>  
 <Specific procedures for tao\_random\_copy 263e>  
 <Specific procedures for tao\_random\_create 261b>  
 <Specific procedures for tao\_random\_luxury 282a>  
 <Specific procedures for tao\_random\_seed 258b>  
 <Step last and reload buffer iff necessary 274c>  
 <Test a(1) = A.2027082 283a>  
 <Trace results of vamp\_sample\_grid 106b>  
 <Trace results of vamp\_sample\_grids 124b>  
 <Trivial ktest.f90 334>  
 <Types in cross\_section 227c>  
 <Unconditionally accept weighted event 135b>  
 <Unconditionally accept weighted multi channel event 137c>  
 <(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 253c>  
 <Variables in 52-bit tao\_random\_numbers 258c>  
 <Variables in cross\_section 221b>

<Variables in divisions 46a>  
 <Variables in exceptions 246c>  
 <Variables in histograms 295e>  
 <Variables in mpi90 (never defined)>  
 <Variables in tao\_random\_numbers 268a>  
 <Variables in utils 312b>  
 <Variables in vamp 79a>  
 <Variables in vamp\_test0 218b>  
 <Variables local to 52-bit tao\_random\_seed 259b>  
 < $V' = V \cdot P(\phi; p, q)$  320d>  
 <Warm up state 257f>  
 <XXX Implementation of cross\_section procedures 222e>  
 <XXX Variables in cross\_section 222a>  
 <application.f90 221a>  
 <basic.f90 23a>  
 <52-bit  $p(z) \rightarrow p(z)^2$  (modulo  $z^K + z^L + 1$ ) 259f>  
 <52-bit  $p(z) \rightarrow zp(z)$  (modulo  $z^K + z^L + 1$ ) 260a>  
 <call copy\_division (gs%div(j), g%div(j)) 99b>  
 <call fork\_division (g%div(j), gs%div(j), g%calls\_per\_cell, ...) 98d>  
 <call join\_division (g%div(j), gs%div(j)) 100a>  
 <call sum\_division (g%div(j), gs%div(j)) 100b>  
 < $c_0/2, c_1, c_2, \dots, c_{15}$  for  $\Gamma(x)$  288a>  
 <constants.f90 244b>  
 <coordinates.f90 336>  
 <ctest.f90 133c>  
 <divisions.f90 37a>  
 <eps = 1 315a>  
 <eps = - eps 315b>  
 <exceptions.f90 246a>  
 <f = wgt \* func (x, weights, channel), iff x inside true\_domain 88c>  
 <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 225c>  
 <mpi90.f90 344a>  
 <pivots = 0 and eps = 0 315c>  
 < $p_1 \leftrightarrow p_2$  for channel #2 226a>  
 <products.f90 323>  
 < $p(z) \rightarrow p(z)^2$  (modulo  $z^K + z^L + 1$ ) 257a>

$\langle p(z) \rightarrow zp(z) \text{ (modulo } z^K + z^L + 1) \text{ 257c} \rangle$   
 $\langle \text{specfun.f90 286a} \rangle$   
 $\langle \text{stest.f90 288b} \rangle$   
 $\langle \text{tao52\_random\_numbers.f90 273a} \rangle$   
 $\langle \text{tao\_random\_numbers.f90 272c} \rangle$   
 $\langle \text{tao\_test.f90 285} \rangle$   
 $\langle \text{utils.f90 304a} \rangle$   
 $\langle \text{vamp0\_} * \Rightarrow \text{vamp\_} * \text{ 167c} \rangle$   
 $\langle \text{vamp.f90 70c} \rangle$   
 $\langle \text{vampi.f90 166b} \rangle$   
 $\langle \text{vampi\_test.f90 201a} \rangle$   
 $\langle \text{vampi\_test0.f90 219b} \rangle$   
 $\langle \text{vamp\_kinds.f90 244a} \rangle$   
 $\langle \text{vamp\_stat.f90 291a} \rangle$   
 $\langle \text{vamp\_test.f90 191a} \rangle$   
 $\langle \text{vamp\_test0.f90 203b} \rangle$   
 $\langle \text{vamp\_test.out 203a} \rangle$   
 $\langle \text{vamp\_test0.out 220} \rangle$   
 $\langle \text{weights: } \alpha_i \rightarrow w_{\max,i} \alpha_i \text{ 137a} \rangle$

# INDEX

deficiencies in Fortran90 and F, 74,  
85  
deficiencies of Fortran90 that have  
been fixed in Fortran95, 247  
dependences on external modules,  
85  
  
Fortran problem, 68  
Fortran sucks, 109  
functional programming rules, 109  
  
IEEE hacks, 45  
inconvenient F constraints, 113, 313  
  
more empirical studies helpful, 129  
  
optimizations not implemented yet,  
101  
  
Problems with MPICH, 183, 184  
  
remove from finalized program, 331  
  
system dependencies, 45, 265  
  
unfinished business, 123

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