

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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Program Summary:

- **Title of program:** VAMP, Version 1.0 (October 1999)
- **Program obtainable** by anonymous `ftp` from the host `crunch.ikp.physik.th-darmstadt.de` in the directory `pub/ohl/vamp`.
- **Licensing provisions:** Free software under the GNU General Public License.
- **Programming language used:** From version 2.2.0 of the program: Fortran2003 [8] Until version 2.1.x of the program: Fortran95 [9] (Fortran90 [7] and F [14] versions available as well)
- **Number of program lines in distributed program, including test data, etc.:** ≈ 4300 (excluding comments)
- **Computer/Operating System:** Any with a Fortran95 (or Fortran90 or F) programming environment.
- **Memory required to execute with typical data:** Negligible on the scale of typical applications calling the library.
- **Typical running time:** A small fraction (typically a few percent) of the running time of applications calling the library.
- **Purpose of program:**
- **Nature of physical problem:**
- **Method of solution:**
- **Keywords:** adaptive integration, event generation, parallel processing

—1—

INTRODUCTION

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

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


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1 <Copyleft notice 1>≡ (37a 70c 167b 192a 202a 204b 220b 222a 245 247a 273c 274a 287a 289b 292a 295a 305a 307a 309a 311a 313a 315a 317a 319a 321a 323a 325a 327a 329a 331a 333a 335a 337a 339a 341a 343a 345a 347a 349a 351a 353a 355a 357a 359a 361a 363a 365a 367a 369a 371a 373a 375a 377a 379a 381a 383a 385a 387a 389a 391a 393a 395a 397a 399a 401a 403a 405a 407a 409a 411a 413a 415a 417a 419a 421a 423a 425a 427a 429a 431a 433a 435a 437a 439a 441a 443a 445a 447a 449a 451a 453a 455a 457a 459a 461a 463a 465a 467a 469a 471a 473a 475a 477a 479a 481a 483a 485a 487a 489a 491a 493a 495a 497a 499a 501a 503a 505a 507a 509a 511a 513a 515a 517a 519a 521a 523a 525a 527a 529a 531a 533a 535a 537a 539a 541a 543a 545a 547a 549a 551a 553a 555a 557a 559a 561a 563a 565a 567a 569a 571a 573a 575a 577a 579a 581a 583a 585a 587a 589a 591a 593a 595a 597a 599a 601a 603a 605a 607a 609a 611a 613a 615a 617a 619a 621a 623a 625a 627a 629a 631a 633a 635a 637a 639a 641a 643a 645a 647a 649a 651a 653a 655a 657a 659a 661a 663a 665a 667a 669a 671a 673a 675a 677a 679a 681a 683a 685a 687a 689a 691a 693a 695a 697a 699a 701a 703a 705a 707a 709a 711a 713a 715a 717a 719a 721a 723a 725a 727a 729a 731a 733a 735a 737a 739a 741a 743a 745a 747a 749a 751a 753a 755a 757a 759a 761a 763a 765a 767a 769a 771a 773a 775a 777a 779a 781a 783a 785a 787a 789a 791a 793a 795a 797a 799a 801a 803a 805a 807a 809a 811a 813a 815a 817a 819a 821a 823a 825a 827a 829a 831a 833a 835a 837a 839a 841a 843a 845a 847a 849a 851a 853a 855a 857a 859a 861a 863a 865a 867a 869a 871a 873a 875a 877a 879a 881a 883a 885a 887a 889a 891a 893a 895a 897a 899a 901a 903a 905a 907a 909a 911a 913a 915a 917a 919a 921a 923a 925a 927a 929a 931a 933a 935a 937a 939a 941a 943a 945a 947a 949a 951a 953a 955a 957a 959a 961a 963a 965a 967a 969a 971a 973a 975a 977a 979a 981a 983a 985a 987a 989a 991a 993a 995a 997a 999a 1001a 1003a 1005a 1007a 1009a 1011a 1013a 1015a 1017a 1019a 1021a 1023a 1025a 1027a 1029a 1031a 1033a 1035a 1037a 1039a 1041a 1043a 1045a 1047a 1049a 1051a 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2713a 2715a 2717a 2719a 2721a 2723a 2725a 2727a 2729a 2731a 2733a 2735a 2737a 2739a 2741a 2743a 2745a 2747a 2749a 2751a 2753a 2755a 2757a 2759a 2761a 2763a 2765a 2767a 2769a 2771a 2773a 2775a 2777a 2779a 2781a 2783a 2785a 2787a 2789a 2791a 2793a 2795a 2797a 2799a 2801a 2803a 2805a 2807a 2809a 2811a 2813a 2815a 2817a 2819a 2821a 2823a 2825a 2827a 2829a 2831a 2833a 2835a 2837a 2839a 2841a 2843a 2845a 2847a 2849a 2851a 2853a 2855a 2857a 2859a 2861a 2863a 2865a 2867a 2869a 2871a 2873a 2875a 2877a 2879a 2881a 2883a 2885a 2887a 2889a 2891a 2893a 2895a 2897a 2899a 2901a 2903a 2905a 2907a 2909a 2911a 2913a 2915a 2917a 2919a 2921a 2923a 2925a 2927a 2929a 2931a 2933a 2935a 2937a 2939a 2941a 2943a 2945a 2947a 2949a 2951a 2953a 2955a 2957a 2959a 2961a 2963a 2965a 2967a 2969a 2971a 2973a 2975a 2977a 2979a 2981a 2983a 2985a 2987a 2989a 2991a 2993a 2995a 2997a 2999a 3001a 3003a 3005a 3007a 3009a 3011a 3013a 3015a 3017a 3019a 3021a 3023a 3025a 3027a 3029a 3031a 3033a 3035a 3037a 3039a 3041a 3043a 3045a 3047a 3049a 3051a 3053a 3055a 3057a 3059a 3061a 3063a 3065a 3067a 3069a 3071a 3073a 3075a 3077a 3079a 3081a 3083a 3085a 3087a 3089a 3091a 3093a 3095a 3097a 3099a 3101a 3103a 3105a 3107a 3109a 3111a 3113a 3115a 3117a 3119a 3121a 3123a 3125a 3127a 3129a 3131a 3133a 3135a 3137a 3139a 3141a 3143a 3145a 3147a 3149a 3151a 3153a 3155a 3157a 3159a 3161a 3163a 3165a 3167a 3169a 3171a 3173a 3175a 3177a 3179a 3181a 3183a 3185a 3187a 3189a 3191a 3193a 3195a 3197a 3199a 3201a 3203a 3205a 3207a 3209a 3211a 3213a 3215a 3217a 3219a 3221a 3223a 3225a 3227a 3229a 3231a 3233a 3235a 3237a 3239a 3241a 3243a 3245a 3247a 3249a 3251a 3253a 3255a 3257a 3259a 3261a 3263a 3265a 3267a 3269a 3271a 3273a 3275a 3277a 3279a 3281a 3283a 3285a 3287a 3289a 3291a 3293a 3295a 3297a 3299a 3301a 3303a 3305a 3307a 3309a 3311a 3313a 3315a 3317a 3319a 3321a 3323a 3325a 3327a 3329a 3331a 3333a 3335a 3337a 3339a 3341a 3343a 3345a 3347a 3349a 3351a 3353a 3355a 3357a 3359a 3361a 3363a 3365a 3367a 3369a 3371a 3373a 3375a 3377a 3379a 3381a 3383a 3385a 3387a 3389a 3391a 3393a 3395a 3397a 3399a 3401a 3403a 3405a 3407a 3409a 3411a 3413a 3415a 3417a 3419a 3421a 3423a 3425a 3427a 3429a 3431a 3433a 3435a 3437a 3439a 3441a 3443a 3445a 3447a 3449a 3451a 3453a 3455a 3457a 3459a 3461a 3463a 3465a 3467a 3469a 3471a 3473a 3475a 3477a 3479a 3481a 3483a 3485a 3487a 3489a 3491a 3493a 3495a 3497a 3499a 3501a 3503a 3505a 3507a 3509a 3511a 3513a 3515a 3517a 3519a 3521a 3523a 3525a 3527a 3529a 3531a 3533a 3535a 3537a 3539a 3541a 3543a 3545a 3547a 3549a 3551a 3553a 3555a 3557a 3559a 3561a 3563a 3565a 3567a 3569a 3571a 3573a 3575a 3577a 3579a 3581a 3583a 3585a 3587a 3589a 3591a 3593a 3595a 3597a 3599a 3601a 3603a 3605a 3607a 3609a 3611a 3613a 3615a 3617a 3619a 3621a 3623a 3625a 3627a 3629a 3631a 3633a 3635a 3637a 3639a 3641a 3643a 3645a 3647a 3649a 3651a 3653a 3655a 3657a 3659a 3661a 3663a 3665a 3667a 3669a 3671a 3673a 3675a 3677a 3679a 3681a 3683a 3685a 3687a 3689a 3691a 3693a 3695a 3697a 3699a 3701a 3703a 3705a 3707a 3709a 3711a 3713a 3715a 3717a 3719a 3721a 3723a 3725a 3727a 3729a 3731a 3733a 3735a 3737a 3739a 3741a 3743a 3745a 3747a 3749a 3751a 3753a 3755a 3757a 3759a 3761a 3763a 3765a 3767a 3769a 3771a 3773a 3775a 3777a 3779a 3781a 3783a 3785a 3787a 3789a 3791a 3793a 3795a 3797a 3799a 3801a 3803a 3805a 3807a 3809a 3811a 3813a 3815a 3817a 3819a 3821a 3823a 3825a 3827a 3829a 3831a 3833a 3835a 3837a 3839a 3841a 3843a 3845a 3847a 3849a 3851a 3853a 3855a 3857a 3859a 3861a 3863a 3865a 3867a 3869a 3871a 3873a 3875a 3877a 3879a 3881a 3883a 3885a 3887a 3889a 3891a 3893a 3895a 3897a 3899a 3901a 3903a 3905a 3907a 3909a 3911a 3913a 3915a 3917a 3919a 3921a 3923a 3925a 3927a 3929a 3931a 3933a 3935a 3937a 3939a 3941a 3943a 3945a 3947a 3949a 3951a 3953a 3955a 3957a 3959a 3961a 3963a 3965a 3967a 3969a 3971a 3973a 3975a 3977a 3979a 3981a 3983a 3985a 3987a 3989a 3991a 3993a 3995a 3997a 3999a 4001a 4003a 4005a 4007a 4009a 4011a 4013a 4015a 4017a 4019a 4021a 4023a 4025a 4027a 4029a 4031a 4033a 4035a 4037a 4039a 4041a 4043a 4045a 4047a 4049a 4051a 4053a 4055a 4057a 4059a 4061a 4063a 4065a 4067a 4069a 4071a 4073a 4075a 4077a 4079a 4081a 4083a 4085a 4087a 4089a 4091a 4093a 4095a 4097a 4099a 4101a 4103a 4105a 4107a 4109a 4111a 4113a 4115a 4117a 4119a 4121a 4123a 4125a 4127a 4129a 4131a 4133a 4135a 4137a 4139a 4141a 4143a 4145a 4147a 4149a 4151a 4153a 4155a 4157a 4159a 4161a 4163a 4165a 4167a 4169a 4171a 4173a 4175a 4177a 4179a 4181a 4183a 4185a 4187a 4189a 4191a 4193a 4195a 4197a 4199a 4201a 4203a 4205a 4207a 4209a 4211a 4213a 4215a 4217a 4219a 4221a 4223a 4225a 4227a 4229a 4231a 4233a 4235a 4237a 4239a 4241a 4243a 4245a 4247a 4249a 4251a 4253a 4255a 4257a 4259a 4261a 4263a 4265a 4267a 4269a 4271a 4273a 4275a 4277a 4279a 4281a 4283a 4285a 4287a 4289a 4291a 4293a 4295a 4297a 4299a 4301a 4303a 4305a 4307a 4309a 4311a 4313a 4315a 4317a 4319a 4321a 4323a 4325a 4327a 4329a 4331a 4333a 4335a 4337a 4339a 4341a 4343a 4345a 4347a 4349a 4351a 4353a 4355a 4357a 435
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[illegible][illegible]

—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 ϕ 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 ϕ^{-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 π 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 μ_n may be used in the estimation of μ'_n , but a particular S_0 is free to ignore them as well. Using a little notational freedom, we augment \mathbf{R} and A with a special value \cdot , which will always be discarded by S_0 .

In an adaptive integration algorithm, there is also a refinement operation $r : \Gamma \times A \rightarrow \Gamma$ 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 σ .

For parallelization, it is crucial to find a division of S_n or any part of it into *independent* pieces that can be evaluated in parallel. In order to be effective, r has to be applied to *all* of a and therefore a 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 ϕ is a forking operation and ι is a joining operation, we are faced with the technical problem of a parallel random number source ρ . As made explicit in (2.18), S_0 changes the state of the random number general ρ , demanding *identical* results therefore imposes a strict ordering on the operations and defeats parallelization. It is possible to devise implementations of S_0 and ρ that circumvent this problem by distributing subsequences of ρ in such a way among processes that results do not depend on the number of parallel processes.

However, a reordering of the random number sequence will only change the result by the statistical error, as long as the scale of the allowed reorderings is *bounded* and much smaller than the period of the random number generator¹ Below, we will therefore use the notation $x \approx y$ for “equal for an appropriate finite reordering of the ρ used in calculating x and y ”. For our 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 ρ_i are statistically independent. This leaves us with G and a and we have to discuss importance sampling and stratified sampling separately.

¹Arbitrary 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,² such that the adaptive grid is strictly finer than the stratification grid. This procedure is shown in figure 2.3.

2.6.2 State and Message Passing

2.6.3 Random Numbers

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

²The 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  $S_n = S_0(rS_0)^n$  14 $\rangle \equiv$ 
  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 <Parallel implementation of  $S_n = S_0(rS_0)^n$  (HPF) 15>≡
  subroutine vamp_sample_grid_hpf (rng, g, iterations, func)
    type(tao_random_state), dimension(:), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: iterations
    <Interface declaration for func 22>
    type(vamp_grid), dimension(:), allocatable :: gs, gx
    !hpf$ processors p(number_of_processors())
    !hpf$ distribute gs(cyclic(1)) onto p
    integer, dimension(:,:), pointer :: d
    integer :: iteration, num_workers
    iterate: do iteration = 1, iterations
      call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
      num_workers = max (1, product (d(2,:)))
      if (num_workers > 1) then
        allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
        call vamp_create_empty_grid (gs)
        call vamp_fork_grid (g, gs, gx, d)
        !hpf$ independent
        do i = 1, num_workers
          call vamp_sample_grid0 (rng(i), gs(i), func)
        end do
        call vamp_join_grid (g, gs, gx, d)
        call vamp_delete_grid (gs)
        deallocate (gs, gx)
      end if
    end do
  end subroutine
```



```

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

```

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

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

```

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

```

MPI

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

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

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

```

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

```

```

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

```

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

—3—

DESIGN TRADE OFFS

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

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

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

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

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

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

3.1 *Programming Language*

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

Let us consider the alternatives

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

—4— USAGE

4.1 Basic Usage

`type(vamp_grid)`

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

Create a fresh grid for the integration domain

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

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

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

`subroutine vamp_delete_grid (g [, exc])`

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

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

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

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

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

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

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

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

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

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

```
22 <Interface declaration for func 22>≡ (14 15 17 86c 94d 104 113–15 120b 135d 137 139–42 170 176 182 183)
interface
  function func (xi, data, weights, channel, grids) result (f)
    use kinds
    use vamp_grid_type !NODEP!
    import vamp_data_t
    real(kind=default), dimension(:), intent(in) :: xi
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: f
  end function func
end interface
```

4.1.1 Basic Example

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

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

```

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

```

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

```

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

```

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

```

23c <basic.f90 23a>+≡
  type(exception) :: exc
  type(tao_random_state) :: rng
  type(vamp_grid) :: grid
  real(kind=default), dimension(2,7) :: domain
  real(kind=default) :: integral, error, chi2
  domain(1,:) = -1.0
  domain(2,:) = 1.0
23b 24a>

```


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

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

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

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

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

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

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

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

4.2 Advanced Usage



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

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

4.2.1 Types

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

4.2.2 Shared Arguments

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

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

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

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

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

The average χ^2 of the iterations.

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

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

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

Collect covariance data.

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

Exceptional conditions are reported in `exc`.

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

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

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

Diagnostic information for multi channel sampling.

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

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

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

The current best estimate of the integral.

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

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

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

The number of sampling points.

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

Number of divisions of the adaptive grid in each dimension.

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

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

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

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

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

The current best estimate of the error on the integral.

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

Try to use stratified sampling.

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

```
...
```

4.2.3 Single Channel Procedures

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

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

subroutine vamp_create_empty_grid (g)

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

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

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

    func

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

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 \langle Interface declaration for phi 31a $\rangle \equiv$ (113–16 137 183a)

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

31b \langle Interface declaration for ihp 31b $\rangle \equiv$ (113c)

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

31c \langle Interface declaration for jacobian 31c $\rangle \equiv$ (113c 114a)

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

```
function vamp_multi_channel (func, phi, ihp, jacobian, x,
  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>≡ (37a) 58a▷
  type, public :: division_t
  ! private
  !!! Avoiding a g95 bug
```

```

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

```

5.1.1 Creation, Manipulation & Injection

38a *<Declaration of divisions procedures 38a>*≡ (37a) 43a>

```

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

```

38b *<Implementation of divisions procedures 38b>*≡ (37a) 39a>

```

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

```

```

else
  d%x_max_true = x_max
end if
end subroutine create_division

```

39a \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 38b 39b \triangleright

```

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 \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 39a 39c \triangleright

```

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

39c \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 39b 43b \triangleright

```

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

```



```

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

```

40a *<Set m to (1,1,...) or to rebinning weights from d%variance 40a>*≡ (39c)

```

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

```

40b *<Resize arrays, iff necessary 40b>*≡ (39c)

```

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

```

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

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



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



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

n_{dim}	$N_{\text{calls}}^{\text{max}}(n_g = 25)$
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_{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_{div}

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

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

```

if (d%ng >= max_num_div / 2) then
  d%stratified = .true.
  equ_per_adap = d%ng / max_num_div + 1
  num_div = d%ng / equ_per_adap
  if (num_div < 2) then
    d%stratified = .false.
    num_div = 2
    d%ng = 1
  else if (mod (num_div,2) == 1) then
    num_div = num_div - 1
    d%ng = equ_per_adap * num_div
  else
```



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

```

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

```

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

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

```

43a  <Declaration of divisions procedures 38a>+≡ (37a) <38a 44c>
      public :: inject_division, inject_division_short

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

```

```

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

```

44a <Set i, delta_x, x, and wgt from xi 44a>≡ (43b 44b)

```

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

```

44b <Implementation of divisions procedures 38b>+≡ (37a) <43b 44d>

```

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

```

5.1.2 Grid Refinement

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

```

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

```

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

```

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

```

45a \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 44d 45c \triangleright

```

    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 \langle Implementation of divisions procedures (removed from WHIZARD) 45b $\rangle \equiv$ 60d \triangleright

```

    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 \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 45a 45e \triangleright

```

    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 \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \triangleleft 44c 47a \triangleright

```

    public :: refine_division

```

45e \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \triangleleft 45c 46b \triangleright

```

    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` ≥ 6 , we know that `num_div` ≥ 3 .

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

Here the Fortran90 array notation really shines, but we have to handle the cases `nd` ≤ 2 specially, because the `quadrupole` option can lead to small `nds`. The equivalent Fortran77 code [2] is orders of magnitude less obvious¹ Also protect against vanishing d_i that will blow up the logarithm.

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

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

¹Some old timers call this a feature, however.

```

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

```

47a \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 45d 48a \rangle
 private :: rebinning_weights



The NaN test is probably not portable:

47b \langle Bail out if any (d == NaN) 47b $\rangle \equiv$ (46b)
 if (any (d /= d)) then
 m = 1.0
 return
 end if

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

47c \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 46b 48e \rangle
 pure function rebin (m, x, num_div) result (x_new)
 real(kind=default), dimension(:), intent(in) :: m
 real(kind=default), dimension(0:), intent(in) :: x
 integer, intent(in) :: num_div
 real(kind=default), dimension(0:num_div) :: x_new
 integer :: i, k
 real(kind=default) :: step, delta
 step = sum (m) / num_div
 k = 0
 delta = 0.0
 x_new(0) = x(0)
 do i = 1, num_div - 1
 \langle Increment k until $\sum m_k \geq \Delta$ and keep the surplus in δ 48b \rangle
 \langle Interpolate the new x_i from x_k and δ 48c \rangle
 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 $\rangle + \equiv$ (37a) \langle 47a 48d \rangle
`private :: rebin`

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

48b \langle Increment k until $\sum m_k \geq \Delta$ and keep the surplus in δ 48b $\rangle \equiv$ (47c)
`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 δ 48c $\rangle \equiv$ (47c)
`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 $\rangle + \equiv$ (37a) \langle 48a 49a \rangle
`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 $\rangle + \equiv$ (37a) \langle 47c 49b \rangle
`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 \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 48d 49c \rangle
 public :: quadrupole_division
- 49b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 48e 50a \rangle
 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 \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 49a 54c \rangle
 public :: fork_division, join_division, sum_division



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

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

```

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

```

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

```

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

```

```

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

```

Importance Sampling

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

51a *Join importance sampling divisions 51a* \equiv (50a)

```

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

```

and sum up the results in the end:

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

```

call sum_division (d, ds)

```

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

Stratified Sampling

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

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

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

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

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

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

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

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

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



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

Pseudo Stratified Sampling

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

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

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

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

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

```

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

```

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

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

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

```

```

private :: collect

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

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

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

```

Trivia

```

55d  <Implementation of divisions procedures 38b>+≡ (37a) <55c 56b>
pure subroutine sum_division (d, ds)
  type(division_t), intent(inout) :: d
  type(division_t), dimension(:), intent(in) :: ds
  integer :: i

```



```

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

```

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

```

public :: debug_division
public :: dump_division

```

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

```

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

```

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

```

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

```

end subroutine dump_division

5.1.6 Inquiry

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

- 57a \langle Declaration of divisions procedures 38a $\rangle + \equiv$ (37a) \langle 56a 58b \rangle
public :: inside_division, stratified_division
public :: volume_division, rigid_division, adaptive_division
- 57b \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 56c 57c \rangle
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 \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57b 57d \rangle
elemental function stratified_division (d) result (yorn)
type(division_t), intent(in) :: d
logical :: yorn
yorn = d%stratified
end function stratified_division
- 57d \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57c 57e \rangle
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 \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57d 57f \rangle
elemental function rigid_division (d) result (n)
type(division_t), intent(in) :: d
integer :: n
n = d%ng
end function rigid_division
- 57f \langle Implementation of divisions procedures 38b $\rangle + \equiv$ (37a) \langle 57e 58c \rangle
elemental function adaptive_division (d) result (n)
type(division_t), intent(in) :: d
integer :: n
n = ubound (d%x, dim=1)
end function adaptive_division

5.1.7 Diagnostics

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

```

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

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

```

public :: copy_history, summarize_division

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

```

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

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

```

private :: probabilities

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

```

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

```

```

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

```

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

```

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

```

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

```

subroutine write_history (u, h, tag)
  integer, intent(in) :: u
  type(div_history), dimension(:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  character(len=BUFFER_SIZE) :: pfx
  character(len=1) :: s
  integer :: i
  if (present (tag)) then
    pfx = tag
  else
    pfx = "[vamp]"
  end if
  if ((minval (h%x_min) == maxval (h%x_min)) &
    .and. (minval (h%x_max) == maxval (h%x_max))) then
    write (u, "(1X,A11,1X,2X,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
      h(1)%x_min, " <= ", h(1)%x_min_true, &
      " < x < ", h(1)%x_max_true, " <= ", h(1)%x_max
  else
    do i = 1, size (h)
      write (u, "(1X,A11,1X,I2,1X,2(ES10.3,A4,ES10.3,A7))") pfx, &
        i, h(i)%x_min, " <= ", h(i)%x_min_true, &
        " < x < ", h(i)%x_max_true, " <= ", h(i)%x_max
    end do
  end if
  write (u, "(1X,A11,1X,A2,2(1X,A3),A1,6(1X,A8))") pfx, &
    "it", "nd", "ng", "", &
    "spr(f/p)", "dev(f/p)", "spr(m)", "dev(m)", "spr(p)", "dev(p)"
  iterations: do i = 1, size (h)
    if (h(i)%stratified) then
      s = "*"
    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>+≡ (37a) <46a 62a>*
integer, private, parameter :: BUFFER_SIZE = 50

60b *<Declaration of divisions procedures 38a>+≡ (37a) <58d 61a>*
public :: print_history, write_history

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

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

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

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

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

```

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

```

5.1.8 I/O

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

```

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

```

61b *<Interfaces of divisions procedures 61b>≡* (37a)

```

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

```

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

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

```

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

```

```

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

```

62a *<Variables in divisions 46a>+≡* (37a) *<60a*

```

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

```

62b *<Implementation of divisions procedures 38b>+≡* (37a) *<61c 63b>*

```

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

```

```

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

```



What happened to d%efficiency?

- 63a *<Insure that ubound (d%x, dim=1) == num_div 63a>≡* (62b 65b 67b)
- ```

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

```
- 63b *<Implementation of divisions procedures 38b>+≡* (37a) <62b 64a>
- ```

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

```



```

        call write_division_unit (d, unit, write_integrals)
        close (unit = unit)
    end subroutine write_division_name
64a  <Implementation of divisions procedures 38b>+≡ (37a) <63b 64b>
    subroutine read_division_name (d, name, read_integrals)
        type(division_t), intent(inout) :: d
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: read_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", file = name)
        call read_division_unit (d, unit, read_integrals)
        close (unit = unit)
    end subroutine read_division_name
64b  <Implementation of divisions procedures 38b>+≡ (37a) <64a 65b>
    subroutine write_division_raw_unit (d, unit, write_integrals)
        type(division_t), intent(in) :: d
        integer, intent(in) :: unit
        logical, intent(in), optional :: write_integrals
        logical :: write_integrals0
        integer :: i
        write_integrals0 = .false.
        if (present(write_integrals)) write_integrals0 = write_integrals
        write (unit = unit) MAGIC_DIVISION_BEGIN
        write (unit = unit) ubound (d%x, dim=1)
        write (unit = unit) d%ng
        write (unit = unit) d%stratified
        write (unit = unit) d%dx
        write (unit = unit) d%dxg
        write (unit = unit) d%x_min
        write (unit = unit) d%x_max
        write (unit = unit) d%x_min_true
        write (unit = unit) d%x_max_true
        do i = 0, ubound (d%x, dim=1)
            if (write_integrals0 .and. i/=0) then
                write (unit = unit) d%x(i), d%integral(i), d%variance(i)
            else
                write (unit = unit) d%x(i)
            end if
        end do
        write (unit = unit) MAGIC_DIVISION_END
    end subroutine write_division_raw_unit

```

```

65a  <Constants in divisions 65a>≡ (37a)
      integer, parameter, private :: MAGIC_DIVISION = 11111111
      integer, parameter, private :: MAGIC_DIVISION_BEGIN = MAGIC_DIVISION + 1
      integer, parameter, private :: MAGIC_DIVISION_END = MAGIC_DIVISION + 2

65b  <Implementation of divisions procedures 38b>+≡ (37a) <64b 66a>
      subroutine read_division_raw_unit (d, unit, read_integrals)
        type(division_t), intent(inout) :: d
        integer, intent(in) :: unit
        logical, intent(in), optional :: read_integrals
        logical :: read_integrals0
        integer :: i, num_div, magic
        character(len=*), parameter :: FN = "read_division_raw_unit"
        read_integrals0 = .false.
        if (present(read_integrals)) read_integrals0 = read_integrals
        read (unit = unit) magic
        if (magic /= MAGIC_DIVISION_BEGIN) then
          print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_BEGIN, &
            ", found ", magic
          stop
        end if
        read (unit = unit) num_div
        <Insure that ubound (d%x, dim=1) == num_div 63a>
        read (unit = unit) d%ng
        read (unit = unit) d%stratified
        read (unit = unit) d%dx
        read (unit = unit) d%dxg
        read (unit = unit) d%x_min
        read (unit = unit) d%x_max
        read (unit = unit) d%x_min_true
        read (unit = unit) d%x_max_true
        do i = 0, ubound (d%x, dim=1)
          if (read_integrals0 .and. i/=0) then
            read (unit = unit) d%x(i), d%integral(i), d%variance(i)
          else
            read (unit = unit) d%x(i)
          end if
        end do
        if (.not.read_integrals0) then
          d%integral = 0.0
          d%variance = 0.0
        !   d%efficiency = 0.0
        end if
        read (unit = unit) magic

```

```

        if (magic /= MAGIC_DIVISION_END) then
            print *, FN, " fatal: expecting magic ", MAGIC_DIVISION_END, &
                ", found ", magic
            stop
        end if
    end subroutine read_division_raw_unit
66a  <Implementation of divisions procedures 38b>+≡ (37a) <65b 66b>
    subroutine write_division_raw_name (d, name, write_integrals)
        type(division_t), intent(in) :: d
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: write_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", &
            form = "unformatted", file = name)
        call write_division_unit (d, unit, write_integrals)
        close (unit = unit)
    end subroutine write_division_raw_name
66b  <Implementation of divisions procedures 38b>+≡ (37a) <66a 66d>
    subroutine read_division_raw_name (d, name, read_integrals)
        type(division_t), intent(inout) :: d
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: read_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", &
            form = "unformatted", file = name)
        call read_division_unit (d, unit, read_integrals)
        close (unit = unit)
    end subroutine read_division_raw_name

```

5.1.9 Marshaling

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

```

66c  <Declaration of divisions procedures 38a>+≡ (37a) <61a 68a>
    public :: marshal_division_size, marshal_division, unmarshal_division
66d  <Implementation of divisions procedures 38b>+≡ (37a) <66b 67a>
    pure subroutine marshal_division (d, ibuf, dbuf)
        type(division_t), intent(in) :: d

```

```

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

```

67a *<Implementation of divisions procedures 38b>+≡* (37a) <66d 67b>

```

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

```

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

```

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

```

```

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

68a <Declaration of divisions procedures 38a>+≡ (37a) <66c
    public :: marshal_div_history_size, marshal_div_history, unmarshal_div_history

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

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

68d <Implementation of divisions procedures 38b>+≡ (37a) <68c 69>
    pure subroutine unmarshal_div_history (h, ibuf, dbuf)

```

```

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

```

5.1.10 Boring Copying and Deleting of Objects

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

```

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

```

```

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

```

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

```

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

```

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

```

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

```

5.2 The Abstract Datatype *vamp_grid*

70c \langle vamp.f90 70c $\rangle \equiv$ 71a \triangleright

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

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

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

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

⚡ By WK for WHIZARD.

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

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


72a \langle Declaration of `vamp_equivalences` types 71c $\rangle + \equiv$ (71b) \triangleleft 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 \langle Constants in `vamp_equivalences` 72b $\rangle \equiv$ (71b)

```

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

```

72c \langle Implementation of `vamp_equivalences` procedures 72c $\rangle \equiv$ (71b) 72e \triangleright

```

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 \langle Declaration of `vamp_equivalences` procedures 72d $\rangle \equiv$ (71b) 73b \triangleright

```

public :: vamp_equivalences_init

```

72e \langle Implementation of `vamp_equivalences` procedures 72c $\rangle + \equiv$ (71b) \triangleleft 72c 73a \triangleright

```

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

```

```

end subroutine vamp_equivalences_init

73a <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <72e 73c>
subroutine vamp_equivalence_final (eq)
  type(vamp_equivalence_t), intent(inout) :: eq
  deallocate (eq%permutation, eq%mode)
end subroutine vamp_equivalence_final

73b <Declaration of vamp_equivalences procedures 72d>+≡ (71b) <72d 73e>
public :: vamp_equivalences_final

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

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

73e <Declaration of vamp_equivalences procedures 72d>+≡ (71b) <73b 74a>
public :: vamp_equivalences_write

73f <Implementation of vamp_equivalences procedures 72c>+≡ (71b) <73d 74b>
subroutine vamp_equivalences_write (eq, unit)
  type(vamp_equivalences_t), intent(in) :: eq
  integer, intent(in), optional :: unit

```

```

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

```

74a \langle Declaration of vamp_equivalences procedures 72d $\rangle + \equiv$ (71b) \langle 73e 74c \rangle
public :: vamp_equivalence_set

74b \langle Implementation of vamp_equivalences procedures 72c $\rangle + \equiv$ (71b) \langle 73f 75a \rangle
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 \langle Declaration of vamp_equivalences procedures 72d $\rangle + \equiv$ (71b) \langle 74a \rangle
public :: vamp_equivalences_complete

75a *<Implementation of vamp_equivalences procedures 72c>+≡*

(71b) <74b

```

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

```

75b *<vamp.f90 70c>+≡*

<71b 76a>

```

module vamp_rest
  use kinds
  use utils

```

```

    use exceptions
    use divisions
    use tao_random_numbers
    use vamp_stat
    use linalg
    use iso_fortran_env
    use vamp_grid_type !NODEP!
    use vamp_equivalences !NODEP!
    implicit none
    private
    <Declaration of vamp procedures 77a>
    <Interfaces of vamp procedures 96b>
    <Constants in vamp 153a>
    <Declaration of vamp types 77b>
    <Variables in vamp 79a>
    character(len=*), public, parameter :: VAMP_RCS_ID = &
        "$Id: vamp.nw 317 2010-04-18 00:31:03Z ohl $"
contains
    <Implementation of vamp procedures 78b>
end module vamp_rest
76a <vamp.f90 70c>+≡ <75b
    module vamp
        use vamp_grid_type !NODEP!
        use vamp_rest !NODEP!
        use vamp_equivalences !NODEP!
        public
    end module vamp

```

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

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

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

76b <Declaration of vamp_grid_type types 76b>≡ (71a)

```

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

```

77a \langle Declaration of vamp procedures 77a $\rangle \equiv$ (75b) 78a \triangleright
 public :: vamp_copy_grid, vamp_delete_grid

5.2.1 Container for application data



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

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

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

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

77c \langle Declaration of vamp types 77b $\rangle + \equiv$ (75b) \langle 77b 106c \rangle
 type(vamp_data_t), parameter, public :: NO_DATA = vamp_data_t ()

5.2.2 Initialization

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

Create a fresh grid for the integration domain

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

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

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

```

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

```

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

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

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

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

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

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

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

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

79c \langle Implementation of `vamp` procedures 78b $\rangle + \equiv$ (75b) \langle 78b 80a \rangle
 pure subroutine `map_domain` (map, true_xmin, true_xmax, xmin, xmax)
 real(kind=default), dimension(:, :), intent(in) :: map
 real(kind=default), dimension(:), intent(in) :: true_xmin, true_xmax
 real(kind=default), dimension(:), intent(out) :: xmin, xmax
 real(kind=default), dimension(2**size(xmin), size(xmin)) :: corners
 integer, dimension(size(xmin)) :: zero_to_n
 integer :: j, ndim, perm
 ndim = size (xmin)
 zero_to_n = (/ (j, j=0, ndim-1) /)
 do perm = 1, 2**ndim
 corners (perm, :) = &


```

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

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

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

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

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

```

```

    if ((present (num_calls)) &
        .or. (present (num_div)) &
        .or. (present (stratified)) &
        .or. (present (quadrupole)) &
        .or. (present (covariance))) then
        call vamp_reshape_grid &
            (g, g%num_calls, g%num_div, &
             g%stratified, g%quadrupole, covariance, exc)
    end if
end subroutine vamp_discard_integral
81a  <Declaration of vamp procedures 77a>+≡ (75b) <80b 83a>
    private :: set_grid_options
81b  <Implementation of vamp procedures 78b>+≡ (75b) <80c 82>
    pure subroutine set_grid_options &
        (g, num_calls, num_div, stratified, quadrupole, &
         independent, equivalent_to_ch, multiplicity)
    type(vamp_grid), intent(inout) :: g
    integer, intent(in), optional :: num_calls
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole
    logical, intent(in), optional :: independent
    integer, intent(in), optional :: equivalent_to_ch, multiplicity
    if (present (num_calls)) then
        g%num_calls = num_calls
    end if
    if (present (num_div)) then
        g%num_div = num_div
    end if
    if (present (stratified)) then
        g%stratified = stratified
    end if
    if (present (quadrupole)) then
        g%quadrupole = quadrupole
    end if
    if (present (independent)) then
        g%independent = independent
    end if
    if (present (equivalent_to_ch)) then
        g%equivalent_to_ch = equivalent_to_ch
    end if
    if (present (multiplicity)) then
        g%multiplicity = multiplicity
    end if

```

```
end subroutine set_grid_options
```

Setting Up the Initial Grid

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

```
82 <Implementation of vamp procedures 78b>+≡ (75b) <81b 83b>
  pure subroutine vamp_reshape_grid_internal &
    (g, num_calls, num_div, &
     stratified, quadrupole, covariance, exc, use_variance, &
     independent, equivalent_to_ch, multiplicity)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in), optional :: num_calls
  integer, dimension(:), intent(in), optional :: num_div
  logical, intent(in), optional :: stratified, quadrupole, covariance
  type(exception), intent(inout), optional :: exc
  logical, intent(in), optional :: use_variance
  logical, intent(in), optional :: independent
  integer, intent(in), optional :: equivalent_to_ch, multiplicity
  integer :: ndim, num_cells
  integer, dimension(size(g%div)) :: ng
  character(len=*), parameter :: FN = "vamp_reshape_grid_internal"
  ndim = size (g%div)
  call set_grid_options &
    (g, num_calls, num_div, stratified, quadrupole, &
     & independent, equivalent_to_ch, multiplicity)
  <Adjust grid and other state for new num_calls 84a>
  g%all_stratified = all (stratified_division (g%div))
  if (present (covariance)) then
    ndim = size (g%div)
    if (covariance .and. (.not. associated (g%mu_x))) then
      allocate (g%mu_x(ndim), g%mu_xx(ndim,ndim))
      allocate (g%sum_mu_x(ndim), g%sum_mu_xx(ndim,ndim))
      g%sum_mu_x = 0.0
      g%sum_mu_xx = 0.0
    else if ((.not. covariance) .and. (associated (g%mu_x))) then
      deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
    end if
  end if
end subroutine vamp_reshape_grid_internal
```

The `use_variance` argument is too dangerous for careless users, because the variance in the divisions will contain garbage before sampling and after

reshaping. Build a fence with another routine.

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

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

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

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

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

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

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

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

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

NB:

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

84a \langle Adjust grid and other state for new num_calls 84a $\rangle \equiv$ (82) 84b \triangleright

```

  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 = Volume / N_calls

```

(5.15)

and

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

84b \langle Adjust grid and other state for new num_calls 84a $\rangle + \equiv$ (82) \triangleleft 84a 84c \triangleright

```

  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 \langle Adjust grid and other state for new num_calls 84a $\rangle + \equiv$ (82) \triangleleft 84b

```

  call vamp_nullify_f_limits (g)

```

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

84d \langle Declaration of vamp procedures 77a $\rangle + \equiv$ (75b) \triangleleft 83a 85a \triangleright

```

  public :: vamp_nullify_f_limits

```

84e \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \triangleleft 83b 85b \triangleright

```

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

```

85a *<Declaration of vamp procedures 77a>+≡* (75b) <84d 86b>
public :: vamp_rigid_divisions
public :: vamp_get_covariance, vamp_nullify_covariance
public :: vamp_get_variance, vamp_nullify_variance

85b *<Implementation of vamp procedures 78b>+≡* (75b) <84e 85c>
pure function vamp_rigid_divisions (g) result (ng)
type(vamp_grid), intent(in) :: g
integer, dimension(size(g%div)) :: ng
ng = rigid_division (g%div)
end function vamp_rigid_divisions

85c *<Implementation of vamp procedures 78b>+≡* (75b) <85b 85d>
pure function vamp_get_covariance (g) result (cov)
type(vamp_grid), intent(in) :: g
real(kind=default), dimension(size(g%div),size(g%div)) :: cov
if (associated (g%mu_x)) then
if (abs (g%sum_weights) <= tiny (cov(1,1))) then
where (g%sum_mu_xx == 0.0_default)
cov = 0.0
elsewhere
cov = huge (cov(1,1))
endwhere
else
cov = g%sum_mu_xx / g%sum_weights &
- outer_product (g%sum_mu_x, g%sum_mu_x) / g%sum_weights**2
end if
else
cov = 0.0
end if
end function vamp_get_covariance

85d *<Implementation of vamp procedures 78b>+≡* (75b) <85c 85e>
elemental subroutine vamp_nullify_covariance (g)
type(vamp_grid), intent(inout) :: g
if (associated (g%mu_x)) then
g%sum_mu_x = 0
g%sum_mu_xx = 0
end if
end subroutine vamp_nullify_covariance

85e *<Implementation of vamp procedures 78b>+≡* (75b) <85d 86a>
elemental function vamp_get_variance (g) result (v)
type(vamp_grid), intent(in) :: g
real(kind=default) :: v
if (abs (g%sum_weights) <= tiny (v)) then

```

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

```

86a \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 85e 86c \rangle

```

    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 \langle Declaration of vamp procedures 77a $\rangle + \equiv$ (75b) \langle 85a 92b \rangle

```

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

```

Simple Non-Adaptive Sampling: S_0

86c \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 86a 92c \rangle

```

    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
         $\langle$ Interface declaration for func 22 $\rangle$ 
        character(len=*), parameter :: FN = "vamp_sample_grid0"
        logical, intent(in), optional :: negative_weights
         $\langle$ Local variables in vamp_sample_grid0 87c $\rangle$ 
        integer :: ndim
        logical :: neg_w

```

```

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

```

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

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

```

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

```

87b <Reset counters in vamp_sample_grid0 87b>≡ (86c)

```

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

```

87c <Local variables in vamp_sample_grid0 87c>≡ (86c) 88a>

```

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

```



```

88a  <Local variables in vamp_sample_grid0 87c>+≡ (86c) <87c 89c>
      integer :: j, k
      integer, dimension(size(g%div)) :: cell

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

```

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

```

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

```

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

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

```

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

```

```

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

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

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

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

```

```

real(kind=default), dimension(size(g%div)):: x, x_mid, wgts
real(kind=default), dimension(size(g%div)):: r
integer, dimension(size(g%div)) :: ia

```

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

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

```

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

```

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

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

90b *⟨Collect results of vamp_sample_grid0 90b⟩*≡ (86c) 91▷

```

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

```

```

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

```

91 *<Collect results of vamp_sample_grid0 90b>+≡* (86c) <90b

```


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

```

```

end if
if (present (channel)) then
    g%sum_mu_gi = g%sum_mu_gi + g%mu_gi / g%mu(2)
end if
else
if (present(channel) .and. g%mu(1)==0) then
    write (buffer, "(I6)") channel
    call raise_exception (exc, EXC_WARN, "! vamp", &
        "Function identically zero in channel " // buffer)
else if (present(channel) .and. g%mu(1)<0) then
    write (buffer, "(I6)") channel
    call raise_exception (exc, EXC_ERROR, "! vamp", &
        "Negative integral in channel " // buffer)
end if
g%sum_integral = 0
g%sum_chi2 = 0
g%sum_weights = 0
end if
92a <Check optional arguments in vamp_sample_grid0 92a>≡ (86c)
    if (present (channel) .neqv. present (weights)) then
        call raise_exception (exc, EXC_FATAL, FN, &
            "channel and weights required together")
        return
    end if
92b <Declaration of vamp procedures 77a>+≡ (75b) <86b 96a>
    public :: vamp_probability
92c <Implementation of vamp procedures 78b>+≡ (75b) <86c 92d>
    pure function vamp_probability (g, x) result (p)
        type(vamp_grid), intent(in) :: g
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default) :: p
        p = product (probability (g%div, x))
    end function vamp_probability

```

 %variance should be private to division

```

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

```

```

n_ch = size (g%grids)
if (n_ch == 0) return
n_dim = size (g%grids(1)%div)
allocate (n_bin(n_ch, n_dim))
do ch = 1, n_ch
  do dim = 1, n_dim
    n_bin(ch, dim) = size (g%grids(ch)%div(dim)%variance)
  end do
end do
allocate (var_tmp (maxval(n_bin), n_dim, n_ch))
var_tmp = 0
do i=1, eq%n_eq
  ch = eq%eq(i)%left
  ch_src = eq%eq(i)%right
  do dim=1, n_dim
    nb = n_bin(ch_src, dim)
    dim_src = eq%eq(i)%permutation(dim)
    select case (eq%eq(i)%mode(dim))
    case (VEQ_IDENTITY)
      var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
        & + g%grids(ch_src)%div(dim_src)%variance
    case (VEQ_INVERT)
      var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
        & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)
    case (VEQ_SYMMETRIC)
      var_tmp(:nb,dim,ch) = var_tmp(:nb,dim,ch) &
        & + g%grids(ch_src)%div(dim_src)%variance / 2 &
        & + g%grids(ch_src)%div(dim_src)%variance(nb:1:-1)/2
    case (VEQ_INVARIANT)
      var_tmp(:nb,dim,ch) = 1
    end select
  end do
end do
do ch=1, n_ch
  do dim=1, n_dim
    g%grids(ch)%div(dim)%variance = var_tmp(:n_bin(ch, dim),dim,ch)
  end do
end do
deallocate (var_tmp)
deallocate (n_bin)
end subroutine vamp_apply_equivalences

```

Grid Refinement: r

$$n_{\text{div},j} \rightarrow \frac{Q_j n_{\text{div},j}}{\left(\prod_j Q_j\right)^{1/n_{\text{dim}}}} \quad (5.19)$$

where

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

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

```

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

```

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

```

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

```

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

```

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

```

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

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

```

subroutine vamp_sample_grid &
  (rng, g, func, data, iterations, &

```

```

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

```

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

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

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

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

95 <Implementation of vamp procedures 78b>+≡ (75b) <94d 97d>
 elemental subroutine vamp_average_iterations_grid &
 (g, iteration, integral, std_dev, avg_chi2)


```

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

```

96a \langle Declaration of vamp procedures 77a $\rangle \equiv$ (75b) \langle 92b 97b \rangle

```

public :: vamp_average_iterations
private :: vamp_average_iterations_grid

```

96b \langle Interfaces of vamp procedures 96b $\rangle \equiv$ (75b) 97c \rangle

```

interface vamp_average_iterations
    module procedure vamp_average_iterations_grid
end interface

```

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

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

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

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

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

96c \langle Copy results of vamp_sample_grid to dummy variables 96c $\rangle \equiv$ (94d 104 120b)

```

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

```

```

        std_dev = local_std_dev
    end if
    if (present (avg_chi2)) then
        avg_chi2 = local_avg_chi2
    end if
97a <Exit iterate if accuracy has been reached 97a>≡ (94d 104 120b)
    if (present (accuracy)) then
        if (local_std_dev <= accuracy * local_integral) then
            call raise_exception (exc, EXC_INFO, FN, &
                "requested accuracy reached")
            exit iterate
        end if
    end if
end if

```

5.2.4 Forking and Joining

```

97b <Declaration of vamp procedures 77a>+≡ (75b) <96a 102b>
    public :: vamp_fork_grid
    private :: vamp_fork_grid_single, vamp_fork_grid_multi
    public :: vamp_join_grid
    private :: vamp_join_grid_single, vamp_join_grid_multi

97c <Interfaces of vamp procedures 96b>+≡ (75b) <96b 107c>
    interface vamp_fork_grid
        module procedure vamp_fork_grid_single, vamp_fork_grid_multi
    end interface
    interface vamp_join_grid
        module procedure vamp_join_grid_single, vamp_join_grid_multi
    end interface

```

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

```

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

```

```

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

Divide the sampling points among identical grids
98a <Handle g%calls_per_cell for d == 0 98a>≡ (97d)
    if (any (stratified_division (g%div))) then
        call raise_exception (exc, EXC_FATAL, FN, &
            "d == 0 incompatible w/ stratification")
    else
        gs(2:)%calls_per_cell = ceiling (real (g%calls_per_cell) / num_grids)
        gs(1)%calls_per_cell = g%calls_per_cell - sum (gs(2:)%calls_per_cell)
    end if

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

Reset results
98c <Copy the rest of g to the gs 98b>+≡ (97d) <98b 99a>
    gs%mu(1) = 0.0
    gs%mu(2) = 0.0
    gs%mu_plus(1) = 0.0
    gs%mu_plus(2) = 0.0

```

```

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

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

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

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

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

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

```

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

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

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

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

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

```

    call join_division (g%div(j), d_tmp, exc)
    deallocate (d_tmp)
    <Bail out if exception exc raised 99d>

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

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

```

The following is made a little bit hairy by the fact that `vamp_fork_grid` can't join grids onto a non-existing grid² therefore we have to keep a tree of joints. Maybe it would be the right thing to handle this tree of joints as a tree with pointers, but since we need the leaves flattened anyway (as food for multiple `vamp_sample_grid`) we use a similar storage layout for the joints.

```

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

```

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

```

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

```

102a \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \triangleleft 100c 102c \triangleright

```

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

```

102b \langle Declaration of vamp procedures 77a $\rangle + \equiv$ (75b) \triangleleft 97b 103b \triangleright

```

public :: vamp_fork_grid_joints

```

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

102c \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \triangleleft 102a 103a \triangleright

```

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

```

103a \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 102c 104 \rangle

```

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

```

5.2.5 Parallel Execution

103b \langle Declaration of vamp procedures 77a $\rangle + \equiv$ (75b) \langle 102b 107b \rangle


```

public :: vamp_sample_grid_parallel
public :: vamp_distribute_work

```

HPF [10, 11, 15]:

```

104 <Implementation of vamp procedures 78b>+≡ (75b) <103a 105b>
subroutine vamp_sample_grid_parallel &
    (rng, g, func, data, iterations, &
     integral, std_dev, avg_chi2, accuracy, &
     channel, weights, grids, exc, history)
type(tao_random_state), dimension(:), intent(inout) :: rng
type(vamp_grid), intent(inout) :: g
class(vamp_data_t), intent(in) :: data
integer, intent(in) :: iterations
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: channel
real(kind=default), dimension(:), intent(in), optional :: weights
type(vamp_grid), dimension(:), intent(in), optional :: grids
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_sample_grid_parallel"
real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
type(exception), dimension(size(rng)) :: excs
type(vamp_grid), dimension(:), allocatable :: gs, gx
!hpf$ processors p(number_of_processors())
!hpf$ distribute gs(cyclic(1)) onto p
integer, dimension(:,:), pointer :: d
integer :: iteration, i
integer :: num_workers
nullify (d)
call clear_exception (excs)
iterate: do iteration = 1, iterations
    call vamp_distribute_work (size (rng), vamp_rigid_divisions (g), d)
    num_workers = max (1, product (d(2,:)))
    if (num_workers > 1) then
        allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
        call vamp_create_empty_grid (gs)
        ! vamp_fork_grid is certainly not local. Speed freaks might
        ! want to tune it to the processor topology, but the gain will be small.
        call vamp_fork_grid (g, gs, gx, d, exc)
        !hpf$ independent
        do i = 1, num_workers
            call vamp_sample_grid0 &

```

```

        (rng(i), gs(i), func, data, &
         channel, weights, grids, exc)
    end do
    <Gather exceptions in vamp_sample_grid_parallel 105a>
    call vamp_join_grid (g, gs, gx, d, exc)
    call vamp_delete_grid (gs)
    deallocate (gs, gx)
else
    call vamp_sample_grid0 &
        (rng(1), g, func, data, channel, weights, grids, exc)
end if
<Bail out if exception exc raised 99d>
call vamp_average_iterations &
    (g, iteration, local_integral, local_std_dev, local_avg_chi2)
<Trace results of vamp_sample_grid 107a>
<Exit iterate if accuracy has been reached 97a>
if (iteration < iterations) call vamp_refine_grid (g)
end do iterate
deallocate (d)
<Copy results of vamp_sample_grid to dummy variables 96c>
end subroutine vamp_sample_grid_parallel
105a <Gather exceptions in vamp_sample_grid_parallel 105a>≡ (104)
    if ((present (exc)) .and. (any (excs(1:num_workers)%level > 0))) then
        call gather_exceptions (exc, excs(1:num_workers))
    end if

```

We could sort d such that (5.23) is minimized

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

but the gain will be negligible.

```

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

```

```

        j = sum (maxloc (ng / num_forks))
        nfork = num_forks(j) * factors(i)
        if (nfork <= ng(j)) then
            num_forks(j) = nfork
        else
            cycle try
        end if
    end do
    <Accept distribution among n workers 106a>
end do try
end subroutine vamp_distribute_work
106a <Accept distribution among n workers 106a>≡ (105b) 106b>
    j = count (num_forks > 1)
    if (associated (d)) then
        if (size (d, dim = 2) /= j) then
            deallocate (d)
            allocate (d(2,j))
        end if
    else
        allocate (d(2,j))
    end if
106b <Accept distribution among n workers 106a>+≡ (105b) <106a
    j = 1
    do i = 1, size (ng)
        if (num_forks(i) > 1) then
            d(:,j) = (/ i, num_forks(i) /)
            j = j + 1
        end if
    end do
    return

```

5.2.6 Diagnostics

```

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

```

```

end type vamp_history

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

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

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

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

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

```

```

        h%calls = 0.0
    end subroutine vamp_terminate_history

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

108b  <Adjust h%div iff necessary 108b>≡ (108a)
    if (associated (h%div)) then
        if (size (h%div) /= size (g%div)) then
            deallocate (h%div)
            allocate (h%div(size(g%div)))
        end if
    else
        allocate (h%div(size(g%div)))
    end if

108c  <Declaration of vamp procedures 77a>+≡ (75b) <107b 113b>
    public :: vamp_print_history, vamp_write_history
    private :: vamp_print_one_history, vamp_print_histories
    ! private :: vamp_write_one_history, vamp_write_histories

108d  <Interfaces of vamp procedures 96b>+≡ (75b) <107c 124d>
    interface vamp_print_history
        module procedure vamp_print_one_history, vamp_print_histories
    end interface
    interface vamp_write_history
        module procedure vamp_write_one_history_unit, vamp_write_histories_unit
    end interface

```

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

```

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

```

```

        end do
        if (present (tag)) then
            write (unit = pfx, fmt = "(A,A1,I2.2)" &
                trim (tag(1:min(len_trim(tag),8))), "#", j
        else
            write (unit = pfx, fmt = "(A,A1,I2.2)" "[vamp]", "#", j
        end if
        call print_history (h_tmp, tag = pfx)
        print "(1X,A78)", repeat ("-", 78)
    end do dimensions
    deallocate (h_tmp)
end if
end if
flush (output_unit)
end subroutine vamp_print_one_history
110a <Variables in vamp 79a>+≡ (75b) <94c 146a>
    integer, private, parameter :: BUFFER_SIZE = 50
110b <Implementation of vamp procedures 78b>+≡ (75b) <109 110c>
    subroutine vamp_print_histories (h, tag)
        type(vamp_history), dimension(:,,:), intent(in) :: h
        character(len=*), intent(in), optional :: tag
        character(len=BUFFER_SIZE) :: pfx
        integer :: i
        print "(1X,A78)", repeat ("=", 78)
        channels: do i = 1, size (h, dim=2)
            if (present (tag)) then
                write (unit = pfx, fmt = "(A4,A1,I3.3)" tag, "#", i
            else
                write (unit = pfx, fmt = "(A4,A1,I3.3)" "chan", "#", i
            end if
            call vamp_print_one_history (h(:,i), pfx)
        end do channels
        print "(1X,A78)", repeat ("=", 78)
        flush (output_unit)
    end subroutine vamp_print_histories

```



WK

```

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

```

```

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

```



```

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

```

5.2.7 Multi Channel

[23]

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

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

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

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

Therefore...

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

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

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

113a \langle Declaration of **vamp** types 77b $\rangle + \equiv$ (75b) \triangleleft 106c

```

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

```

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

113b \langle Declaration of **vamp** procedures 77a $\rangle + \equiv$ (75b) \triangleleft 108c 114b \rangle

```

public :: vamp_multi_channel, vamp_multi_channel0

```

113c \langle Implementation of **vamp** procedures 78b $\rangle + \equiv$ (75b) \triangleleft 110c 114a \rangle

```

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
   $\langle$ Interface declaration for func 22 $\rangle$ 
   $\langle$ Interface declaration for phi 31a $\rangle$ 
   $\langle$ Interface declaration for ihp 31b $\rangle$ 
   $\langle$ Interface declaration for jacobian 31c $\rangle$ 
  real(kind=default) :: w_x
  integer :: i

```

```

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

```

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

```

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

```



WK

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

```

public :: vamp_jacobian, vamp_check_jacobian

```

114c *<Implementation of vamp procedures 78b>+≡* (75b) <114a 115>

```

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

```

```

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

```

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

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

(75b) \langle 114c 117b \rangle

```

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

```

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

116a <Declaration of vamp procedures (removed from WHIZARD) 116a>≡
 private :: numeric_jacobian

116b <Implementation of vamp procedures (removed from WHIZARD) 116b>≡
 pure subroutine numeric_jacobian (phi, channel, x, region, jacobian, delta_x)
 integer, intent(in) :: channel
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:, :), intent(in) :: region
 real(kind=default), intent(out) :: jacobian
 real(kind=default), intent(in), optional :: delta_x
 <Interface declaration for phi 31a>

```

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

```

117a *<Declaration of vamp procedures 77a>+≡* (75b) <114b 118b>
 public :: vamp_create_grids, vamp_create_empty_grids
 public :: vamp_copy_grids, vamp_delete_grids

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

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

```

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

```

118a *<Implementation of vamp procedures 78b>+≡* (75b) *<117b 118c>*

```

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

```

118b *<Declaration of vamp procedures 77a>+≡* (75b) *<117a 119a>*

```

public :: vamp_discard_integrals

```

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

```

pure subroutine vamp_discard_integrals &
  (g, num_calls, num_div, stratified, quadrupole, exc, eq)
type(vamp_grids), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
type(vamp_equivalences_t), intent(in), optional :: eq
integer :: ch
character(len=*), parameter :: FN = "vamp_discard_integrals"

```

```

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

```

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

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

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

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

119d *<Implementation of vamp procedures 78b>+≡* (75b) <119b 120b>
 pure subroutine vamp_reshape_grids &


```

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

```

120a \langle Declaration of vamp procedures 77a $\rangle + \equiv$ (75b) \langle 119c 123a \rangle
 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 \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 119d 123b \rangle
 subroutine vamp_sample_grids &

```

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

```

```

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

```

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

```

122 <Sample the grid g%grids(ch) 122>≡ (120b)
    call vamp_sample_grid0 &
      (rng, g%grids(ch), func, data, &
        ch, weights, g%grids, excs(ch), neg_w)
    if (present (exc) .and. present (warn_error)) then
      if (warn_error) call handle_exception (excs(ch))
    end if
    call vamp_average_iterations &
      (g%grids(ch), iteration, integrals(ch), std_devs(ch), local_avg_chi2)
    if (present (histories)) then
      if (iteration <= ubound (histories, dim=1)) then
        call vamp_get_history &
          (histories(iteration,ch), g%grids(ch), &
            integrals(ch), std_devs(ch), local_avg_chi2)
      else
        call raise_exception (exc, EXC_WARN, FN, "history too short")
      end if
      call vamp_terminate_history (histories(iteration+1:,ch))
    end if

```

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

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

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

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

where (5.30b) is actually

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

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

123b \langle Implementation of `vamp` procedures 78b $\rangle + \equiv$ (75b) \langle 120b 124b \rangle
`pure subroutine vamp_reduce_channels (g, integrals, std_devs, active)`
`type(vamp_grids), intent(inout) :: g`
`real(kind=default), dimension(:), intent(in) :: integrals, std_devs`
`logical, dimension(:), intent(in) :: active`
`real(kind=default) :: this_integral, this_weight, total_calls`
`real(kind=default) :: total_variance`
`if (.not.any(active)) return`
`total_calls = sum (g%num_calls, mask=active)`
`if (total_calls > 0) then`
`this_integral = sum (g%num_calls * integrals, mask=active) / total_calls`
`else`
`this_integral = 0`
`end if`
`total_variance = sum ((g%num_calls*std_devs)**2, mask=active)`
`if (total_variance > 0) then`
`this_weight = total_calls**2 / total_variance`
`else`
`this_weight = 0`
`end if`
`g%sum_weights = g%sum_weights + this_weight`
`g%sum_integral = g%sum_integral + this_weight * this_integral`
`g%sum_chi2 = g%sum_chi2 + this_weight * this_integral**2`
`end subroutine vamp_reduce_channels`

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

124b \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 123b 124e \rangle
elemental subroutine vamp_average_iterations_grids &
(g, iteration, integral, std_dev, avg_chi2)
type(vamp_grids), intent(in) :: g
integer, intent(in) :: iteration
real(kind=default), intent(out) :: integral, std_dev, avg_chi2
real(kind=default), parameter :: eps = 1000 * epsilon (1._default)
if (g%sum_weights>0) then
integral = g%sum_integral / g%sum_weights
std_dev = sqrt (1.0 / g%sum_weights)
avg_chi2 = &
max ((g%sum_chi2 - g%sum_integral * integral) / (iteration-0.99), &
0.0_default)
if (avg_chi2 < eps * g%sum_chi2) avg_chi2 = 0
else
integral = 0
std_dev = 0
avg_chi2 = 0
end if
end subroutine vamp_average_iterations_grids

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

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

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

124e \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \langle 124b 125d \rangle
pure subroutine vamp_refine_weights (g, power)
type(vamp_grids), intent(inout) :: g
real(kind=default), intent(in), optional :: power
real(kind=default) :: local_power
real(kind=default), parameter :: DEFAULT_POWER = 0.5_default
if (present (power)) then
local_power = power
else
local_power = DEFAULT_POWER
end if
call vamp_update_weights &

```

        (g, g%weights * vamp_get_variance (g%grids) ** local_power)
    end subroutine vamp_refine_weights
125a <Trace results of vamp_sample_grids 125a>≡ (120b)
    if (present (history)) then
        if (iteration <= size (history)) then
            call vamp_get_history &
                (history(iteration), g, local_integral, local_std_dev, &
                 local_avg_chi2)
        else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
        end if
        call vamp_terminate_history (history(iteration+1:))
    end if
125b <Declaration of vamp procedures 77a>+≡ (75b) <124c 126a>
    private :: vamp_get_history_multi
125c <Interfaces of vamp procedures 96b>+≡ (75b) <124d 131b>
    interface vamp_get_history
        module procedure vamp_get_history_multi
    end interface
125d <Implementation of vamp procedures 78b>+≡ (75b) <124e 126b>
    pure subroutine vamp_get_history_multi (h, g, integral, std_dev, avg_chi2)
        type(vamp_history), intent(inout) :: h
        type(vamp_grids), intent(in) :: g
        real(kind=default), intent(in) :: integral, std_dev, avg_chi2
        h%calls = sum (g%grids%calls)
        h%stratified = all (g%grids%all_stratified)
        h%integral = 0.0
        h%std_dev = 0.0
        h%avg_integral = integral
        h%avg_std_dev = std_dev
        h%avg_chi2 = avg_chi2
        h%f_min = 0.0
        h%f_max = huge (h%f_max)
        if (h%verbose) then
            h%verbose = .false.
            if (associated (h%div)) then
                deallocate (h%div)
            end if
        end if
    end subroutine vamp_get_history_multi

```



WK

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

126b \langle Implementation of `vamp` procedures 78b $\rangle + \equiv$ (75b) \langle 125d 127c \rangle
`function vamp_sum_channels (x, weights, func, data, grids) result (g)`
`real(kind=default), dimension(:), intent(in) :: x, weights`
`class(vamp_data_t), intent(in) :: data`
`type(vamp_grid), dimension(:), intent(in), optional :: grids`
`interface`
`function func (xi, data, weights, channel, grids) result (f)`
`use kinds`
`use vamp_grid_type !NODEP!`
`import vamp_data_t`
`real(kind=default), dimension(:), intent(in) :: xi`
`class(vamp_data_t), intent(in) :: data`
`real(kind=default), dimension(:), intent(in), optional :: weights`
`integer, intent(in), optional :: channel`
`type(vamp_grid), dimension(:), intent(in), optional :: grids`
`real(kind=default) :: f`
`end function func`
`end interface`
`real(kind=default) :: g`
`integer :: ch`
`g = 0.0`
`do ch = 1, size (weights)`
`g = g + weights(ch) * func (x, data, weights, ch, grids)`
`end do`
`end function vamp_sum_channels`

5.2.8 Mapping

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

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

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

where

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

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

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

After call `diagonalize_real_symmetric (cov, evals, evecs)`, we have $\text{evals}(j) = \lambda_j$ and $\text{evecs}(:, j) = v_j$. This is equivalent with $\text{evecs}(i, j) = R_{ij}$.

This approach will not work in high dimensions, however. In general, R will *not* leave most of the axes invariant, even if the covariance matrix is almost isotropic in these directions. In this case the benefit from the rotation is rather small and offset by the negative effects from the misalignment of the integration region.

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

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

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

```

127a <Declaration of vamp procedures 77a>+≡ (75b) <126a 128a>
    public :: select_rotation_axis
    public :: select_rotation_subspace

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

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

```



```

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

```

128a \langle Declaration of `vamp` procedures 77a $\rangle + \equiv$ (75b) \langle 127a 131c \rangle
 private :: more_pancake_than_cigar

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

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

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

128b \langle Set `i(1)`, `i(2)` to the axes of the optimal plane 128b $\rangle \equiv$ (129d) 129a \rangle
`abs_evec = abs (evecs(:,iv))`
`i(1) = sum (maxloc (abs_evec))`
`abs_evec(i(1)) = -1.0`
`i(2) = sum (maxloc (abs_evec))`

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

128c \langle Set `i(1)`, `i(2)` to the axes of the optimal plane (broken!) 128c $\rangle \equiv$
`abs_evec = abs (evecs(:,iv))`
`i(1) = sum (maxloc (abs_evec))`
`i(2) = sum (maxloc (abs_evec, mask = abs_evec < abs_evec(i(1))))`

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

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

```
print *, iv, evals(iv), " => ", evcs(:,iv)
print *, i(1), abs_evec(i(1)), ", ", i(2), abs_evec(i(2))
print *, i(1), evcs(i(1),iv), ", ", i(2), evcs(i(2),iv)
```

129b \langle Get $\cos \theta$ and $\sin \theta$ from evcs 129b $\rangle \equiv$ (129d)

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

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

129c \langle Construct $\hat{R}(\theta; i, j)$ 129c $\rangle \equiv$ (129d)

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

129d \langle Implementation of vamp procedures 78b $\rangle + \equiv$ (75b) \triangleleft 127c 130b \rangle

```
subroutine select_rotation_axis (cov, r, pancake, cigar)
  real(kind=default), dimension(:, :), intent(in) :: cov
  real(kind=default), dimension(:, :), intent(out) :: r
  integer, intent(in), optional :: pancake, cigar
  integer :: num_pancake, num_cigar
  logical :: like_pancake
  real(kind=default), dimension(size(cov,dim=1),size(cov,dim=2)) :: evcs
  real(kind=default), dimension(size(cov,dim=1)) :: evals, abs_evec
  integer :: iv
  integer, dimension(2) :: i
  real(kind=default) :: cos_theta, sin_theta, norm
   $\langle$ Handle optional pancake and cigar 130a $\rangle$ 
  call diagonalize_real_symmetric (cov, evals, evcs)
   $\langle$ Set iv to the index of the optimal eigenvector 127b $\rangle$ 
   $\langle$ Set  $i(1)$ ,  $i(2)$  to the axes of the optimal plane 128b $\rangle$ 
   $\langle$ Get  $\cos \theta$  and  $\sin \theta$  from evcs 129b $\rangle$ 
   $\langle$ Construct  $\hat{R}(\theta; i, j)$  129c $\rangle$ 
end subroutine select_rotation_axis
```

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

```

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

```

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

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

```

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

```

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

```

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

```

```

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

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

131b  <Interfaces of vamp procedures 96b>+≡ (75b) <125c 135b>
        interface select_rotation_subspace
            module procedure select_subspace_explicit, select_subspace_guess
        end interface

131c  <Declaration of vamp procedures 77a>+≡ (75b) <128a 131d>
        private :: select_subspace_explicit
        private :: select_subspace_guess

131d  <Declaration of vamp procedures 77a>+≡ (75b) <131c 132a>
        public :: vamp_print_covariance

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

```

```

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

```

Condensing Eigenvalues

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


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

```

! private :: condense
public :: condense

```

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

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

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

```

cl_pos = x
cl_num = size (cl_pos)
cl = spread ((/ (i, i=1,cl_num) /), dim = 2, ncopies = 2)

```

It appears that the logarithmic metric

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

performs better than the linear metric

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

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

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

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

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

```

133a  <Join closest clusters 133a>≡ (133c) 133b>
      if (linear_metric) then
        gap = sum (minloc (cl_pos(2:cl_num) - cl_pos(1:cl_num-1)))
      else
        gap = sum (minloc (cl_pos(2:cl_num) / cl_pos(1:cl_num-1)))
      end if
      wgt0 = cl(gap,2) - cl(gap,1) + 1
      wgt1 = cl(gap+1,2) - cl(gap+1,1) + 1
      cl_pos(gap) = (wgt0 * cl_pos(gap) + wgt1 * cl_pos(gap+1)) / (wgt0 + wgt1)
      cl(gap,2) = cl(gap+1,2)

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

133c  <Implementation of vamp procedures 78b>+≡ (75b) <131e 134b>
      subroutine condense (x, cluster_pos, clusters, linear)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), dimension(:), intent(out) :: cluster_pos
        integer, dimension(:,:), intent(out) :: clusters
        logical, intent(in), optional :: linear
        logical :: linear_metric
        real(kind=default), dimension(size(x)) :: cl_pos
        real(kind=default) :: wgt0, wgt1
        integer :: cl_num
        integer, dimension(size(x),2) :: cl
        integer :: i, gap
        linear_metric = .false.
        if (present (linear)) then
          linear_metric = linear
        end if
        <Initialize clusters 132b>
        do cl_num = size (cl_pos), size (cluster_pos) + 1, -1
          <Join closest clusters 133a>
          print *, cl_num, ": action = ", condense_action (x, cl)

```

```

        end do
        cluster_pos = cl_pos(1:cl_num)
        clusters = cl(1:cl_num,:)
    end subroutine condense
134a  <Declaration of vamp procedures 77a>+≡ (75b) <132a 135a>
    ! private :: condense_action
    public :: condense_action

```

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

```

134b  <Implementation of vamp procedures 78b>+≡ (75b) <133c 135d>
    function condense_action (positions, clusters) result (s)
        real(kind=default), dimension(:), intent(in) :: positions
        integer, dimension(:,:), intent(in) :: clusters
        real(kind=default) :: s
        integer :: i
        integer, parameter :: POWER = 2
        s = 0
        do i = 1, size (clusters, dim = 1)
            s = s + standard_deviation (positions(clusters(i,1) &
                                                    :clusters(i,2))) ** POWER
        end do
    end function condense_action
134c  <ctest.f90 134c>≡
    program ctest
        use kinds
        use utils
        use vamp_stat
        use tao_random_numbers
        use vamp
        implicit none
        integer, parameter :: N = 16, NC = 2
        real(kind=default), dimension(N) :: eval
        real(kind=default), dimension(NC) :: cluster_pos
        integer, dimension(NC,2) :: clusters
        integer :: i
        call tao_random_number (eval)
        call sort (eval)
        print *, eval
        eval(1:N/2) = 0.95*eval(1:N/2)
        eval(N/2+1:N) = 1.0 - 0.95*(1.0 - eval(N/2+1:N))
        print *, eval
        call condense (eval, cluster_pos, clusters, linear=.true.)

```

```

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

```

5.2.9 Event Generation

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

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

135b *<Interfaces of vamp procedures 96b>+≡* (75b) <131b 140b>
 interface vamp_next_event
 module procedure vamp_next_event_single, vamp_next_event_multi
 end interface

135c *<Declaration of vamp procedures 77a>+≡* (75b) <135a 139a>
 private :: vamp_next_event_single, vamp_next_event_multi

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

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


```

real(kind=default), dimension(size(g%div)):: wgts
real(kind=default), dimension(size(g%div)):: r
integer, dimension(size(g%div)):: ia
real(kind=default) :: f, wgt
real(kind=default) :: r0
rejection: do
  <Choose a x and calculate f(x) 136a>
  if (present (weight)) then
    <Unconditionally accept weighted event 136b>
  else
    <Maybe accept unweighted event 136c>
  end if
end do rejection
end subroutine vamp_next_event_single
136a <Choose a x and calculate f(x) 136a>≡ (135d)
call tao_random_number (rng, r)
call inject_division_short (g%div, real(r, kind=default), x, ia, wgts)
wgt = g%jacobi * product (wgts)
wgt = g%calls * wgt ! the calling procedure will divide by #calls
if (associated (g%map)) then
  x = matmul (g%map, x)
end if
<f = wgt * func (x, weights, channel), iff x inside true.domain 88d>
! call record_efficiency (g%div, ia, f/g%f_max)
136b <Unconditionally accept weighted event 136b>≡ (135d)
weight = f
exit rejection
136c <Maybe accept unweighted event 136c>≡ (135d)
if (f > g%f_max) then
  g%f_max = f
  call raise_exception (exc, EXC_WARN, FN, "weight > 1")
  exit rejection
end if
call tao_random_number (rng, r0)
if (r0 * g%f_max <= f) then
  exit rejection
end if

```

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

$$f(x) = \sum_i \alpha_i g_i(x) w(x) \quad (5.39)$$

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

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

```

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

```

We can either reject with the weights

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

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

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

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

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

 if (any (g%grids%f_max > 0)) then
 weights = g%weights * g%grids%f_max
 else
 weights = g%weights
 end if
 weights = weights / sum (weights)

```
- 138b  $\langle \text{Select channel from weights 138b} \rangle \equiv$  (137)
- ```

    call tao_random_number (rng, r)
    select_channel: do channel = 1, size (g%weights)
        r = r - weights(channel)
        if (r <= 0.0) then
            exit select_channel
        end if
    end do select_channel
    channel = min (channel, size (g%weights)) ! for r = 1 and rounding errors

```
- 138c $\langle \text{Unconditionally accept weighted multi channel event 138c} \rangle \equiv$ (137)
- ```

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

```
- 138d  $\langle \text{Maybe accept unweighted multi channel event 138d} \rangle \equiv$  (137)
- ```

    if (abs (wgt) > g%grids(channel)%f_max) then
        if (present(excess)) then
            excess = abs (wgt) / g%grids(channel)%f_max - 1
        else
            call raise_exception (exc, EXC_WARN, FN, "weight > 1")
            !      print *, "weight > 1 (", wgt/g%grids(channel)%f_max, &
            !          & ") in channel ", channel

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

```
- 138e $\langle \text{Maybe accept unweighted multi channel event (old version) 138e} \rangle \equiv$

```

if (wgt > g%grids(channel)%f_max) then
  g%grids(channel)%f_max = wgt
   $\langle \text{weights: } \alpha_i \rightarrow w_{\max,i} \alpha_i \text{ 138a} \rangle$ 
  call raise_exception (exc, EXC_WARN, FN, "weight > 1")
  exit rejection
end if
call tao_random_number (rng, r)
if (r * g%grids(channel)%f_max <= wgt) then
  exit rejection
end if

```

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

139a $\langle \text{Declaration of vamp procedures 77a} \rangle + \equiv$ (75b) $\langle 135c \ 140a \rangle$
 public :: vamp_warmup_grid, vamp_warmup_grids

139b $\langle \text{Implementation of vamp procedures 78b} \rangle + \equiv$ (75b) $\langle 137 \ 139c \rangle$
 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
 $\langle \text{Interface declaration for func 22} \rangle$
 call vamp_sample_grid &
 (rng, g, func, data, &
 iterations - 1, exc = exc, history = history)
 call vamp_sample_grid0 (rng, g, func, data, exc = exc)
 end subroutine vamp_warmup_grid



WHERE ... END WHERE alert!

139c $\langle \text{Implementation of vamp procedures 78b} \rangle + \equiv$ (75b) $\langle 139b \ 140c \rangle$

```

subroutine vamp_warmup_grids &
  (rng, g, func, data, iterations, history, histories, exc)
  type(tao_random_state), intent(inout) :: rng
  type(vamp_grids), intent(inout) :: g
  class(vamp_data_t), intent(in) :: data
  integer, intent(in) :: iterations

```

```

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

```

5.2.10 Convenience Routines

- 140a <Declaration of vamp procedures 77a>+≡ (75b) <139a 142a>
 public :: vamp_integrate
 private :: vamp_integrate_grid, vamp_integrate_region
- 140b <Interfaces of vamp procedures 96b>+≡ (75b) <135b 142b>
 interface vamp_integrate
 module procedure vamp_integrate_grid, vamp_integrate_region
 end interface
- 140c <Implementation of vamp procedures 78b>+≡ (75b) <139c 141>
 subroutine vamp_integrate_grid &
 (rng, g, func, data, calls, integral, std_dev, avg_chi2, num_div, &
 stratified, quadrupole, accuracy, exc, history)
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid), intent(inout) :: g
 class(vamp_data_t), intent(in) :: data
 integer, dimension(:, :), intent(in) :: calls

```

real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_integrate_grid"
integer :: step, last_step, it
last_step = size (calls, dim = 2)
it = 1
do step = 1, last_step - 1
    call vamp_discard_integral (g, calls(2,step), num_div, &
                                stratified, quadrupole, exc = exc)
    call vamp_sample_grid (rng, g, func, data, calls(1,step), &
                           exc = exc, history = history(it:))
    <Bail out if exception exc raised 99d>
    it = it + calls(1,step)
end do
call vamp_discard_integral (g, calls(2,last_step), exc = exc)
call vamp_sample_grid (rng, g, func, data, calls(1,last_step), &
                       integral, std_dev, avg_chi2, accuracy, exc = exc, &
                       history = history(it:))
end subroutine vamp_integrate_grid
141 <Implementation of vamp procedures 78b>+≡ (75b) <140c 142c>
subroutine vamp_integrate_region &
    (rng, region, func, data, calls, &
     integral, std_dev, avg_chi2, num_div, &
     stratified, quadrupole, accuracy, map, covariance, exc, history)
type(tao_random_state), intent(inout) :: rng
real(kind=default), dimension(:,:), intent(in) :: region
class(vamp_data_t), intent(in) :: data
integer, dimension(:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
real(kind=default), dimension(:,:), intent(in), optional :: map
real(kind=default), dimension(:,:), intent(out), optional :: covariance
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_integrate_region"

```

```

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

```

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

```

public :: vamp_integratex
private :: vamp_integratex_region

```

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

```

interface vamp_integratex
    module procedure vamp_integratex_region
end interface

```

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

```

subroutine vamp_integratex_region &
    (rng, region, func, data, calls, integral, std_dev, avg_chi2, &
     num_div, stratified, quadrupole, accuracy, pancake, cigar, &
     exc, history)
type(tao_random_state), intent(inout) :: rng
real(kind=default), dimension(:,,:), intent(in) :: region
class(vamp_data_t), intent(in) :: data
integer, dimension(:,:,:), intent(in) :: calls
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: pancake, cigar
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
real(kind=default), dimension(size(region,dim=2)) :: eval
real(kind=default), dimension(size(region,dim=2),size(region,dim=2)) :: evec
type(vamp_grid) :: g
integer :: step, last_step, it
it = 1

```

```

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

```

5.2.11 I/O

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

```

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

```



```

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

144a <Declaration of vamp procedures 77a>+≡ (75b) <143 158a>
public :: vamp_read_grids_raw
private :: read_grids_raw_unit, read_grids_raw_name
public :: vamp_read_grid_raw
private :: read_grid_raw_unit, read_grid_raw_name
public :: vamp_write_grids_raw
private :: write_grids_raw_unit, write_grids_raw_name
public :: vamp_write_grid_raw
private :: write_grid_raw_unit, write_grid_raw_name

144b <Interfaces of vamp procedures 96b>+≡ (75b) <142b 144c>
interface vamp_write_grid
  module procedure write_grid_unit, write_grid_name
end interface
interface vamp_read_grid
  module procedure read_grid_unit, read_grid_name
end interface
interface vamp_write_grids
  module procedure write_grids_unit, write_grids_name
end interface
interface vamp_read_grids
  module procedure read_grids_unit, read_grids_name
end interface

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

144d <Implementation of vamp procedures 78b>+≡ (75b) <142c 146b>
  subroutine write_grid_unit (g, unit, write_integrals)

```

```

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

```

```

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

```

146a *<Variables in vamp 79a>+≡* (75b) <110a

```

character(len=*), parameter, private :: &
    descr_fmt = "(1x,a)", &
    integer_fmt = "(1x,a17,1x,i15)", &
    integer_array_fmt = "(1x,i17,1x,i15)", &
    logical_fmt = "(1x,a17,1x,l1)", &
    double_fmt = "(1x,a17,1x,e30.22e4)", &
    double_array_fmt = "(1x,i17,1x,e30.22e4)", &
    double_array2_fmt = "(2(1x,i8),1x,e30.22e4)"

```

146b *<Implementation of vamp procedures 78b>+≡* (75b) <144d 149a>

```

subroutine read_grid_unit (g, unit, read_integrals)
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: read_integrals
    character(len=*), parameter :: FN = "vamp_read_grid"
    character(len=80) :: chdum
    integer :: ndim, i, j, idum, jdum
    read (unit = unit, fmt = descr_fmt) chdum
    read (unit = unit, fmt = integer_fmt) chdum, ndim
    <Insure that size (g%div) == ndim 148a>
    call create_array_pointer (g%num_div, ndim)
    read (unit = unit, fmt = integer_fmt) chdum, g%num_calls

```

```

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

```

```

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

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

148b <Insure that associated (g%map) == .false. 148b>≡ (146b 153b 160b)
if (associated (g%map)) then
  deallocate (g%map)
end if

148c <Insure that associated (g%mu_x) == .false. 148c>≡ (146b 153b 160b)
if (associated (g%mu_x)) then
  deallocate (g%mu_x)
end if
if (associated (g%mu_xx)) then

```

```

        deallocate (g%mu_xx)
    end if
    if (associated (g%sum_mu_x)) then
        deallocate (g%sum_mu_x)
    end if
    if (associated (g%sum_mu_xx)) then
        deallocate (g%sum_mu_xx)
    end if
149a <Implementation of vamp procedures 78b>+≡ (75b) <146b 149b>
    subroutine write_grid_name (g, name, write_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: write_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", file = name)
        call write_grid_unit (g, unit, write_integrals)
        close (unit = unit)
    end subroutine write_grid_name
149b <Implementation of vamp procedures 78b>+≡ (75b) <149a 149c>
    subroutine read_grid_name (g, name, read_integrals)
        type(vamp_grid), intent(inout) :: g
        character(len=*), intent(in) :: name
        logical, intent(in), optional :: read_integrals
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", file = name)
        call read_grid_unit (g, unit, read_integrals)
        close (unit = unit)
    end subroutine read_grid_name
149c <Implementation of vamp procedures 78b>+≡ (75b) <149b 150>
    subroutine write_grids_unit (g, unit, write_integrals)
        type(vamp_grids), intent(in) :: g
        integer, intent(in) :: unit
        logical, intent(in), optional :: write_integrals
        integer :: i
        write (unit = unit, fmt = descr_fmt) "begin type(vamp_grids) :: g"
        write (unit = unit, fmt = integer_fmt) "size (g%grids) = ", size (g%grids)
        write (unit = unit, fmt = double_fmt) "sum_integral = ", g%sum_integral
        write (unit = unit, fmt = double_fmt) "sum_weights = ", g%sum_weights
        write (unit = unit, fmt = double_fmt) "sum_chi2 = ", g%sum_chi2
        write (unit = unit, fmt = descr_fmt) "begin g%weights"

```

```

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

```

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

```

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

```

```

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

```

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

```

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

```

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

```

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

```

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

```

subroutine write_grid_raw_unit (g, unit, write_integrals)
    type(vamp_grid), intent(in) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: write_integrals
    integer :: i, j

```



```

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

```

```

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

```

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

```

integer, parameter, private :: MAGIC_GRID = 22222222
integer, parameter, private :: MAGIC_GRID_BEGIN = MAGIC_GRID + 1
integer, parameter, private :: MAGIC_GRID_END = MAGIC_GRID + 2
integer, parameter, private :: MAGIC_GRID_EMPTY = MAGIC_GRID + 3
integer, parameter, private :: MAGIC_GRID_MAP = MAGIC_GRID + 4
integer, parameter, private :: MAGIC_GRID_MU_X = MAGIC_GRID + 5

```

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

```

subroutine read_grid_raw_unit (g, unit, read_integrals)
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: unit
    logical, intent(in), optional :: read_integrals
    character(len=*), parameter :: FN = "vamp_read_raw_grid"
    integer :: ndim, i, j, magic
    read (unit = unit) magic
    if (magic /= MAGIC_GRID_BEGIN) then
        print *, FN, " fatal: expecting magic ", MAGIC_GRID_BEGIN, &
            ", found ", magic
        stop
    end if
    read (unit = unit) ndim
    <Insure that size (g%div) == ndim 148a>
    call create_array_pointer (g%num_div, ndim)
    read (unit = unit) g%num_calls
    read (unit = unit) g%calls_per_cell
    read (unit = unit) g%stratified
    read (unit = unit) g%all_stratified
    read (unit = unit) g%quadrupole
    read (unit = unit) g%mu(1)
    read (unit = unit) g%mu(2)
    read (unit = unit) g%mu_plus(1)
    read (unit = unit) g%mu_plus(2)

```

```

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

```

```

        read (unit = unit) g%mu_xx(i,j)
        read (unit = unit) g%sum_mu_xx(i,j)
    end do
end do
else if (magic == MAGIC_GRID_EMPTY) then
    <Insure that associated (g%mu_x) == .false. 148c>
else
    print *, FN, " fatal: expecting magic ", MAGIC_GRID_EMPTY, &
        " or ", MAGIC_GRID_MU_X, " found ", magic
    stop
end if
read (unit = unit) magic
if (magic /= MAGIC_GRID_END) then
    print *, FN, " fatal: expecting magic ", MAGIC_GRID_END, &
        " found ", magic
    stop
end if
end subroutine read_grid_raw_unit
155a <Implementation of vamp procedures 78b>+≡ (75b) <153b 155b>
subroutine write_grid_raw_name (g, name, write_integrals)
    type(vamp_grid), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: write_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "write", status = "replace", &
        form = "unformatted", file = name)
    call write_grid_raw_unit (g, unit, write_integrals)
    close (unit = unit)
end subroutine write_grid_raw_name
155b <Implementation of vamp procedures 78b>+≡ (75b) <155a 156a>
subroutine read_grid_raw_name (g, name, read_integrals)
    type(vamp_grid), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: read_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "read", status = "old", &
        form = "unformatted", file = name)
    call read_grid_raw_unit (g, unit, read_integrals)
    close (unit = unit)
end subroutine read_grid_raw_name

```

```

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

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

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

```

```

        deallocate (g%grids, g%weights, g%num_calls)
        allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
        call vamp_create_empty_grid (g%grids)
    end if
else
    allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
    call vamp_create_empty_grid (g%grids)
end if
read (unit = unit) g%sum_integral
read (unit = unit) g%sum_weights
read (unit = unit) g%sum_chi2
do i = 1, nch
    read (unit = unit) g%weights(i)
end do
do i = 1, nch
    read (unit = unit) g%num_calls(i)
end do
do i = 1, nch
    call read_grid_raw_unit (g%grids(i), unit, read_integrals)
end do
read (unit = unit) magic
if (magic /= MAGIC_GRIDS_END) then
    print *, FN, " fatal: expecting magic ", MAGIC_GRIDS_END, &
        " found ", magic
    stop
end if
end subroutine read_grids_raw_unit
157a <Implementation of vamp procedures 78b>+≡ (75b) <156c 157b>
subroutine write_grids_raw_name (g, name, write_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name
    logical, intent(in), optional :: write_integrals
    integer :: unit
    call find_free_unit (unit)
    open (unit = unit, action = "write", status = "replace", &
        form = "unformatted", file = name)
    call write_grids_raw_unit (g, unit, write_integrals)
    close (unit = unit)
end subroutine write_grids_raw_name
157b <Implementation of vamp procedures 78b>+≡ (75b) <157a 158b>
subroutine read_grids_raw_name (g, name, read_integrals)
    type(vamp_grids), intent(inout) :: g
    character(len=*), intent(in) :: name

```

```

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

```

5.2.12 Marshaling

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

```

158a <Declaration of vamp procedures 77a>+≡ (75b) <144a 161>
      public :: vamp_marshall_grid_size, vamp_marshall_grid, vamp_unmarshal_grid

158b <Implementation of vamp procedures 78b>+≡ (75b) <157b 160a>
      pure subroutine vamp_marshall_grid (g, ibuf, dbuf)
        type(vamp_grid), intent(in) :: g
        integer, dimension(:), intent(inout) :: ibuf
        real(kind=default), dimension(:), intent(inout) :: dbuf
        integer :: i, iwords, dwords, iidx, didx, ndim
        ndim = size (g%div)
        ibuf(1) = g%num_calls
        ibuf(2) = g%calls_per_cell
        ibuf(3) = ndim
        if (g%stratified) then
          ibuf(4) = 1
        else
          ibuf(4) = 0
        end if
        if (g%all_stratified) then
          ibuf(5) = 1
        else
          ibuf(5) = 0
        end if
        if (g%quadrupole) then
          ibuf(6) = 1
        else
          ibuf(6) = 0
        end if
        dbuf(1:2) = g%mu
        dbuf(3) = g%sum_integral

```

```

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

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

```



```

        iidx = iidx + 1
    end subroutine vamp_marshall_grid
160a  <Implementation of vamp procedures 78b>+≡ (75b) <158b 160b>
    pure subroutine vamp_marshall_grid_size (g, iwords, dwords)
        type(vamp_grid), intent(in) :: g
        integer, intent(out) :: iwords, dwords
        integer :: i, ndim, iw, dw
        ndim = size (g%div)
        iwords = 6 + ndim
        dwords = 12
        do i = 1, ndim
            call marshal_division_size (g%div(i), iw, dw)
            iwords = iwords + 2 + iw
            dwords = dwords + dw
        end do
        iwords = iwords + 1
        if (associated (g%map)) then
            dwords = dwords + ndim**2
        end if
        iwords = iwords + 1
        if (associated (g%mu_x)) then
            dwords = dwords + 2 * (ndim + ndim**2)
        end if
    end subroutine vamp_marshall_grid_size
160b  <Implementation of vamp procedures 78b>+≡ (75b) <160a 162a>
    pure subroutine vamp_unmarshal_grid (g, ibuf, dbuf)
        type(vamp_grid), intent(inout) :: g
        integer, dimension(:), intent(in) :: ibuf
        real(kind=default), dimension(:), intent(in) :: dbuf
        integer :: i, iwords, dwords, iidx, didx, ndim
        g%num_calls = ibuf(1)
        g%calls_per_cell = ibuf(2)
        ndim = ibuf(3)
        g%stratified = ibuf(4) /= 0
        g%all_stratified = ibuf(5) /= 0
        g%quadrupole = ibuf(6) /= 0
        g%mu = dbuf(1:2)
        g%sum_integral = dbuf(3)
        g%sum_weights = dbuf(4)
        g%sum_chi2 = dbuf(5)
        g%calls = dbuf(6)
        g%dv2g = dbuf(7)
        g%jacobi = dbuf(8)

```

```

g%f_min = dbuf(9)
g%f_max = dbuf(10)
g%mu_gi = dbuf(11)
g%sum_mu_gi = dbuf(12)
call copy_array_pointer (g%num_div, ibuf(7:6+ndim))
<Insure that size (g%div) == ndim 148a>
iidx = 7 + ndim
didx = 13
do i = 1, ndim
  iwords = ibuf(iidx)
  dwords = ibuf(iidx+1)
  iidx = iidx + 2
  call unmarshal_division (g%div(i), ibuf(iidx:iidx-1+iwords), &
                           dbuf(didx:didx-1+dwords))

  iidx = iidx + iwords
  didx = didx + dwords
end do
if (ibuf(iidx) > 0) then
  call copy_array_pointer &
    (g%map, reshape (dbuf(didx:didx-1+ibuf(iidx)), (/ ndim, ndim /)))
  didx = didx + ibuf(iidx)
else
  <Insure that associated (g%map) == .false. 148b>
end if
iidx = iidx + 1
if (ibuf(iidx) > 0) then
  call copy_array_pointer (g%mu_x, dbuf(didx:didx-1+ndim))
  didx = didx + ndim
  call copy_array_pointer (g%sum_mu_x, dbuf(didx:didx-1+ndim))
  didx = didx + ndim
  call copy_array_pointer &
    (g%mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
  didx = didx + ndim**2
  call copy_array_pointer &
    (g%sum_mu_xx, reshape (dbuf(didx:didx-1+ndim**2), (/ ndim, ndim /)))
  didx = didx + ndim**2
else
  <Insure that associated (g%mu_x) == .false. 148c>
end if
iidx = iidx + 1
end subroutine vamp_unmarshal_grid

```

161 <Declaration of vamp procedures 77a>+≡ (75b) <158a
public :: vamp_marshal_history_size, vamp_marshal_history

```

public :: vamp_unmarshal_history

162a <Implementation of vamp procedures 78b>+≡ (75b) <160b 162b>
pure subroutine vamp_marshall_history (h, ibuf, dbuf)
  type(vamp_history), intent(in) :: h
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=default), dimension(:), intent(inout) :: dbuf
  integer :: j, ndim, iidx, didx, iwords, dwords
  if (h%verbose .and. (associated (h%div))) then
    ndim = size (h%div)
  else
    ndim = 0
  end if
  ibuf(1) = ndim
  ibuf(2) = h%calls
  if (h%stratified) then
    ibuf(3) = 1
  else
    ibuf(3) = 0
  end if
  dbuf(1) = h%integral
  dbuf(2) = h%std_dev
  dbuf(3) = h%avg_integral
  dbuf(4) = h%avg_std_dev
  dbuf(5) = h%avg_chi2
  dbuf(6) = h%f_min
  dbuf(7) = h%f_max
  iidx = 4
  didx = 8
  do j = 1, ndim
    call marshal_div_history_size (h%div(j), iwords, dwords)
    ibuf(iidx) = iwords
    ibuf(iidx+1) = dwords
    iidx = iidx + 2
    call marshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                             dbuf(didx:didx-1+dwords))

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

162b <Implementation of vamp procedures 78b>+≡ (75b) <162a 163>
pure subroutine vamp_marshall_history_size (h, iwords, dwords)
  type(vamp_history), intent(in) :: h
  integer, intent(out) :: iwords, dwords

```

```

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

```

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

```

pure subroutine vamp_unmarshal_history (h, ibuf, dbuf)
type(vamp_history), intent(inout) :: h
integer, dimension(:), intent(in) :: ibuf
real(kind=default), dimension(:), intent(in) :: dbuf
integer :: j, ndim, iidx, didx, iwords, dwords
ndim = ibuf(1)
h%calls = ibuf(2)
h%stratified = ibuf(3) /= 0
h%integral = dbuf(1)
h%std_dev = dbuf(2)
h%avg_integral = dbuf(3)
h%avg_std_dev = dbuf(4)
h%avg_chi2 = dbuf(5)
h%f_min = dbuf(6)
h%f_max = dbuf(7)
if (ndim > 0) then
    if (associated (h%div)) then
        if (size (h%div) /= ndim) then
            deallocate (h%div)
            allocate (h%div(ndim))
        end if
    else
        allocate (h%div(ndim))
    end if
    iidx = 4
    didx = 8
    do j = 1, ndim
        iwords = ibuf(iidx)

```

```

        dwords = ibuf(iidx+1)
        iidx = iidx + 2
        call unmarshal_div_history (h%div(j), ibuf(iidx:iidx-1+iwords), &
                                   dbuf(didx:didx-1+dwords))

        iidx = iidx + iwords
        didx = didx + dwords
    end do
end if
end subroutine vamp_unmarshal_history

```

5.2.13 Boring Copying and Deleting of Objects

164 \langle Implementation of `vamp` procedures 78b $\rangle + \equiv$ (75b) \langle 163 165a \rangle

```

elemental subroutine vamp_copy_grid (lhs, rhs)
    type(vamp_grid), intent(inout) :: lhs
    type(vamp_grid), intent(in) :: rhs
    integer :: ndim
    ndim = size (rhs%div)
    lhs%mu = rhs%mu
    lhs%mu_plus = rhs%mu_plus
    lhs%mu_minus = rhs%mu_minus
    lhs%sum_integral = rhs%sum_integral
    lhs%sum_weights = rhs%sum_weights
    lhs%sum_chi2 = rhs%sum_chi2
    lhs%calls = rhs%calls
    lhs%num_calls = rhs%num_calls
    call copy_array_pointer (lhs%num_div, rhs%num_div)
    lhs%dv2g = rhs%dv2g
    lhs%jacobi = rhs%jacobi
    lhs%f_min = rhs%f_min
    lhs%f_max = rhs%f_max
    lhs%mu_gi = rhs%mu_gi
    lhs%sum_mu_gi = rhs%sum_mu_gi
    lhs%calls_per_cell = rhs%calls_per_cell
    lhs%stratified = rhs%stratified
    lhs%all_stratified = rhs%all_stratified
    lhs%quadrupole = rhs%quadrupole
    if (associated (lhs%div)) then
        if (size (lhs%div) /= ndim) then
            call delete_division (lhs%div)
            deallocate (lhs%div)
            allocate (lhs%div(ndim))
        end if
    end if

```

```

else
    allocate (lhs%div(ndim))
end if
call copy_division (lhs%div, rhs%div)
if (associated (rhs%map)) then
    call copy_array_pointer (lhs%map, rhs%map)
else if (associated (lhs%map)) then
    deallocate (lhs%map)
end if
if (associated (rhs%mu_x)) then
    call copy_array_pointer (lhs%mu_x, rhs%mu_x)
    call copy_array_pointer (lhs%mu_xx, rhs%mu_xx)
    call copy_array_pointer (lhs%sum_mu_x, rhs%sum_mu_x)
    call copy_array_pointer (lhs%sum_mu_xx, rhs%sum_mu_xx)
else if (associated (lhs%mu_x)) then
    deallocate (lhs%mu_x, lhs%mu_xx, lhs%sum_mu_x, lhs%sum_mu_xx)
end if
end subroutine vamp_copy_grid

```

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

```

elemental subroutine vamp_delete_grid (g)
    type(vamp_grid), intent(inout) :: g
    if (associated (g%div)) then
        call delete_division (g%div)
        deallocate (g%div, g%num_div)
    end if
    if (associated (g%map)) then
        deallocate (g%map)
    end if
    if (associated (g%mu_x)) then
        deallocate (g%mu_x, g%mu_xx, g%sum_mu_x, g%sum_mu_xx)
    end if
end subroutine vamp_delete_grid

```

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

```

elemental subroutine vamp_copy_grids (lhs, rhs)
    type(vamp_grids), intent(inout) :: lhs
    type(vamp_grids), intent(in) :: rhs
    integer :: nch
    nch = size (rhs%grids)
    lhs%sum_integral = rhs%sum_integral
    lhs%sum_chi2 = rhs%sum_chi2
    lhs%sum_weights = rhs%sum_weights
    if (associated (lhs%grids)) then

```

```

        if (size (lhs%grids) /= nch) then
            deallocate (lhs%grids)
            allocate (lhs%grids(nch))
            call vamp_create_empty_grid (lhs%grids(nch))
        end if
    else
        allocate (lhs%grids(nch))
        call vamp_create_empty_grid (lhs%grids(nch))
    end if
    call vamp_copy_grid (lhs%grids, rhs%grids)
    call copy_array_pointer (lhs%weights, rhs%weights)
    call copy_array_pointer (lhs%num_calls, rhs%num_calls)
end subroutine vamp_copy_grids

```

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

```

    elemental subroutine vamp_delete_grids (g)
        type(vamp_grids), intent(inout) :: g
        if (associated (g%grids)) then
            call vamp_delete_grid (g%grids)
            deallocate (g%weights, g%grids, g%num_calls)
        end if
    end subroutine vamp_delete_grids

```

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

```

    elemental subroutine vamp_copy_history (lhs, rhs)
        type(vamp_history), intent(inout) :: lhs
        type(vamp_history), intent(in) :: rhs
        lhs%calls = rhs%calls
        lhs%stratified = rhs%stratified
        lhs%verbose = rhs%verbose
        lhs%integral = rhs%integral
        lhs%std_dev = rhs%std_dev
        lhs%avg_integral = rhs%avg_integral
        lhs%avg_std_dev = rhs%avg_std_dev
        lhs%avg_chi2 = rhs%avg_chi2
        lhs%f_min = rhs%f_min
        lhs%f_max = rhs%f_max
        if (rhs%verbose) then
            if (associated (lhs%div)) then
                if (size (lhs%div) /= size (rhs%div)) then
                    deallocate (lhs%div)
                    allocate (lhs%div(size(rhs%div)))
                end if
            else
                allocate (lhs%div(size(rhs%div)))
            end if
        end if
    end subroutine vamp_copy_history

```

```

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

```

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

```

    elemental subroutine vamp_delete_history (h)
        type(vamp_history), intent(inout) :: h
        if (associated (h%div)) then
            deallocate (h%div)
        end if
    end subroutine vamp_delete_history

```

5.3 Interface to MPI

The module **vamp** makes no specific assumptions about the hardware and software supporting parallel execution. In this section, we present a specific example of a parallel implementation of multi channel sampling using the message passing paradigm.

The modules **vamp_serial_mpi** and **vamp_parallel_mpi** are not intended to be used directly by application programs. For this purpose, the module **vampi** is provided. **vamp_serial_mpi** is identical to **vamp**, but some types, procedures and variables are renamed so that **vamp_parallel_mpi** can redefine them:

167b \langle vampi.f90 167b $\rangle \equiv$ 167c \triangleright

```

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

```

vamp_parallel_mpi contains the non trivial MPI code and will be discussed in detail below.

167c \langle vampi.f90 167b $\rangle + \equiv$ \triangleleft 167b 168a \triangleright

```

module vamp_parallel_mpi
    use kinds
    use utils

```



```

use tao_random_numbers
use exceptions
use mpi90
use divisions
use vamp_serial_mpi !NODEP!
use iso_fortran_env
implicit none
private
<Declaration of vampi procedures 168b>
<Interfaces of vampi procedures 173a>
<Parameters in vampi 169b>
<Declaration of vampi types 173d>
character(len=*), public, parameter :: VAMPI_RCS_ID = &
    "$Id: vampi.nw 314 2010-04-17 20:32:33Z ohl $"
contains
    <Implementation of vampi procedures 169a>
end module vamp_parallel_mpi

```

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

```

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

```

5.3.1 Parallel Execution

Single Channel

```

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

168c <vamp0.* => vamp.* 168c>≡ (167b) 172c>
    vamp0_create_grid => vamp_create_grid, &
    vamp0_discard_integral => vamp_discard_integral, &
    vamp0_reshape_grid => vamp_reshape_grid, &
    vamp0_sample_grid => vamp_sample_grid, &

```

```

vamp0_delete_grid => vamp_delete_grid, &
169a  <Implementation of vampi procedures 169a>≡ (167c) 169c>
subroutine vamp_create_grid &
  (g, domain, num_calls, num_div, &
   stratified, quadrupole, covariance, map, exc)
type(vamp_grid), intent(inout) :: g
real(kind=default), dimension(:,:), intent(in) :: domain
integer, intent(in) :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
real(kind=default), dimension(:,:), intent(in), optional :: map
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
  call vamp0_create_grid &
    (g, domain, num_calls, num_div, &
     stratified, quadrupole, covariance, map, exc)
else
  call vamp_create_empty_grid (g)
end if
end subroutine vamp_create_grid
169b  <Parameters in vampi 169b>≡ (167c) 177a>
integer, public, parameter :: VAMP_ROOT = 0
169c  <Implementation of vampi procedures 169a>+≡ (167c) <169a 169d>
subroutine vamp_discard_integral &
  (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
  call vamp0_discard_integral &
    (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
end if
end subroutine vamp_discard_integral
169d  <Implementation of vampi procedures 169a>+≡ (167c) <169c 170>
subroutine vamp_reshape_grid &
  (g, num_calls, num_div, stratified, quadrupole, covariance, exc)

```

```

type(vamp_grid), intent(inout) :: g
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole, covariance
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_reshape_grid &
        (g, num_calls, num_div, stratified, quadrupole, covariance, exc)
end if
end subroutine vamp_reshape_grid

```

NB: grids has to have intent(inout) because we will call vamp_broadcast_grid on it.

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

```

subroutine vamp_sample_grid &
    (rng, g, func, iterations, integral, std_dev, avg_chi2, accuracy, &
    channel, weights, grids, exc, history)
type(tao_random_state), intent(inout) :: rng
type(vamp_grid), intent(inout) :: g
integer, intent(in) :: iterations
real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
real(kind=default), intent(in), optional :: accuracy
integer, intent(in), optional :: channel
real(kind=default), dimension(:), intent(in), optional :: weights
type(vamp_grid), dimension(:), intent(inout), optional :: grids
type(exception), intent(inout), optional :: exc
type(vamp_history), dimension(:), intent(inout), optional :: history
<Interface declaration for func 22>
character(len=*), parameter :: FN = "vamp_sample_grid"
real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
type(vamp_grid), dimension(:), allocatable :: gs, gx
integer, dimension(:,:), pointer :: d
integer :: iteration, i
integer :: num_proc, proc_id, num_workers
nullify (d)
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
iterate: do iteration = 1, iterations
    if (proc_id == VAMP_ROOT) then
        call vamp_distribute_work (num_proc, vamp_rigid_divisions (g), d)
        num_workers = max (1, product (d(2,:)))
    end if
end if

```

```

call mpi90_broadcast (num_workers, VAMP_ROOT)
if ((present (grids)) .and. (num_workers > 1)) then
    call vamp_broadcast_grid (grids, VAMP_ROOT)
end if
if (proc_id == VAMP_ROOT) then
    allocate (gs(num_workers), gx(vamp_fork_grid_joints (d)))
    call vamp_create_empty_grid (gs)
    call vamp_fork_grid (g, gs, gx, d, exc)
    do i = 2, num_workers
        call vamp_send_grid (gs(i), i-1, 0)
    end do
else if (proc_id < num_workers) then
    call vamp_receive_grid (g, VAMP_ROOT, 0)
end if
if (proc_id == VAMP_ROOT) then
    if (num_workers > 1) then
        call vamp_sample_grid0 &
            (rng, gs(1), func, channel, weights, grids, exc)
    else
        call vamp_sample_grid0 &
            (rng, g, func, channel, weights, grids, exc)
    end if
else if (proc_id < num_workers) then
    call vamp_sample_grid0 &
        (rng, g, func, channel, weights, grids, exc)
end if
if (proc_id == VAMP_ROOT) then
    do i = 2, num_workers
        call vamp_receive_grid (gs(i), i-1, 0)
    end do
    call vamp_join_grid (g, gs, gx, d, exc)
    call vamp0_delete_grid (gs)
    deallocate (gs, gx)
    call vamp_refine_grid (g)
    call vamp_average_iterations &
        (g, iteration, local_integral, local_std_dev, local_avg_chi2)
    if (present (history)) then
        if (iteration <= size (history)) then
            call vamp_get_history &
                (history(iteration), g, &
                    local_integral, local_std_dev, local_avg_chi2)
        else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
        end if
    end if
end if

```

```

        end if
        call vamp_terminate_history (history(iteration+1:))
    end if
    if (present (accuracy)) then
        if (local_std_dev <= accuracy * local_integral) then
            call raise_exception (exc, EXC_INFO, FN, &
                "requested accuracy reached")
            exit iterate
        end if
    end if
    else if (proc_id < num_workers) then
        call vamp_send_grid (g, VAMP_ROOT, 0)
    end if
end do iterate
if (proc_id == VAMP_ROOT) then
    deallocate (d)
    if (present (integral)) then
        integral = local_integral
    end if
    if (present (std_dev)) then
        std_dev = local_std_dev
    end if
    if (present (avg_chi2)) then
        avg_chi2 = local_avg_chi2
    end if
end if
end subroutine vamp_sample_grid
172a <Implementation of vampi procedures 169a>+≡ (167c) <170 173b>
subroutine vamp_delete_grid (g)
    type(vamp_grid), intent(inout) :: g
    integer :: proc_id
    call mpi90_rank (proc_id)
    if (proc_id == VAMP_ROOT) then
        call vamp0_reshape_grid (g)
    end if
end subroutine vamp_delete_grid
172b <Declaration of vampi procedures 168b>+≡ (167c) <168b 173f>
public :: vamp_print_history
private :: vamp_print_one_history, vamp_print_histories
172c <vamp0.* => vamp.* 168c>+≡ (167b) <168c 173e>
vamp0_print_history => vamp_print_history, &

```

173a \langle Interfaces of `vampi` procedures 173a $\rangle \equiv$ (167c) 182c \triangleright

```

interface vamp_print_history
  module procedure vamp_print_one_history, vamp_print_histories
end interface

```

173b \langle Implementation of `vampi` procedures 169a $\rangle + \equiv$ (167c) \triangleleft 172a 173c \triangleright

```

subroutine vamp_print_one_history (h, tag)
  type(vamp_history), dimension(:), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_print_history (h, tag)
  end if
end subroutine vamp_print_one_history

```

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

```

subroutine vamp_print_histories (h, tag)
  type(vamp_history), dimension(:, :), intent(in) :: h
  character(len=*), intent(in), optional :: tag
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_print_history (h, tag)
  end if
end subroutine vamp_print_histories

```

Multi Channel

173d \langle Declaration of `vampi` types 173d $\rangle \equiv$ (167c)

```

type, public :: vamp_grids
  !!! private
  type(vamp0_grids) :: g0
  logical, dimension(:), pointer :: active
  integer, dimension(:), pointer :: proc
  real(kind=default), dimension(:), pointer :: integrals, std_devs
end type vamp_grids

```

173e \langle vamp0.* => vamp.* 168c $\rangle + \equiv$ (167b) \triangleleft 172c 174a \triangleright
 vamp0_grids => vamp_grids, &
 Partially duplicate the API of `vamp`:

173f \langle Declaration of `vampi` procedures 168b $\rangle + \equiv$ (167c) \triangleleft 172b 179c \triangleright

```

public :: vamp_create_grids
public :: vamp_discard_integrals

```

```

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

```

174a $\langle \text{vamp0_} * \Rightarrow \text{vamp_} * \text{ 168c} \rangle + \equiv$ (167b) $\langle \text{173e 182b} \rangle$

```

vamp0_create_grids => vamp_create_grids, &
vamp0_discard_integrals => vamp_discard_integrals, &
vamp0_update_weights => vamp_update_weights, &
vamp0_refine_weights => vamp_refine_weights, &
vamp0_delete_grids => vamp_delete_grids, &
vamp0_sample_grids => vamp_sample_grids, &

```

Call **vamp_create_grids** just like the serial version. It will create the actual grids on the root processor and create stubs on the other processors

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

```

subroutine vamp_create_grids (g, domain, num_calls, weights, maps, &
                             num_div, stratified, quadrupole, exc)
    type(vamp_grids), intent(inout) :: g
    real(kind=default), dimension(:, :), intent(in) :: domain
    integer, intent(in) :: num_calls
    real(kind=default), dimension(:), intent(in) :: weights
    real(kind=default), dimension(:, :, :), intent(in), optional :: maps
    integer, dimension(:), intent(in), optional :: num_div
    logical, intent(in), optional :: stratified, quadrupole
    type(exception), intent(inout), optional :: exc
    integer :: proc_id, nch
    call mpi90_rank (proc_id)
    nch = size (weights)
    allocate (g%active(nch), g%proc(nch), g%integrals(nch), g%std_devs(nch))
    if (proc_id == VAMP_ROOT) then
        call vamp0_create_grids (g%g0, domain, num_calls, weights, maps, &
                                num_div, stratified, quadrupole, exc)
    else
        allocate (g%g0%grids(nch), g%g0%weights(nch), g%g0%num_calls(nch))
        call vamp_create_empty_grid (g%g0%grids)
    end if
end subroutine vamp_create_grids

```

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

```

subroutine vamp_discard_integrals &
    (g, num_calls, num_div, stratified, quadrupole, exc)
    type(vamp_grids), intent(inout) :: g
    integer, intent(in), optional :: num_calls
    integer, dimension(:), intent(in), optional :: num_div

```

```

logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_discard_integrals &
        (g%g0, num_calls, num_div, stratified, quadrupole, exc)
end if
end subroutine vamp_discard_integrals
175a <Implementation of vampi procedures 169a>+≡ (167c) <174c 175b>
subroutine vamp_update_weights &
    (g, weights, num_calls, num_div, stratified, quadrupole, exc)
type(vamp_grids), intent(inout) :: g
real(kind=default), dimension(:), intent(in) :: weights
integer, intent(in), optional :: num_calls
integer, dimension(:), intent(in), optional :: num_div
logical, intent(in), optional :: stratified, quadrupole
type(exception), intent(inout), optional :: exc
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_update_weights &
        (g%g0, weights, num_calls, num_div, stratified, quadrupole, exc)
end if
end subroutine vamp_update_weights
175b <Implementation of vampi procedures 169a>+≡ (167c) <175a 175c>
subroutine vamp_refine_weights (g, power)
type(vamp_grids), intent(inout) :: g
real(kind=default), intent(in), optional :: power
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_refine_weights (g%g0, power)
end if
end subroutine vamp_refine_weights
175c <Implementation of vampi procedures 169a>+≡ (167c) <175b 176>
subroutine vamp_delete_grids (g)
type(vamp_grids), intent(inout) :: g
character(len=*), parameter :: FN = "vamp_delete_grids"
deallocate (g%active, g%proc, g%integrals, g%std_devs)
call vamp0_delete_grids (g%g0)
end subroutine vamp_delete_grids

```


Call `vamp_sample_grids` just like `vamp0_sample_grids`.

```

176 <Implementation of vampi procedures 169a>+≡ (167c) <175c 179d>
  subroutine vamp_sample_grids &
    (rng, g, func, iterations, integral, std_dev, avg_chi2, &
     accuracy, history, histories, exc)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: iterations
    real(kind=default), intent(out), optional :: integral, std_dev, avg_chi2
    real(kind=default), intent(in), optional :: accuracy
    type(vamp_history), dimension(:), intent(inout), optional :: history
    type(vamp_history), dimension(:, :), intent(inout), optional :: histories
    type(exception), intent(inout), optional :: exc
    <Interface declaration for func 22>
    character(len=*), parameter :: FN = "vamp_sample_grids"
    integer :: num_proc, proc_id, nch, ch, iteration
    real(kind=default), dimension(size(g%g0%weights)) :: weights
    real(kind=default) :: local_integral, local_std_dev, local_avg_chi2
    real(kind=default) :: current_accuracy, waste
    logical :: distribute_complete_grids
    call mpi90_size (num_proc)
    call mpi90_rank (proc_id)
    nch = size (g%g0%weights)
    if (proc_id == VAMP_ROOT) then
      g%active = (g%g0%num_calls >= 2)
      where (g%active)
        weights = g%g0%num_calls
      elsewhere
        weights = 0.0
      endwhere
      weights = weights / sum (weights)
      call schedule (weights, num_proc, g%proc, waste)
      distribute_complete_grids = (waste <= VAMP_MAX_WASTE)
    end if
    call mpi90_broadcast (weights, VAMP_ROOT)
    call mpi90_broadcast (g%active, VAMP_ROOT)
    call mpi90_broadcast (distribute_complete_grids, VAMP_ROOT)
    if (distribute_complete_grids) then
      call mpi90_broadcast (g%proc, VAMP_ROOT)
    end if
    iterate: do iteration = 1, iterations
      if (distribute_complete_grids) then
        call vamp_broadcast_grid (g%g0%grids, VAMP_ROOT)

```

```

        <Distribute complete grids among processes 177b>
    else
        <Distribute each grid among processes 181b>
    end if
    <Exit iterate if accuracy has been reached (MPI) 180a>
end do iterate
<Copy results of vamp_sample_grids to dummy variables 179f>
end subroutine vamp_sample_grids

```

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

```

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

177b <Distribute complete grids among processes 177b>≡ (176) 177c>
    do ch = 1, nch
        if (g%active(ch)) then
            if (proc_id == g%proc(ch)) then
                call vamp0_discard_integral (g%g0%grids(ch))
                <Sample g%g0%grids(ch) 177d>
            end if
        else
            call vamp_nullify_variance (g%g0%grids(ch))
            call vamp_nullify_covariance (g%g0%grids(ch))
        end if
    end do

```

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

```

177c <Distribute complete grids among processes 177b>+≡ (176) <177b 178a>
    do ch = 1, nch
        if (g%active(ch) .and. (proc_id == g%proc(ch))) then
            call vamp_refine_grid (g%g0%grids(ch))
            if (proc_id /= VAMP_ROOT) then
                <Ship the result for channel #ch back to the root 179a>
            end if
        end if
    end do

```

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

```

177d <Sample g%g0%grids(ch) 177d>≡ (177b)
    call vamp_sample_grid0 &
        (rng, g%g0%grids(ch), func, ch, weights, g%g0%grids, exc)
    call vamp_average_iterations &
        (g%g0%grids(ch), iteration, g%integrals(ch), g%std_devs(ch), local_avg_chi2)

```

```

if (present (histories)) then
  if (iteration <= ubound (histories, dim=1)) then
    call vamp_get_history &
      (histories(iteration,ch), g%g0%grids(ch), &
        g%integrals(ch), g%std_devs(ch), local_avg_chi2)
  else
    call raise_exception (exc, EXC_WARN, FN, "history too short")
  end if
  call vamp_terminate_history (histories(iteration+1:,ch))
end if

178a <Distribute complete grids among processes 177b>+≡ (176) <177c
if (proc_id == VAMP_ROOT) then
  do ch = 1, nch
    if (g%active(ch) .and. (g%proc(ch) /= proc_id)) then
      <Receive the result for channel #ch at the root 179b>
    end if
  end do
  call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
  call vamp_average_iterations &
    (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
  if (present (history)) then
    if (iteration <= size (history)) then
      call vamp_get_history &
        (history(iteration), g%g0, local_integral, local_std_dev, &
          local_avg_chi2)
    else
      call raise_exception (exc, EXC_WARN, FN, "history too short")
    end if
    call vamp_terminate_history (history(iteration+1:))
  end if
end if

```

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

```

178b <Ship g%g0%grids from the root to the assigned processor 178b>≡
do ch = 1, nch
  if (g%active(ch) .and. (g%proc(ch) /= VAMP_ROOT)) then
    if (proc_id == VAMP_ROOT) then
      call vamp_send_grid &
        (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
    else if (proc_id == g%proc(ch)) then
      call vamp_receive_grid &
        (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
    end if
  end if
end do

```

```

        end if
    end if
end do

179a  <Ship the result for channel #ch back to the root 179a>≡ (177c)
    call mpi90_send (g%integrals(ch), VAMP_ROOT, object (ch, TAG_INTEGRAL))
    call mpi90_send (g%std_devs(ch), VAMP_ROOT, object (ch, TAG_STD_DEV))
    call vamp_send_grid (g%g0%grids(ch), VAMP_ROOT, object (ch, TAG_GRID))
    if (present (histories)) then
        call vamp_send_history &
            (histories(iteration,ch), VAMP_ROOT, object (ch, TAG_HISTORY))
    end if

179b  <Receive the result for channel #ch at the root 179b>≡ (178a)
    call mpi90_receive (g%integrals(ch), g%proc(ch), object (ch, TAG_INTEGRAL))
    call mpi90_receive (g%std_devs(ch), g%proc(ch), object (ch, TAG_STD_DEV))
    call vamp_receive_grid (g%g0%grids(ch), g%proc(ch), object (ch, TAG_GRID))
    if (present (histories)) then
        call vamp_receive_history &
            (histories(iteration,ch), g%proc(ch), object (ch, TAG_HISTORY))
    end if

179c  <Declaration of vampi procedures 168b>+≡ (167c) <173f 180b>
    private :: object

179d  <Implementation of vampi procedures 169a>+≡ (167c) <176 180c>
    pure function object (ch, obj) result (tag)
        integer, intent(in) :: ch, obj
        integer :: tag
        tag = 100 * ch + obj
    end function object

179e  <Parameters in vampi 169b>+≡ (167c) <177a
    integer, public, parameter :: &
        TAG_INTEGRAL = 1, &
        TAG_STD_DEV = 2, &
        TAG_GRID = 3, &
        TAG_HISTORY = 6, &
        TAG_NEXT_FREE = 9

179f  <Copy results of vamp_sample_grids to dummy variables 179f>≡ (176)
    if (present (integral)) then
        call mpi90_broadcast (local_integral, VAMP_ROOT)
        integral = local_integral
    end if
    if (present (std_dev)) then
        call mpi90_broadcast (local_std_dev, VAMP_ROOT)

```

```

        std_dev = local_std_dev
    end if
    if (present (avg_chi2)) then
        call mpi90_broadcast (local_avg_chi2, VAMP_ROOT)
        avg_chi2 = local_avg_chi2
    end if

```

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

```

    if (present (accuracy)) then
        if (proc_id == VAMP_ROOT) then
            current_accuracy = local_std_dev / local_integral
        end if
        call mpi90_broadcast (current_accuracy, VAMP_ROOT)
        if (current_accuracy <= accuracy) then
            call raise_exception (exc, EXC_INFO, FN, &
                "requested accuracy reached")
            exit iterate
        end if
    end if

```

A very simple minded scheduler: maximizes processor utilization and, does not pay attention to communication costs.

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

We disfavor the root process a little bit (by starting up with a fake filling ratio of 10%) so that it is likely to be ready to answer all communication requests.

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

```

    pure subroutine schedule (jobs, num_procs, assign, waste)
        real(kind=default), dimension(:), intent(in) :: jobs
        integer, intent(in) :: num_procs
        integer, dimension(:), intent(out) :: assign
        real(kind=default), intent(out), optional :: waste
        integer, dimension(size(jobs)) :: idx
        real(kind=default), dimension(size(jobs)) :: sjobs
        real(kind=default), dimension(num_procs) :: fill
        integer :: job, proc
        sjobs = jobs / sum (jobs) * num_procs
        idx = (/ (job, job = 1, size(jobs)) /)
        call sort (sjobs, idx, reverse = .true.)
        fill = 0.0
        fill(VAMP_ROOT+1) = 0.1
        do job = 1, size (sjobs)
            proc = sum (minloc (fill))

```

```

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

```

Assuming equivalent processors and uniform computation costs, the waste is given by the fraction of the time that it spent by the other processors waiting for the processor with the biggest assignment:

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

```

    if (present (waste)) then
        waste = 1.0 - sum (fill) / (num_procs * maxval (fill))
    end if

```

Accordingly, if the waste caused by distributing only complete grids, we switch to splitting the grids, just like in single channel sampling. This is *not* the default, because the communication costs are measurably higher for many grids and many processors.



This version is broken!

181b *<Distribute each grid among processes 181b>*≡ (176)

```

    do ch = 1, size (g%g0%grids)
        if (g%active(ch)) then
            call vamp_discard_integral (g%g0%grids(ch))
            if (present (histories)) then
                call vamp_sample_grid &
                    (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
                     channel = ch, weights = weights, grids = g%g0%grids, &
                     history = histories(iteration:iteration,ch))
            else
                call vamp_sample_grid &
                    (rng, g%g0%grids(ch), func, 1, g%integrals(ch), g%std_devs(ch), &
                     channel = ch, weights = weights, grids = g%g0%grids)
            end if
        else
            if (proc_id == VAMP_ROOT) then
                call vamp_nullify_variance (g%g0%grids(ch))
                call vamp_nullify_covariance (g%g0%grids(ch))
            end if
        end if
    end do
    if (proc_id == VAMP_ROOT) then
        call vamp_reduce_channels (g%g0, g%integrals, g%std_devs, g%active)
        call vamp_average_iterations &

```

```

        (g%g0, iteration, local_integral, local_std_dev, local_avg_chi2)
    if (present (history)) then
        if (iteration <= size (history)) then
            call vamp_get_history &
                (history(iteration), g%g0, local_integral, local_std_dev, &
                 local_avg_chi2)
        else
            call raise_exception (exc, EXC_WARN, FN, "history too short")
        end if
        call vamp_terminate_history (history(iteration+1:))
    end if
end if

```

5.3.2 Event Generation

This is currently only a syntactical translation ...

- 182a *<Declaration of vampi procedures 168b>+≡* (167c) <180b 184a>
 public :: vamp_warmup_grid
 public :: vamp_warmup_grids
 public :: vamp_next_event
 private :: vamp_next_event_single, vamp_next_event_multi
- 182b *<vamp0.* => vamp.* 168c>+≡* (167b) <174a 184b>
 vamp0_warmup_grid => vamp_warmup_grid, &
 vamp0_warmup_grids => vamp_warmup_grids, &
 vamp0_next_event => vamp_next_event, &
- 182c *<Interfaces of vampi procedures 173a>+≡* (167c) <173a 184c>
 interface vamp_next_event
 module procedure vamp_next_event_single, vamp_next_event_multi
 end interface
- 182d *<Implementation of vampi procedures 169a>+≡* (167c) <180c 183a>
 subroutine vamp_next_event_single &
 (x, rng, g, func, weight, channel, weights, grids, exc)
 real(kind=default), dimension(:), intent(out) :: x
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid), intent(inout) :: g
 real(kind=default), intent(out), optional :: weight
 integer, intent(in), optional :: channel
 real(kind=default), dimension(:), intent(in), optional :: weights
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>

```

integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_next_event &
        (x, rng, g, func, weight, channel, weights, grids, exc)
end if
end subroutine vamp_next_event_single
183a <Implementation of vampi procedures 169a>+≡ (167c) <182d 183b>
subroutine vamp_next_event_multi (x, rng, g, func, phi, weight, exc)
    real(kind=default), dimension(:), intent(out) :: x
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids), intent(inout) :: g
    real(kind=default), intent(out), optional :: weight
    type(exception), intent(inout), optional :: exc
    <Interface declaration for func 22>
    <Interface declaration for phi 31a>
    integer :: proc_id
    call mpi90_rank (proc_id)
    if (proc_id == VAMP_ROOT) then
        call vamp0_next_event (x, rng, g%g0, func, phi, weight, exc)
    end if
end subroutine vamp_next_event_multi
183b <Implementation of vampi procedures 169a>+≡ (167c) <183a 183c>
subroutine vamp_warmup_grid (rng, g, func, iterations, exc, history)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grid), intent(inout) :: g
    integer, intent(in) :: iterations
    type(exception), intent(inout), optional :: exc
    type(vamp_history), dimension(:), intent(inout), optional :: history
    <Interface declaration for func 22>
    call vamp_sample_grid &
        (rng, g, func, iterations - 1, exc = exc, history = history)
    call vamp_sample_grid0 (rng, g, func, exc = exc)
end subroutine vamp_warmup_grid
183c <Implementation of vampi procedures 169a>+≡ (167c) <183b 184d>
subroutine vamp_warmup_grids &
    (rng, g, func, iterations, history, histories, exc)
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids), intent(inout) :: g
    integer, intent(in) :: iterations
    type(vamp_history), dimension(:), intent(inout), optional :: history
    type(vamp_history), dimension(:, :), intent(inout), optional :: histories

```



```

type(exception), intent(inout), optional :: exc
<Interface declaration for func 22>
integer :: ch
call vamp0_sample_grids (rng, g%g0, func, iterations - 1, exc = exc, &
                        history = history, histories = histories)
do ch = 1, size (g%g0%grids)
  ! if (g%g0%grids(ch)%num_calls >= 2) then
    call vamp_sample_grid0 (rng, g%g0%grids(ch), func, exc = exc)
  ! end if
end do
end subroutine vamp_warmup_grids

```

5.3.3 I/O

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

```

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

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

```

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

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

```

interface vamp_write_grid
  module procedure write_grid_unit, write_grid_name
end interface
interface vamp_read_grid
  module procedure read_grid_unit, read_grid_name
end interface

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

```

subroutine write_grid_unit (g, unit)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: unit
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_write_grid (g, unit)
  end if
end subroutine write_grid_unit

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

```

subroutine read_grid_unit (g, unit)
  type(vamp_grid), intent(inout) :: g

```

```

integer, intent(in) :: unit
integer :: proc_id
call mpi90_rank (proc_id)
if (proc_id == VAMP_ROOT) then
    call vamp0_read_grid (g, unit)
end if
end subroutine read_grid_unit
185a <Implementation of vampi procedures 169a>+≡ (167c) <184e 185b>
subroutine write_grid_name (g, name)
    type(vamp_grid), intent(inout) :: g
    character(len=*), intent(in) :: name
    integer :: proc_id
    call mpi90_rank (proc_id)
    if (proc_id == VAMP_ROOT) then
        call vamp0_write_grid (g, name)
    end if
end subroutine write_grid_name
185b <Implementation of vampi procedures 169a>+≡ (167c) <185a 186a>
subroutine read_grid_name (g, name)
    type(vamp_grid), intent(inout) :: g
    character(len=*), intent(in) :: name
    integer :: proc_id
    call mpi90_rank (proc_id)
    if (proc_id == VAMP_ROOT) then
        call vamp0_read_grid (g, name)
    end if
end subroutine read_grid_name
185c <Declaration of vampi procedures 168b>+≡ (167c) <184a 187a>
public :: vamp_write_grids, vamp_read_grids
private :: write_grids_unit, write_grids_name
private :: read_grids_unit, read_grids_name
185d <vamp0.* => vamp.* 168c>+≡ (167b) <184b>
vamp0_write_grids => vamp_write_grids, &
vamp0_read_grids => vamp_read_grids, &
185e <Interfaces of vampi procedures 173a>+≡ (167c) <184c 189a>
interface vamp_write_grids
    module procedure write_grids_unit, write_grids_name
end interface
interface vamp_read_grids
    module procedure read_grids_unit, read_grids_name
end interface

```

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

```

subroutine write_grids_unit (g, unit)
  type(vamp_grids), intent(in) :: g
  integer, intent(in) :: unit
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_write_grids (g%g0, unit)
  end if
end subroutine write_grids_unit

```

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

```

subroutine read_grids_unit (g, unit)
  type(vamp_grids), intent(inout) :: g
  integer, intent(in) :: unit
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_read_grids (g%g0, unit)
  end if
end subroutine read_grids_unit

```

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

```

subroutine write_grids_name (g, name)
  type(vamp_grids), intent(inout) :: g
  character(len=*), intent(in) :: name
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_write_grids (g%g0, name)
  end if
end subroutine write_grids_name

```

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

```

subroutine read_grids_name (g, name)
  type(vamp_grids), intent(inout) :: g
  character(len=*), intent(in) :: name
  integer :: proc_id
  call mpi90_rank (proc_id)
  if (proc_id == VAMP_ROOT) then
    call vamp0_read_grids (g%g0, name)
  end if

```

```
end subroutine read_grids_name
```

5.3.4 Communicating Grids

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

```
public :: vamp_send_grid
public :: vamp_receive_grid
public :: vamp_broadcast_grid
public :: vamp_broadcast_grids
```



The next two are still kludged. Nicer implementations with one message less per call below, but MPICH does funny things during `mpi_get_count`, which is called by `mpi90_receive_pointer`.

Caveat: this `vamp_send_grid` uses *three* tags: `tag`, `tag+1` and `tag+2`:

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

```
subroutine vamp_send_grid (g, target, tag, domain, error)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: target, tag
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call vamp_marshall_grid_size (g, words(1), words(2))
  allocate (ibuf(words(1)), dbuf(words(2)))
  call vamp_marshall_grid (g, ibuf, dbuf)
  call mpi90_send (words, target, tag, domain, error)
  call mpi90_send (ibuf, target, tag+1, domain, error)
  call mpi90_send (dbuf, target, tag+2, domain, error)
  deallocate (ibuf, dbuf)
end subroutine vamp_send_grid
```

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

```
subroutine vamp_receive_grid (g, source, tag, domain, status, error)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: source, tag
  integer, intent(in), optional :: domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  integer, dimension(2) :: words
  integer, dimension(:), allocatable :: ibuf
```

```

real(kind=default), dimension(:), allocatable :: dbuf
call mpi90_receive (words, source, tag, domain, status, error)
allocate (ibuf(words(1)), dbuf(words(2)))
call mpi90_receive (ibuf, source, tag+1, domain, status, error)
call mpi90_receive (dbuf, source, tag+2, domain, status, error)
call vamp_unmarshal_grid (g, ibuf, dbuf)
deallocate (ibuf, dbuf)
end subroutine vamp_receive_grid

```


Caveat: the real `vamp_send_grid` uses *two* tags: `tag` and `tag+1`:

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

```

subroutine vamp_send_grid (g, target, tag, domain, error)
  type(vamp_grid), intent(in) :: g
  integer, intent(in) :: target, tag
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: iwords, dwords
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  call vamp_marshall_grid_size (g, iwords, dwords)
  allocate (ibuf(iwords), dbuf(dwords))
  call vamp_marshall_grid (g, ibuf, dbuf)
  call mpi90_send (ibuf, target, tag, domain, error)
  call mpi90_send (dbuf, target, tag+1, domain, error)
  deallocate (ibuf, dbuf)
end subroutine vamp_send_grid

```

 There's something wrong with MPICH: if I call `mpi90_receive_pointer` in the opposite order, the low level call to `mpi_get_count` bombs for no apparent reason!

 There are also funky things going on with tag: `mpi90_receive_pointer` should leave it alone, but ...

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

```

subroutine vamp_receive_grid (g, source, tag, domain, status, error)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: source, tag
  integer, intent(in), optional :: domain
  type(mpi90_status), intent(out), optional :: status
  integer, intent(out), optional :: error
  integer, dimension(:), pointer :: ibuf

```

```

real(kind=default), dimension(:), pointer :: dbuf
nullify (ibuf, dbuf)
call mpi90_receive_pointer (dbuf, source, tag+1, domain, status, error)
call mpi90_receive_pointer (ibuf, source, tag, domain, status, error)
call vamp_unmarshal_grid (g, ibuf, dbuf)
deallocate (ibuf, dbuf)
end subroutine vamp_receive_grid

```

This is not a good idea, with respect to communication costs. For SMP machines, it appears to be negligible however.

189a *<Interfaces of vampi procedures 173a>+≡* (167c) <185e

```

interface vamp_broadcast_grid
  module procedure &
    vamp_broadcast_one_grid, vamp_broadcast_many_grids
end interface

```

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

```

subroutine vamp_broadcast_one_grid (g, root, domain, error)
  type(vamp_grid), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer, dimension(:), allocatable :: ibuf
  real(kind=default), dimension(:), allocatable :: dbuf
  integer :: iwords, dwords, me
  call mpi90_rank (me)
  if (me == root) then
    call vamp_marshal_grid_size (g, iwords, dwords)
  end if
  call mpi90_broadcast (iwords, root, domain, error)
  call mpi90_broadcast (dwords, root, domain, error)
  allocate (ibuf(iwords), dbuf(dwords))
  if (me == root) then
    call vamp_marshal_grid (g, ibuf, dbuf)
  end if
  call mpi90_broadcast (ibuf, root, domain, error)
  call mpi90_broadcast (dbuf, root, domain, error)
  if (me /= root) then
    call vamp_unmarshal_grid (g, ibuf, dbuf)
  end if
  deallocate (ibuf, dbuf)
end subroutine vamp_broadcast_one_grid

```

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

```

subroutine vamp_broadcast_many_grids (g, root, domain, error)
  type(vamp_grid), dimension(:), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: i
  do i = 1, size(g)
    call vamp_broadcast_one_grid (g(i), root, domain, error)
  end do
end subroutine vamp_broadcast_many_grids

```

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

```

subroutine vamp_broadcast_grids (g, root, domain, error)
  type(vamp0_grids), intent(inout) :: g
  integer, intent(in) :: root
  integer, intent(in), optional :: domain
  integer, intent(out), optional :: error
  integer :: nch, me
  call mpi90_broadcast (g%sum_chi2, root, domain, error)
  call mpi90_broadcast (g%sum_integral, root, domain, error)
  call mpi90_broadcast (g%sum_weights, root, domain, error)
  call mpi90_rank (me)
  if (me == root) then
    nch = size (g%grids)
  end if
  call mpi90_broadcast (nch, root, domain, error)
  if (me /= root) then
    if (associated (g%grids)) then
      if (size (g%grids) /= nch) then
        call vamp0_delete_grid (g%grids)
        deallocate (g%grids, g%weights, g%num_calls)
        allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
        call vamp_create_empty_grid (g%grids)
      end if
    else
      allocate (g%grids(nch), g%weights(nch), g%num_calls(nch))
      call vamp_create_empty_grid (g%grids)
    end if
  end if
  call vamp_broadcast_grid (g%grids, root, domain, error)
  call mpi90_broadcast (g%weights, root, domain, error)
  call mpi90_broadcast (g%num_calls, root, domain, error)
end subroutine vamp_broadcast_grids

```

191a *<Declaration of vampi procedures 168b>+≡* (167c) <187a
 public :: vamp_send_history
 public :: vamp_receive_history

191b *<Implementation of vampi procedures 169a>+≡* (167c) <190 191c>
 subroutine vamp_send_history (g, target, tag, domain, error)
 type(vamp_history), intent(in) :: g
 integer, intent(in) :: target, tag
 integer, intent(in), optional :: domain
 integer, intent(out), optional :: error
 integer, dimension(2) :: words
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call vamp_marshall_history_size (g, words(1), words(2))
 allocate (ibuf(words(1)), dbuf(words(2)))
 call vamp_marshall_history (g, ibuf, dbuf)
 call mpi90_send (words, target, tag, domain, error)
 call mpi90_send (ibuf, target, tag+1, domain, error)
 call mpi90_send (dbuf, target, tag+2, domain, error)
 deallocate (ibuf, dbuf)
end subroutine vamp_send_history

191c *<Implementation of vampi procedures 169a>+≡* (167c) <191b
 subroutine vamp_receive_history (g, source, tag, domain, status, error)
 type(vamp_history), intent(inout) :: g
 integer, intent(in) :: source, tag
 integer, intent(in), optional :: domain
 type(mpi90_status), intent(out), optional :: status
 integer, intent(out), optional :: error
 integer, dimension(2) :: words
 integer, dimension(:), allocatable :: ibuf
 real(kind=default), dimension(:), allocatable :: dbuf
 call mpi90_receive (words, source, tag, domain, status, error)
 allocate (ibuf(words(1)), dbuf(words(2)))
 call mpi90_receive (ibuf, source, tag+1, domain, status, error)
 call mpi90_receive (dbuf, source, tag+2, domain, status, error)
 call vamp_unmarshall_history (g, ibuf, dbuf)
 deallocate (ibuf, dbuf)
end subroutine vamp_receive_history

—6—

SELF TEST

6.1 No Mapping Mode

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

6.1.1 Serial Test

```

192a <vamp_test.f90 192a>≡
! vamp_test.f90 --
<Copyleft notice 1>
<Module vamp_test_functions 192b>
<Module vamp_tests 196b>
200c>

192b <Module vamp_test_functions 192b>≡ (192a 202a)
module vamp_test_functions
  use kinds
  use constants, only: PI
  use coordinates
  use vamp, only: vamp_grid, vamp_multi_channel
  use vamp, only: vamp_data_t
  implicit none
  private
  public :: f, j, phi, ihp, w
  public :: lorentzian
  private :: lorentzian_normalized
  real(kind=default), public :: width
contains
  <Implementation of vamp_test_functions procedures 193a>

```

```
end module vamp_test_functions
```

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

193a \langle Implementation of vamp_test_functions procedures 193a $\rangle \equiv$ (192b) 193b \rangle

```
pure function lorentzian_normalized (x, x0, x1, x2, a) result (f)
  real(kind=default), intent(in) :: x, x0, x1, x2, a
  real(kind=default) :: f
  if (x1 <= x .and. x <= x2) then
    f = 1 / ((x - x0)**2 + a**2) &
      * a / (atan2 (x2 - x0, a) - atan2 (x1 - x0, a))
  else
    f = 0
  end if
end function lorentzian_normalized
```

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

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

```
pure function lorentzian (x, x0, x1, x2, r0, a) result (f)
  real(kind=default), dimension(:), intent(in) :: x, x0, x1, x2
  real(kind=default), intent(in) :: r0, a
  real(kind=default) :: f
  real(kind=default) :: r, r1, r2
  integer :: n
  n = size (x)
  if (n > 1) then
    r = sqrt (dot_product (x-x0, x-x0))
    r1 = 0.4_default
    r2 = min (minval (x2-x0), minval (x0-x1))
    if (r1 <= r .and. r <= r2) then
      f = lorentzian_normalized (r, r0, r1, r2, a) * r**(1-n) / surface (n)
    else
      f = 0
    end if
  else
    f = lorentzian_normalized (x(1), x0(1), x1(1), x2(1), a)
  endif
end function lorentzian
```

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

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

```

real(kind=default), dimension(:), intent(in), optional :: weights
integer, intent(in), optional :: channel
type(vamp_grid), dimension(:), intent(in), optional :: grids
real(kind=default) :: f_x
real(kind=default), dimension(size(x)) :: minus_one, plus_one, zero, w_i, f_i
integer :: n, i
n = size(x)
minus_one = -1
zero = 0
plus_one = 1
w_i = 1
do i = 1, n
  if (all (abs (x(i+1:)) <= 1)) then
    f_i = lorentzian (x(1:i), zero(1:i), minus_one(1:i), plus_one(1:i), &
      0.7_default, width) &
      / 2.0_default**(n-i)
  else
    f_i = 0
  end if
end do
f_x = dot_product (w_i, f_i) / sum (w_i)
end function f

```

194 \langle Implementation of vamp_test functions procedures 193a $\rangle + \equiv$ (192b) \langle 193c 195a \rangle

```

pure function phi (xi, channel) result (x)
real(kind=default), dimension(:), intent(in) :: xi
integer, intent(in) :: channel
real(kind=default), dimension(size(xi)) :: x
real(kind=default) :: r
real(kind=default), dimension(0) :: dummy
integer :: n
n = size(x)
if (channel == 1) then
  x = xi
else if (channel == 2) then
  r = (xi(1) + 1) / 2 * sqrt (2.0_default)
  x(1:2) = spherical_cos_to_cartesian (r, PI * xi(2), dummy)
  x(3:) = xi(3:)
else if (channel < n) then
  r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))
  x(1:channel) = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:channel))
  x(channel+1:) = xi(channel+1:)
else if (channel == n) then
  r = (xi(1) + 1) / 2 * sqrt (real (channel, kind=default))

```

```

        x = spherical_cos_to_cartesian (r, PI * xi(2), xi(3:))
    else
        x = 0
    end if
end function phi
195a <Implementation of vamp_test_functions procedures 193a>+≡ (192b) <194 195b>
pure function ihp (x, channel) result (xi)
    real(kind=default), dimension(:), intent(in) :: x
    integer, intent(in) :: channel
    real(kind=default), dimension(size(x)) :: xi
    real(kind=default) :: r, phi
    integer :: n
    n = size(x)
    if (channel == 1) then
        xi = x
    else if (channel == 2) then
        call cartesian_to_spherical_cos (x(1:2), r, phi)
        xi(1) = 2 * r / sqrt (2.0_default) - 1
        xi(2) = phi / PI
        xi(3:) = x(3:)
    else if (channel < n) then
        call cartesian_to_spherical_cos (x(1:channel), r, phi, xi(3:channel))
        xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
        xi(2) = phi / PI
        xi(channel+1:) = x(channel+1:)
    else if (channel == n) then
        call cartesian_to_spherical_cos (x, r, phi, xi(3:))
        xi(1) = 2 * r / sqrt (real (channel, kind=default)) - 1
        xi(2) = phi / PI
    else
        xi = 0
    end if
end function ihp
195b <Implementation of vamp_test_functions procedures 193a>+≡ (192b) <195a 196a>
pure function j (x, data, channel) result (j_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: channel
    real(kind=default) :: j_x
    if (channel == 1) then
        j_x = 1
    else if (channel > 1) then
        j_x = 2 / sqrt (real (channel, kind=default)) ! 1/|dr/dξ1|
    end if
end function j

```

```

        j_x = j_x / PI ! 1/|dφ/dξ2|
        j_x = j_x * cartesian_to_spherical_cos_j (x(1:channel))
    else
        j_x = 0
    end if
end function j

```

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

```

function w (x, data, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    w_x = vamp_multi_channel (f, data, phi, ihp, j, x, weights, channel, grids)
end function w

```

196b \langle Module `vamp_tests` 196b $\rangle \equiv$ (192a)

```

module vamp_tests
    use kinds
    use exceptions
    use histograms
    use tao_random_numbers
    use coordinates
    use vamp
    use vamp_test_functions !NODEP!
    implicit none
    private
     $\langle$ Declaration of procedures in vamp_tests 196c $\rangle$ 
contains
     $\langle$ Implementation of procedures in vamp_tests 197a $\rangle$ 
end module vamp_tests

```

Verification

196c \langle Declaration of procedures in `vamp_tests` 196c $\rangle \equiv$ (196b 202b) 198a \triangleright

```

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

```

196d \langle Implementation of procedures in `vamp_tests` (broken?) 196d $\rangle \equiv$

```

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

```

197a *<Implementation of procedures in vamp_tests 197a>≡ (196b 202b) 197b>*

```

subroutine check_inverses (rng, region, weights, samples)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,,:), intent(in) :: region
    real(kind=default), dimension(:), intent(in) :: weights
    integer, intent(in) :: samples
    real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx
    real(kind=default) :: dx, dx_max
    integer :: ch, i
    dx_max = 0
    x_dx = 0
    do ch = 1, size(weights)
        do i = 1, samples
            call tao_random_number (rng, x1)
            x2 = ihp (phi (x1, ch), ch)
            dx = sqrt (dot_product (x1-x2, x1-x2))
            if (dx > dx_max) then
                dx_max = dx
                x_dx = x1
            end if
        end do
        print *, "channel", ch, ": |x-x|=", real(dx), ", @x=", real (x_dx)
    end do
end subroutine check_inverses

```

197b *<Implementation of procedures in vamp_tests 197a>+≡ (196b 202b) <197a 198b>*

```

subroutine check_inverses3 (rng, region, samples)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,,:), intent(in) :: region
    integer, intent(in) :: samples
    real(kind=default), dimension(size(region,dim=2)) :: x1, x2, x_dx, x_dj
    real(kind=default) :: r, phi, jac, caj, dx, dx_max, dj, dj_max
    real(kind=default), dimension(size(x1)-2) :: cos_theta
    integer :: i
    dx_max = 0

```

```

x_dx = 0
dj_max = 0
x_dj = 0
do i = 1, samples
  call tao_random_number (rng, x1)
  call cartesian_to_spherical_cos_2 (x1, r, phi, cos_theta, jac)
  call spherical_cos_to_cartesian_2 (r, phi, cos_theta, x2, caj)
  dx = sqrt (dot_product (x1-x2, x1-x2))
  dj = jac*caj - 1
  if (dx > dx_max) then
    dx_max = dx
    x_dx = x1
  end if
  if (dj > dj_max) then
    dj_max = dj
    x_dj = x1
  end if
end do
print *, "channel 3 : j*j-1=", real(dj), ", @x=", real (x_dj)
print *, "channel 3 : |x-x|=", real(dx), ", @x=", real (x_dx)
end subroutine check_inverses3

```

Integration

198a *<Declaration of procedures in vamp_tests 196c>+≡ (196b 202b) <196c 200a>*
 public :: single_channel, multi_channel

198b *<Implementation of procedures in vamp_tests 197a>+≡ (196b 202b) <197b 199a>*
 subroutine single_channel (rng, region, samples, iterations, &
 integral, standard_dev, chi_squared)
 type(tao_random_state), intent(inout) :: rng
 real(kind=default), dimension(:,:), intent(in) :: region
 integer, dimension(:), intent(in) :: samples, iterations
 real(kind=default), intent(out) :: integral, standard_dev, chi_squared
 type(vamp_grid) :: gr
 type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
 call vamp_create_history (history)
 call vamp_create_grid (gr, region, samples(1))
 call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
 call vamp_discard_integral (gr, samples(2))
 call vamp_sample_grid &
 (rng, gr, f, NO_DATA, iterations(2), &
 integral, standard_dev, chi_squared, &
 history = history(iterations(1)+1:))

```

    call vamp_write_grid (gr, "vamp_test.grid")
    call vamp_delete_grid (gr)
    call vamp_print_history (history, "single")
    call vamp_delete_history (history)
end subroutine single_channel
199a <Implementation of procedures in vamp_tests 197a>+≡ (196b 202b) <198b 200b>
subroutine multi_channel (rng, region, weights, samples, iterations, powers, &
    integral, standard_dev, chi_squared)
    type(tao_random_state), intent(inout) :: rng
    real(kind=default), dimension(:,:), intent(in) :: region
    real(kind=default), dimension(:), intent(inout) :: weights
    integer, dimension(:), intent(in) :: samples, iterations
    real(kind=default), dimension(:), intent(in) :: powers
    real(kind=default), intent(out) :: integral, standard_dev, chi_squared
    type(vamp_grids) :: grs
    <Body of multi_channel 199b>
end subroutine multi_channel
199b <Body of multi_channel 199b>≡ (199a 213a) 213b>
    type(vamp_history), dimension(iterations(1)+iterations(2)+size(powers)-1) :: &
        history
    type(vamp_history), dimension(size(history),size(weights)) :: histories
    integer :: it, nit
    nit = size (powers)
    call vamp_create_history (history)
    call vamp_create_history (histories)
    call vamp_create_grids (grs, region, samples(1), weights)
    call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
        history = history, histories = histories)
    call vamp_print_history (history, "multi")
    call vamp_print_history (histories, "multi")
    do it = 1, nit
        call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
            history = history(iterations(1)+it-1:), &
            histories = histories(iterations(1)+it-1:,:))
        call vamp_print_history (history(iterations(1)+it-1:), "multi")
        call vamp_print_history (histories(iterations(1)+it-1:,:), "multi")
        call vamp_refine_weights (grs, powers(it))
    end do
    call vamp_discard_integrals (grs, samples(2))
    call vamp_sample_grids &
        (rng, grs, w, NO_DATA, iterations(2), &
            integral, standard_dev, chi_squared, &
            history = history(iterations(1)+nit:), &

```



```

        histories = histories(iterations(1)+nit:,:)
call vamp_print_history (history(iterations(1)+nit:), "multi")
call vamp_print_history (histories(iterations(1)+nit:,:), "multi")
call vamp_write_grids (grs, "vamp_test.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)

```

Input/Output

- 200a *<Declaration of procedures in vamp_tests 196c>+≡ (196b 202b) <198a*
public :: print_results
- 200b *<Implementation of procedures in vamp_tests 197a>+≡ (196b 202b) <199a*
subroutine print_results (prefix, prev_ticks, &
integral, std_dev, chi2, acceptable, failures)
character(len=*), intent(in) :: prefix
integer, intent(in) :: prev_ticks
real(kind=default), intent(in) :: integral, std_dev, chi2, acceptable
integer, intent(inout) :: failures
integer :: ticks, ticks_per_second
real(kind=default) :: pull
call system_clock (ticks, ticks_per_second)
pull = (integral - 1) / std_dev
print "(1X,A,A,F6.2,A)", prefix, &
": time = ", real (ticks - prev_ticks) / ticks_per_second, " secs"
print *, prefix, ": int, err, chi2: ", &
real (integral), real (std_dev), real (chi2)
if (abs (pull) > acceptable) then
failures = failures + 1
print *, prefix, ": unacceptable pull:", real (pull)
else
print *, prefix, ": acceptable pull:", real (pull)
end if
end subroutine print_results

Main Program

- 200c *<vamp_test.f90 192a>+≡ <192a*
program vamp_test
use kinds
use tao_random_numbers

```

use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp
use vamp_test_functions !NODEP!
use vamp_tests !NODEP!
implicit none
integer :: start_ticks, status
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type(tao_random_state) :: rng
real(kind=default), parameter :: ACCEPTABLE = 4
integer :: failures
failures = 0
call tao_random_create (rng, 0)
call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
if (status == 0) then
    call system_clock (start_ticks)
else
    start_ticks = 42
end if
call tao_random_seed (rng, start_ticks)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
print *, "Starting VAMP 1.0 self test..."
print *, "serial code"
print *, VAMP_RCS_ID
print *, DIVISIONS_RCS_ID
call system_clock (start_ticks)
call single_channel (rng, region, samples, iterations, &
    single_integral, single_standard_dev, single_chi_squared)
call print_results ("SINGLE", start_ticks, &
    single_integral, single_standard_dev, single_chi_squared, &
    10*ACCEPTABLE, failures)
weight_vector = 1
powers = 0.25_default
call system_clock (start_ticks)

```

```

call multi_channel (rng, region, weight_vector, samples, iterations, &
    powers, multi_integral, multi_standard_dev, multi_chi_squared)
call print_results ("MULTI", start_ticks, &
    multi_integral, multi_standard_dev, multi_chi_squared, &
    ACCEPTABLE, failures)
call system_clock (start_ticks)
! call check_jacobians (rng, region, weight_vector, samples(1))
call check_inverses (rng, region, weight_vector, samples(1))
call check_inverses3 (rng, region, samples(1))
if (failures == 0) then
    stop 0
else if (failures == 1) then
    stop 1
else
    stop 2
end if
end program vamp_test

```

6.1.2 Parallel Test

202a \langle vampi_test.f90 202a $\rangle \equiv$ 202b \triangleright

```

! vampi_test.f90 --
<Copyleft notice 1>
<Module vamp_test_functions 192b>

```

The following is identical to **vamp_tests**, except for use **vampi**:

202b \langle vampi_test.f90 202a $\rangle + \equiv$ \triangleleft 202a 202c \triangleright

```

module vampi_tests
    use kinds
    use exceptions
    use histograms
    use tao_random_numbers
    use coordinates
    use vampi
    use vamp_test_functions !NODEP!
    implicit none
    private
    <Declaration of procedures in vamp_tests 196c>
contains
    <Implementation of procedures in vamp_tests 197a>
end module vampi_tests

```

202c \langle vampi_test.f90 202a $\rangle + \equiv$ \triangleleft 202b

```

program vampi_test

```

```

use kinds
use tao_random_numbers
use coordinates
use divisions, only: DIVISIONS_RCS_ID
use vamp, only: VAMP_RCS_ID
use vampi
use mpi90
use vamp_test_functions !NODEP!
use vampi_tests !NODEP!
implicit none
integer :: num_proc, proc_id, start_ticks
logical :: perform_io
integer, dimension(2) :: iterations, samples
real(kind=default), dimension(2,5) :: region
real(kind=default), dimension(5) :: weight_vector
real(kind=default), dimension(10) :: powers
real(kind=default) :: single_integral, single_standard_dev, single_chi_squared
real(kind=default) :: multi_integral, multi_standard_dev, multi_chi_squared
type( tao_random_state ) :: rng
integer :: iostat, command
character(len=72) :: command_line
integer, parameter :: &
    CMD_ERROR = -1, CMD_END = 0, &
    CMD_NOP = 1, CMD_SINGLE = 2, CMD_MULTI = 3, CMD_CHECK = 4
call tao_random_create (rng, 0)
call mpi90_init ()
call mpi90_size (num_proc)
call mpi90_rank (proc_id)
perform_io = (proc_id == 0)
call system_clock (start_ticks)
call tao_random_seed (rng, start_ticks + proc_id)
iterations = (/ 4, 3 /)
samples = (/ 20000, 200000 /)
samples = (/ 200000, 2000000 /)
region(1,:) = -1.0
region(2,:) = 1.0
width = 0.0001
if (perform_io) then
    print *, "Starting VAMP 1.0 self test..."
    if (num_proc > 1) then
        print *, "parallel code running on ", num_proc, " processors"
    else
        print *, "parallel code running serially"
    end if
end if

```

```

        end if
        print *, VAMP_RCS_ID
        print *, VAMPI_RCS_ID
        print *, DIVISIONS_RCS_ID
    end if
    command_loop: do
        <Parse the commandline in vamp_test and set command (never defined)>
        call mpi90_broadcast (command, 0)
        call system_clock (start_ticks)
        select case (command)
            <Execute command in vamp_test (never defined)>
            case (CMD_END)
                exit command_loop
            case (CMD_NOP)
                ! do nothing
            case (CMD_ERROR)
                ! do nothing
            end select
        end do command_loop
        call mpi90_finalize ()
    end program vampi_test

```

6.1.3 Output

204a *<vamp_test.out 204a>*≡

6.2 Mapped Mode

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

6.2.1 Serial Test

204b *<vamp_test0.f90 204b>*≡ 211a>
 ! vamp_test0.f90 --
<Copyleft notice 1>
<Module vamp_test0_functions 205>

Single Channel

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

205 \langle Module vamp_test0_functions 205 $\rangle \equiv$ (204b 220b)

```

module vamp_test0_functions
  use kinds
  use vamp, only: vamp_grid, vamp_multi_channel0
  use vamp, only: vamp_data_t
  implicit none
  private
  public :: f, g, phi, w
  public :: create_sample, delete_sample
  private :: f0, psi, g0, f_norm
  real(kind=default), dimension(:), allocatable, private :: c, x_min, x_max
  real(kind=default), dimension(:, :, :), allocatable, public :: x0, gamma
contains
  (Implementation of vamp_test0_functions procedures 206a)
end module vamp_test0_functions

```

We start from a model of n_p interfering resonances in one variable (cf. section ??)

$$f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = \frac{1}{N(x_{\min}, x_{\max}, x_0, \gamma)} \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.3)$$

where

$$N(x_{\min}, x_{\max}, x_0, \gamma) = \int_{x_{\min}}^{x_{\max}} dx \left| \sum_{p=1}^{n_p} \frac{1}{x - x_{0,p} + i\gamma_p} \right|^2 \quad (6.4)$$

such that

$$\int_{x_{\min}}^{x_{\max}} dx f_0(x|x_{\min}, x_{\max}, x_0, \gamma) = 1 \quad (6.5)$$

NB: the $N(x_{\min}, x_{\max}, x_0, \gamma)$ should be calculated once and tabulated to save processing time, but we are lazy here.

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

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

```

pure function f0 (x, x_min, x_max, x0, g) result (f_x)
  real(kind=default), intent(in) :: x, x_min, x_max
  real(kind=default), dimension(:), intent(in) :: x0, g
  real(kind=default) :: f_x
  complex(kind=default) :: amp
  real(kind=default) :: norm
  integer :: i, j
  amp = sum (1.0 / 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.

206b \langle Implementation of vamp_test0_functions procedures 206a $\rangle + \equiv$ (205) \triangleleft 206a 207a \triangleright

```

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.

207a \langle Implementation of `vamp_test0.functions` procedures 206a $\rangle + \equiv$ (205) \langle 206b 207b \rangle

```
pure function f (x, data, weights, channel, grids) result (f_x)
  real(kind=default), dimension(:), intent(in) :: x
  class(vamp_data_t), intent(in) :: data
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: f_x
  real(kind=default) :: fi_x
  integer :: i, j
  f_x = 0.0
  do i = 1, size (c)
    fi_x = 1.0
    do j = 1, size (x)
      if (all (gamma(:,i,j) > 0)) then
        fi_x = fi_x * f0 (x(j), x_min(j), x_max(j), &
                          x0(:,i,j), gamma(:,i,j))
      else
        fi_x = fi_x / (x_max(j) - x_min(j))
      end if
    end do
    f_x = f_x + c(i) * fi_x
  end do
  f_x = f_x / sum (c)
end function f
```

207b \langle Implementation of `vamp_test0.functions` procedures 206a $\rangle + \equiv$ (205) \langle 207a 207c \rangle

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

207c \langle Implementation of `vamp_test0.functions` procedures 206a $\rangle + \equiv$ (205) \langle 207b 208 \rangle

```
subroutine create_sample (num_poles, weights, region)
  integer, intent(in) :: num_poles
  real(kind=default), dimension(:), intent(in) :: weights
```



```

real(kind=default), dimension(:,,:), intent(in) :: region
integer :: nd, nc
nd = size (region, dim=2)
nc = size (weights)
allocate (c(nc), x_min(nd), x_max(nd))
allocate (x0(num_poles,nc,nd), gamma(num_poles,nc,nd))
x_min = region(1,:)
x_max = region(2,:)
c = weights
end subroutine create_sample

```

Multi Channel

We start from the usual mapping for Lorentzian peaks

$$\begin{aligned} \psi(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ \xi \mapsto x = \psi(\xi | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.9)$$

where

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

208 \langle Implementation of `vamp_test0` functions procedures 206a $\rangle + \equiv$ (205) \triangleleft 207c 209a \triangleright

```

pure function psi (xi, x_min, x_max, x0, gamma) result (x)
  real(kind=default), intent(in) :: xi, x_min, x_max, x0, gamma
  real(kind=default) :: x
  x = x0 + gamma &
    * tan (((xi - x_min) * atan ((x_max - x0) / gamma) &
      - (x_max - xi) * atan ((x0 - x_min) / gamma)) &
      / (x_max - x_min))
end function psi

```

The inverse mapping is

$$\begin{aligned} \psi^{-1}(x_{\min}, x_{\max}, x_0, \gamma) : [x_{\min}, x_{\max}] &\rightarrow [x_{\min}, x_{\max}] \\ x \mapsto \xi = \psi^{-1}(x | x_{\min}, x_{\max}, x_0, \gamma) \end{aligned} \quad (6.11)$$

with

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

with Jacobian

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

209a *<Implementation of vamp_test0_functions procedures 206a>+≡ (205) <208 209c>*

```

pure function g0 (x, x_min, x_max, x0, gamma) result (g_x)
  real(kind=default), intent(in) :: x, x_min, x_max, x0, gamma
  real(kind=default) :: g_x
  g_x = gamma / (atan ((x_max - x0) / gamma) - atan ((x_min - x0) / gamma)) &
    * (x_max - x_min) / ((x - x0)**2 + gamma**2)
end function g0

```

The function f has $n_c n_p^{n_d}$ peaks and we need a channel for each one, plus a constant function for the background. We encode the position on the grid linearly:

209b *<Decode channel into ch and p(:) 209b>≡ (209c 210a)*

```

ch = channel - 1
do j = 1, size (x)
  p(j) = 1 + modulo (ch, np)
  ch = ch / np
end do
ch = ch + 1

```

The map ϕ is the direct product of ψ s:

209c *<Implementation of vamp_test0_functions procedures 206a>+≡ (205) <209a 210a>*

```

pure function phi (xi, channel) result (x)
  real(kind=default), dimension(:), intent(in) :: xi
  integer, intent(in) :: channel
  real(kind=default), dimension(size(xi)) :: x
  integer, dimension(size(xi)) :: p
  integer :: j, ch, np, nch, nd, channels
  np = size (x0, dim = 1)
  nch = size (x0, dim = 2)
  nd = size (x0, dim = 3)
  channels = nch * np**nd
  if (channel >= 1 .and. channel <= channels) then
    <Decode channel into ch and p(:) 209b>
    do j = 1, size (xi)
      if (all (gamma(:,ch,j) > 0)) then
        x(j) = psi (xi(j), x_min(j), x_max(j), &
          x0(p(j),ch,j), gamma(p(j),ch,j))
      else
        x = xi

```

```

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

```

similarly for the Jacobians:

210a \langle Implementation of `vamp_test0.functions` procedures 206a $\rangle + \equiv$ (205) \triangleleft 209c 210b \triangleright

```

pure recursive function g (x, data, channel) result (g_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    integer, intent(in) :: channel
    real(kind=default) :: g_x
    integer, dimension(size(x)) :: p
    integer :: j, ch, np, nch, nd, channels
    np = size (x0, dim = 1)
    nch = size (x0, dim = 2)
    nd = size (x0, dim = 3)
    channels = nch * np**nd
    if (channel >= 1 .and. channel <= channels) then
         $\langle$ Decode channel into ch and p(:) 209b $\rangle$ 
        g_x = 1.0
        do j = 1, size (x)
            if (all (gamma(:,ch,j) > 0)) then
                g_x = g_x * g0 (x(j), x_min(j), x_max(j), &
                    x0(p(j),ch,j), gamma(p(j),ch,j))
            end if
        end do
    else if (channel == channels + 1) then
        g_x = 1.0
    else
        g_x = 0
    end if
end function g

```

210b \langle Implementation of `vamp_test0.functions` procedures 206a $\rangle + \equiv$ (205) \triangleleft 210a

```

function w (x, data, weights, channel, grids) result (w_x)
    real(kind=default), dimension(:), intent(in) :: x
    class(vamp_data_t), intent(in) :: data
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel

```

```

    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: w_x
    w_x = vamp_multi_channel0 (f, data, phi, g, x, weights, channel)
end function w

```

Driver Routines

```

211a <vamp_test0.f90 204b>+≡ <204b 217>
    module vamp_tests0
        <Modules used by vamp_tests0 211b>
        use vamp
        implicit none
        private
        <Declaration of procedures in vamp_tests0 212a>
    contains
        <Implementation of procedures in vamp_tests0 212b>
    end module vamp_tests0

211b <Modules used by vamp_tests0 211b>≡ (211a 220b)
    use kinds
    use exceptions
    use histograms
    use tao_random_numbers
    use vamp_test0_functions !NODEP!

```

Verification

```

211c <Declaration of procedures in vamp_tests0 (broken?) 211c>≡
    public :: check_jacobians

211d <Implementation of procedures in vamp_tests0 (broken?) 211d>≡
    subroutine check_jacobians (do_print, region, samples, rng)
        logical, intent(in) :: do_print
        real(kind=default), dimension(:,,:), intent(in) :: region
        integer, dimension(:), intent(in) :: samples
        type( tao_random_state ), intent(inout) :: rng
        real(kind=default), dimension(size(region,dim=2)) :: x
        real(kind=default) :: d
        integer :: ch
        do ch = 1, size(x0,dim=2) * size(x0,dim=1)**size(x0,dim=3) + 1
            call vamp_check_jacobian (rng, samples(1), g, phi, ch, region, d, x)
            if (do_print) then
                print *, ch, ": ", d, ", x = ", real (x)
            end if
        end do
    end subroutine

```

```

    end do
end subroutine check_jacobians

```

Integration

```

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

212b <Implementation of procedures in vamp_tests0 212b>≡ (211a 220b) 213a>
    subroutine single_channel (do_print, region, iterations, samples, rng, &
        acceptable, failures)
        logical, intent(in) :: do_print
        real(kind=default), dimension(:,:), intent(in) :: region
        integer, dimension(:), intent(in) :: iterations, samples
        type(tao_random_state), intent(inout) :: rng
        real(kind=default), intent(in) :: acceptable
        integer, intent(inout) :: failures
        type(vamp_grid) :: gr
        type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
        real(kind=default) :: integral, standard_dev, chi_squared, pull
        call vamp_create_history (history)
        call vamp_create_grid (gr, region, samples(1))
        call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
        call vamp_discard_integral (gr, samples(2))
        call vamp_sample_grid &
            (rng, gr, f, NO_DATA, iterations(2), &
             integral, standard_dev, chi_squared, &
             history = history(iterations(1)+1:))
        call vamp_write_grid (gr, "vamp_test0.grid")
        call vamp_delete_grid (gr)
        call vamp_print_history (history, "single")
        call vamp_delete_history (history)
        pull = (integral - 1) / standard_dev
        if (do_print) then
            print *, "    int, err, chi2:", integral, standard_dev, chi_squared
        end if
        if (abs (pull) > acceptable) then
            failures = failures + 1
            print *, " unacceptable pull:", pull
        else
            print *, "    acceptable pull:", pull
        end if
    end subroutine single_channel

```

213a *<Implementation of procedures in vamp_tests0 212b>+≡ (211a 220b) <212b 214b>*
`subroutine multi_channel (do_print, region, iterations, samples, rng, &
acceptable, failures)
logical, intent(in) :: do_print
real(kind=default), dimension(:,:), intent(in) :: region
integer, dimension(:), intent(in) :: iterations, samples
type(tao_random_state), intent(inout) :: rng
real(kind=default), intent(in) :: acceptable
type(vamp_grids) :: grs
integer, intent(inout) :: failures
<Body of multi_channel 199b>
end subroutine multi_channel`

213b *<Body of multi_channel 199b>+≡ (199a 213a) <199b*
`real(kind=default), &
dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
weight_vector
type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
real(kind=default) :: integral, standard_dev, chi_squared, pull
integer :: it
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
history = history, histories = histories)
do it = 1, 5
call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
history = history(iterations(1)+it-1:), &
histories = histories(iterations(1)+it-1:,:))
call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_sample_grids &
(rng, grs, w, NO_DATA, iterations(2), &
integral, standard_dev, chi_squared, &
history = history(iterations(1)+5:), &
histories = histories(iterations(1)+5:,:))
call vamp_write_grids (grs, "vamp_test0.grids")
call vamp_delete_grids (grs)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)`

```

call vamp_delete_history (histories)
if (do_print) then
  print *, integral, standard_dev, chi_squared
end if
pull = (integral - 1) / standard_dev
if (abs (pull) > acceptable) then
  failures = failures + 1
  print *, " unacceptable pull:", pull
else
  print *, "    acceptable pull:", pull
end if

```

Event Generation

214a *<Declaration of procedures in vamp_tests0 212a>+≡ (211a 220b) <212a*
 public :: single_channel_generator, multi_channel_generator

214b *<Implementation of procedures in vamp_tests0 212b>+≡ (211a 220b) <213a 215>*
 subroutine single_channel_generator (do_print, region, iterations, samples, rng)
 logical, intent(in) :: do_print
 real(kind=default), dimension(:,:), intent(in) :: region
 integer, dimension(:), intent(in) :: iterations, samples
 type(tao_random_state), intent(inout) :: rng
 type(vamp_grid) :: gr
 type(vamp_history), dimension(iterations(1)+iterations(2)) :: history
 type(histogram) :: unweighted, reweighted, weighted, weights
 type(exception) :: exc
 real(kind=default) :: weight, integral, standard_dev
 integer :: i
 real(kind=default), dimension(size(region,dim=2)) :: x
 call vamp_create_grid (gr, region, samples(1))
 call vamp_sample_grid (rng, gr, f, NO_DATA, iterations(1), history = history)
 call vamp_discard_integral (gr, samples(2))
 call vamp_warmup_grid &
 (rng, gr, f, NO_DATA, iterations(2), history = history(iterations(1)+1:))
 call vamp_print_history (history, "single")
 call vamp_delete_history (history)
 call create_histogram (unweighted, region(1,1), region(2,1), 100)
 call create_histogram (reweighted, region(1,1), region(2,1), 100)
 call create_histogram (weighted, region(1,1), region(2,1), 100)
 call create_histogram (weights, 0.0_default, 10.0_default, 100)
 ! do i = 1, 1000000
 do i = 1, 100
 call clear_exception (exc)

```

        call vamp_next_event (x, rng, gr, f, NO_DATA, exc = exc)
        call handle_exception (exc)
        call fill_histogram (unweighted, x(1))
        call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
    end do
    integral = 0.0
    standard_dev = 0.0
    do i = 1, 10000
        call clear_exception (exc)
        call vamp_next_event (x, rng, gr, f, NO_DATA, weight, exc = exc)
        call handle_exception (exc)
        call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
        call fill_histogram (weights, x(1), weight)
        integral = integral + weight
        standard_dev = standard_dev + weight**2
    end do
    if (do_print) then
        print *, integral / (i-1), sqrt (standard_dev) / (i-1)
        call write_histogram (unweighted, "u_s.d")
        call write_histogram (reweighted, "r_s.d")
        call write_histogram (weighted, "w_s.d")
        call write_histogram (weights, "ws_s.d")
    end if
    call delete_histogram (unweighted)
    call delete_histogram (reweighted)
    call delete_histogram (weighted)
    call delete_histogram (weights)
    call vamp_delete_grid (gr)
end subroutine single_channel_generator

```

215 *<Implementation of procedures in vamp_tests0 212b>+≡ (211a 220b) <214b*

```

subroutine multi_channel_generator (do_print, region, iterations, samples, rng)
    logical, intent(in) :: do_print
    real(kind=default), dimension(:,:), intent(in) :: region
    integer, dimension(:), intent(in) :: iterations, samples
    type(tao_random_state), intent(inout) :: rng
    type(vamp_grids) :: grs
    real(kind=default), &
        dimension(size(x0,dim=2)*size(x0,dim=1)**size(x0,dim=3)+1) :: &
        weight_vector
    type(vamp_history), dimension(iterations(1)+iterations(2)+4) :: history
    type(vamp_history), dimension(size(history),size(weight_vector)) :: histories
    type(histogram) :: unweighted, reweighted, weighted, weights
    type(exception) :: exc

```



```

real(kind=default) :: weight, integral, standard_dev
real(kind=default), dimension(size(region,dim=2)) :: x
character(len=5) :: pfx
integer :: it, i, j
weight_vector = 1.0
call vamp_create_history (history)
call vamp_create_history (histories)
call vamp_create_grids (grs, region, samples(1), weight_vector)
call vamp_sample_grids (rng, grs, w, NO_DATA, iterations(1) - 1, &
                        history = history, histories = histories)
do it = 1, 5
    call vamp_sample_grids (rng, grs, w, NO_DATA, 1, &
                            history = history(iterations(1)+it-1:), &
                            histories = histories(iterations(1)+it-1:,:))
    call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, samples(2))
call vamp_warmup_grids &
    (rng, grs, w, NO_DATA, iterations(2), &
    history = history(iterations(1)+5:), &
    histories = histories(iterations(1)+5:,:))
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
call vamp_delete_history (history)
call vamp_delete_history (histories)
!!! do i = 1, size (grs%grids)
!!!     do j = 1, size (grs%grids(i)%div)
!!!         write (pfx, "(I2.2,'/',I2.2)") i, j
!!!         call dump_division (grs%grids(i)%div(j), pfx)
!!!     end do
!!! end do
call create_histogram (unweighted, region(1,1), region(2,1), 100)
call create_histogram (reweighted, region(1,1), region(2,1), 100)
call create_histogram (weighted, region(1,1), region(2,1), 100)
call create_histogram (weights, 0.0_default, 10.0_default, 100)
! do i = 1, 1000000
do i = 1, 100
    call clear_exception (exc)
    call vamp_next_event (x, rng, grs, f, NO_DATA, phi, exc = exc)
    call handle_exception (exc)
    call fill_histogram (unweighted, x(1))
    call fill_histogram (reweighted, x(1), 1.0_default / f (x, NO_DATA))
end do

```

```

integral = 0.0
standard_dev = 0.0
do i = 1, 10000
  call clear_exception (exc)
  call vamp_next_event (x, rng, grs, f, NO_DATA, phi, weight, exc = exc)
  call handle_exception (exc)
  call fill_histogram (weighted, x(1), weight / f (x, NO_DATA))
  call fill_histogram (weights, x(1), weight)
  integral = integral + weight
  standard_dev = standard_dev + weight**2
end do
if (do_print) then
  print *, integral / (i-1), sqrt (standard_dev) / (i-1)
  call write_histogram (unweighted, "u_m.d")
  call write_histogram (reweighted, "r_m.d")
  call write_histogram (weighted, "w_m.d")
  call write_histogram (weights, "ws_m.d")
end if
call delete_histogram (unweighted)
call delete_histogram (reweighted)
call delete_histogram (weighted)
call delete_histogram (weights)
call vamp_delete_grids (grs)
end subroutine multi_channel_generator

```

Main Program

```

217  <vamp_test0.f90 204b>+≡ <211a
  program vamp_test0
    <Modules used by vamp_test0 219d>
    implicit none
    <Variables in vamp_test0 219b>
    do_print = .true.
    print *, "Starting VAMP 1.0 self test..."
    print *, "serial code"
    print *, VAMP_RCS_ID
    print *, DIVISIONS_RCS_ID
    call tao_random_create (rng, 0)
    call get_environment_variable (name="VAMP_RANDOM_TESTS", status=status)
    if (status == 0) then
      call system_clock (ticks0)
    else
      ticks0 = 42
    end if
  end program

```

```

end if
call tao_random_seed (rng, ticks0)
<Set up integrand and region in vamp_test0 219f>
<Execute tests in vamp_test0 218a>
<Cleanup in vamp_test0 220a>
if (failures == 0) then
    stop 0
else if (failures == 1) then
    stop 1
else
    stop 2
end if
end program vamp_test0

218a <Execute tests in vamp_test0 218a>≡ (217) 218b>
failures = 0
call system_clock (ticks0)
call single_channel (do_print, region, iterations, samples, rng, 10*ACCEPTABLE, failures)
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
    "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218b <Execute tests in vamp_test0 218a>+≡ (217) <218a 218c>
call system_clock (ticks0)
call single_channel_generator &
    (do_print, region, iterations, samples, rng)
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
    "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218c <Execute tests in vamp_test0 218a>+≡ (217) <218b 218d>
call system_clock (ticks0)
call multi_channel (do_print, region, iterations, samples, rng, ACCEPTABLE, failures)
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
    "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

218d <Execute tests in vamp_test0 218a>+≡ (217) <218c 219a>
call system_clock (ticks0)
call multi_channel_generator &
    (do_print, region, iterations, samples, rng)
call system_clock (ticks, ticks_per_second)
print "(1X,A,F6.2,A)", &
    "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

```

```

219a  <Execute tests in vamp_test0 218a>+≡ (217) <218d
      call system_clock (ticks0)
      ! call check_jacobians (do_print, region, samples, rng)
      call system_clock (ticks, ticks_per_second)
      print "(1X,A,F6.2,A)", &
            "time = ", real (ticks - ticks0) / ticks_per_second, " secs"

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

219c  <Execute command 219c>≡ (220c)

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

219e  <Variables in vamp_test0 219b>+≡ (217 220c) <219b
      integer :: i, j, ticks, ticks_per_second, ticks0, status
      integer, dimension(2) :: iterations, samples
      real(kind=default), dimension(:,,:), allocatable :: region
      type(tao_random_state) :: rng
      real(kind=default), parameter :: ACCEPTABLE = 4
      integer :: failures

219f  <Set up integrand and region in vamp_test0 219f>≡ (217 220c)
      iterations = (/ 4, 3 /)
      samples = (/ 10000, 50000 /)
      allocate (region(2,2))
      region(1,:) = -1.0
      region(2,:) = 2.0
      call create_sample &
            (num_poles = 2, weights = (/ 1.0_default, 2.0_default /), region = region)
      do i = 1, size (x0, dim=2)
        do j = 1, size (x0, dim=3)
          call tao_random_number (rng, x0(:,i,j))
        end do
      end do
      gamma = 0.001
      x0(1, :, :) = 0.2
      x0(2, :, :) = 0.8

```

220a *<Cleanup in vamp_test0 220a>*≡ (217 220c)
 call delete_sample ()
 deallocate (region)

6.2.2 Parallel Test

220b *<vampi_test0.f90 220b>*≡ 220c>
 ! vampi_test0.f90 --
<Copyleft notice 1>
<Module vamp_test0_functions 205>
 module vamp_tests0
<Modules used by vamp_tests0 211b>
 use vampi
 use mpi90
 implicit none
 private
<Declaration of procedures in vamp_tests0 212a>
 contains
<Implementation of procedures in vamp_tests0 212b>
 end module vamp_tests0

220c *<vampi_test0.f90 220b>*+≡ <220b
 program vampi_test0
<Modules used by vamp_test0 219d>
 use mpi90
 use vampi, only: VAMPI_RCS_ID
 implicit none
<Variables in vamp_test0 219b>
 integer :: num_proc, proc_id
 call mpi90_init ()
 call mpi90_size (num_proc)
 call mpi90_rank (proc_id)
 if (proc_id == 0) then
 do_print = .true.
 print *, "Starting VAMP 1.0 self test..."
 if (num_proc > 1) then
 print *, "parallel code running on ", num_proc, " processors"
 else
 print *, "parallel code running serially"
 end if
 print *, VAMP_RCS_ID
 print *, VAMPI_RCS_ID
 print *, DIVISIONS_RCS_ID

```

else
    do_print = .false.
end if
call tao_random_create (rng, 0)
call system_clock (ticks0)
call tao_random_seed (rng, ticks0 + proc_id)
<Set up integrand and region in vamp_test0 219f>
call mpi90_broadcast (x0, 0)
call mpi90_broadcast (gamma, 0)
command_loop: do
    if (proc_id == 0) then
        <Read command line and decode it as command (never defined)>
    end if
    call mpi90_broadcast (command, 0)
    call system_clock (ticks0)
    <Execute command 219c>
    call system_clock (ticks, ticks_per_second)
    if (proc_id == 0) then
        print "(1X,A,F6.2,A)", &
            "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
    end if
end do command_loop
<Cleanup in vamp_test0 220a>
call mpi90_finalize ()
if (proc_id == 0) then
    print *, "bye."
end if
end program vampi_test0

```

6.2.3 Output

221 *<vamp_test0.out 221>*≡

—7—

APPLICATION

7.1 *Cross section*

```

222a <application.f90 222a>≡
! application.f90 --
<Copyleft notice 1>
module cross_section
  use kinds
  use constants
  use utils
  use kinematics
  use tao_random_numbers
  use products, only: dot
  use helicity
  use vamp, only: vamp_grid, vamp_probability
  implicit none
  private
  <Declaration of cross_section procedures 223d>
  <Types in cross_section 228c>
  <Variables in cross_section 222b>
contains
  <Implementation of cross_section procedures 224a>
end module cross_section
239▷

222b <Variables in cross_section 222b>≡
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, &
(222a) 223c▷

```

```
S_0 = 200.0 ** 2
```

223a \langle XXX Variables in cross_section 223a $\rangle \equiv$ 223b \triangleright

```
real(kind=default), private, parameter :: &
  MA_0 = 0.01, &
  MB_0 = 0.01, &
  M1_0 = 0.01, &
  M2_0 = 0.01, &
  M3_0 = 0.01, &
  S_0 = 200.0 ** 2
```

223b \langle XXX Variables in cross_section 223a $\rangle + \equiv$ \triangleleft 223a

```
real(kind=default), private, parameter :: &
  S1_MIN_0 = 0.0 ** 2, &
  S2_MIN_0 = 0.0 ** 2, &
  S3_MIN_0 = 0.0 ** 2, &
  T1_MIN_0 = 0.0 ** 2, &
  T2_MIN_0 = 0.0 ** 2
```

223c \langle Variables in cross_section 222b $\rangle + \equiv$ (222a) \triangleleft 222b 223f \triangleright

```
real(kind=default), private, parameter :: &
  S1_MIN_0 = 1.0 ** 2, &
  S2_MIN_0 = 1.0 ** 2, &
  S3_MIN_0 = 1.0 ** 2, &
  T1_MIN_0 = 10.0 ** 2, &
  T2_MIN_0 = 10.0 ** 2
```

223d \langle Declaration of cross_section procedures 223d $\rangle \equiv$ (222a) 225a \triangleright

```
private :: cuts
```

223e \langle XXX Implementation of cross_section procedures 223e $\rangle \equiv$

```
pure function cuts (k1, k2, p1, p2, q) result (inside)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  logical :: inside
  inside = (abs (dot (k1 - q, k1 - q)) >= T1_MIN_0) &
    .and. (abs (dot (k2 - q, k2 - q)) >= T2_MIN_0) &
    .and. (abs (dot (p1 + q, p1 + q)) >= S1_MIN_0) &
    .and. (abs (dot (p2 + q, p2 + q)) >= S2_MIN_0) &
    .and. (abs (dot (p1 + p2, p1 + p2)) >= S3_MIN_0)
end function cuts
```

223f \langle Variables in cross_section 222b $\rangle + \equiv$ (222a) \triangleleft 223c

```
real(kind=default), private, parameter :: &
```



```

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

```

224a *⟨Implementation of cross_section procedures 224a⟩*≡ (222a) 224b>

```

pure function cuts (k1, k2, p1, p2, q) result (inside)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  logical :: inside
  real(kind=default), dimension(3) :: p1n, p2n, qn
  inside = .false.
  if ((p1(0) < E_MIN) .or. (p2(0) < E_MIN) .or. (q(0) < E_MIN)) then
    return
  end if
  p1n = p1(1:3) / sqrt (dot_product (p1(1:3), p1(1:3)))
  p2n = p2(1:3) / sqrt (dot_product (p2(1:3), p2(1:3)))
  qn = q(1:3) / sqrt (dot_product (q(1:3), q(1:3)))
  if ((abs (qn(3)) > COSTH_BEAM_MAX) &
      .or. (abs (p1n(3)) > COSTH_BEAM_MAX)&
      .or. (abs (p2n(3)) > COSTH_BEAM_MAX)) then
    return
  end if
  if (dot_product (p1n, qn) > COSTH_SEP_MAX) then
    return
  end if
  if (dot_product (p2n, qn) > COSTH_SEP_MAX) then
    return
  end if
  if (dot_product (p1n, p2n) > COSTH_SEP_MAX) then
    return
  end if
  inside = .true.
end function cuts

```

224b *⟨Implementation of cross_section procedures 224a⟩*+≡ (222a) <224a 226b>

```

function xsect (k1, k2, p1, p2, q) result (xs)
  real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
  real(kind=default) :: xs
  complex(kind=default), dimension(-1:1,-1:1,-1:1,-1:1,-1:1) :: amp
  !!! xs = 1.0_double / phase_space_volume (3, k1(0) + k2(0))
  !!! xs = 1.0_double / dot (p1 + q, p1 + q) &
  !!!      + 1.0_double / dot (p2 + q, p2 + q)
  !!! return
  amp = nneeg (k1, k2, p1, p2, q)

```

```

      xs = sum (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2) &
               * conjg (amp(-1:1:2,-1:1:2,-1:1:2,-1:1:2,-1:1:2)))
    end function xsect

```

225a \langle Declaration of cross_section procedures 223d $\rangle + \equiv$ (222a) \langle 223d 227b \rangle

```

private :: xsect

$$\phi : [0, 1]^{\otimes 5} \rightarrow [(m_2 + m_3)^2, (\sqrt{s} - m_1)^2] \otimes [t_1^{\min}(s_2), t_1^{\max}(s_2)]$$


$$\otimes [0, 2\pi] \otimes [-1, 1] \otimes [0, 2\pi]$$


$$(x_1, \dots, x_5) \mapsto (s_2, t_1, \phi, \cos \theta_3, \phi_3)$$


$$= (s_2(x_1), x_2 t_1^{\max}(s_2) + (1 - x_2) t_1^{\min}(s_2), 2\pi x_3, 2x_4 - 1, 2\pi x_5)$$


```

(7.1)

where

$$t_1^{\max/\min}(s_2)$$

$$= m_a^2 + m_1^2 - \frac{(s + m_a^2 - m_b^2)(s - s_2 + m_1^2) \mp \sqrt{\lambda(s, m_a^2, m_b^2)\lambda(s, s_2, m_1^2)}}{2s}$$

(7.2)

225b \langle Set $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$ from (x_1, \dots, x_5) 225b $\rangle \equiv$ (226b)

```

! s2_min = S1_MIN_0
s2_min = (m2 + m3)**2
s2_max = (sqrt(s) - m1)**2
s2 = s2_max * x(1) + s2_min * (1 - x(1))
t1_min = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
+ sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1_max = ma**2 + m1**2 - ((s + ma**2 - mb**2) * (s - s2 + m1**2) &
- sqrt(lambda(s, ma**2, mb**2) * lambda(s, s2, m1**2))) / (2*s)
t1 = t1_max * x(2) + t1_min * (1 - x(2))
phi = 2*PI * x(3)
cos_theta3 = 2 * x(4) - 1
phi3 = 2*PI * x(5)

```

225c \langle Set $(s_2, t_1, \phi, \cos \theta_3, \phi_3)$ from (x_1, \dots, x_5) (massless case) 225c $\rangle \equiv$ (228b)

```

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

```

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

i.e.

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

226a $\langle \text{Adjust Jacobian 226a} \rangle \equiv$ (226b 228b)

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

226b $\langle \text{Implementation of cross_section procedures 224a} \rangle + \equiv$ (222a) $\langle 224b \ 227c \rangle$

```
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
   $\langle m_a \leftrightarrow m_b, m_1 \leftrightarrow m_2 \text{ for channel \#1 226c} \rangle$ 
   $\langle \text{Set } (s_2, t_1, \phi, \cos \theta_3, \phi_3) \text{ from } (x_1, \dots, x_5) \text{ 225b} \rangle$ 
  p = two_to_three(s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3)
   $\langle \text{Adjust Jacobian 226a} \rangle$ 
   $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 227a} \rangle$ 
end function phase_space
```

226c $\langle m_a \leftrightarrow m_b, m_1 \leftrightarrow m_2 \text{ for channel \#1 226c} \rangle \equiv$ (226b)

```
select case (channel)
case (1)
  ma = MA_0
  mb = MB_0
  m1 = M1_0
  m2 = M2_0
  m3 = M3_0
case (2)
  ma = MB_0
  mb = MA_0
  m1 = M2_0
  m2 = M1_0
  m3 = M3_0
case (3)
  ma = MA_0
  mb = MB_0
  m1 = M3_0
```

```

        m2 = M2_0
        m3 = M1_0
    case default
        ma = MA_0
        mb = MB_0
        m1 = M1_0
        m2 = M2_0
        m3 = M3_0
    end select

```

227a $\langle p_1 \leftrightarrow p_2 \text{ for channel \#2 227a} \rangle \equiv$ (226b 228b)

```

    select case (channel)
    case (1)
        ! OK
    case (2)
        call swap (p%p(1,:), p%p(2,:))
    case (3)
        call swap (p%p(1,:), p%p(3,:))
    case default
        ! OK
    end select

```

227b $\langle \text{Declaration of cross_section procedures 223d} \rangle + \equiv$ (222a) \langle 225a 228a \rangle
 private :: jacobian

227c $\langle \text{Implementation of cross_section procedures 224a} \rangle + \equiv$ (222a) \langle 226b 228b \rangle

```

    pure function jacobian (k1, k2, p1, p2, q) result (jac)
    real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
    real(kind=default) :: jac
    real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
    real(kind=default) :: s, s2, s2_min, s2_max, t1_min, t1_max
    ma_2 = max (dot (k1, k1), 0.0_double)
    mb_2 = max (dot (k2, k2), 0.0_double)
    m1_2 = max (dot (p1, p1), 0.0_double)
    m2_2 = max (dot (p2, p2), 0.0_double)
    m3_2 = max (dot (q, q), 0.0_double)
    s = dot (k1 + k2, k1 + k2)
    s2 = dot (p2 + q, p2 + q)
    ! s2_min = S1_MIN_0
    s2_min = (sqrt (m2_2) + sqrt (m3_2))**2
    s2_max = (sqrt (s) - sqrt (m1_2))**2
    t1_min = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
        + sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)
    t1_max = ma_2 + m1_2 - ((s + ma_2 - mb_2) * (s - s2 + m1_2) &
        - sqrt (lambda (s, ma_2, mb_2) * lambda (s, s2, m1_2))) / (2*s)

```

```

    jac = 1.0 / ((2*PI)**5 * 32 * s2) &
      * sqrt (lambda (s2, m2_2, m3_2) / lambda (s, ma_2, mb_2)) &
      * (8.0 * PI**2 * (s2_max - s2_min) * (t1_max - t1_min))
end function jacobian

```

228a \langle Declaration of cross_section procedures 223d $\rangle + \equiv$ (222a) \langle 227b 228e \rangle
 private :: phase_space, phase_space_massless

228b \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 227c 228f \rangle
 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) 225c \rangle
 p = two_to_three (s, t1, s2, phi, cos_theta3, phi3)
 \langle Adjust Jacobian 226a \rangle
 \langle $p_1 \leftrightarrow p_2$ for channel #2 227a \rangle
 end function phase_space_massless

228c \langle Types in cross_section 228c $\rangle \equiv$ (222a) 228d \rangle
 type, public :: LIPS3_m5i2a3
 ! private
 real(kind=default) :: ma, mb, m1, m2, m3
 real(kind=default) :: s, s2, t1
 real(kind=default) :: phi, cos_theta3, phi3
 real(kind=default) :: jacobian
 end type LIPS3_m5i2a3

228d \langle Types in cross_section 228c $\rangle + \equiv$ (222a) \langle 228c \rangle
 type, public :: x5
 ! private
 real(kind=default), dimension(5) :: x
 real(kind=default) :: jacobian
 end type x5

228e \langle Declaration of cross_section procedures 223d $\rangle + \equiv$ (222a) \langle 228a 231a \rangle
 private :: invariants_from_p, invariants_to_p
 private :: invariants_from_x, invariants_to_x

228f \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 228b 229a \rangle
 pure function invariants_from_p (p, k1, k2) result (q)
 type(LIPS3), intent(in) :: p

```

real(kind=default), dimension(0:), intent(in) :: k1, k2
type(LIPS3_m5i2a3) :: q
real(kind=default) :: ma_2, mb_2, m1_2, m2_2, m3_2
real(kind=default), dimension(0:3) :: k1k2, p2p3, k1p1, p3_23
k1k2 = k1 + k2
k1p1 = - k1 + p%p(1,:)
p2p3 = p%p(2,:) + p%p(3,:)
ma_2 = max (dot (k1, k1), 0.0_double)
mb_2 = max (dot (k2, k2), 0.0_double)
m1_2 = max (dot (p%p(1,:), p%p(1:)), 0.0_double)
m2_2 = max (dot (p%p(2,:), p%p(2:)), 0.0_double)
m3_2 = max (dot (p%p(3,:), p%p(3:)), 0.0_double)
q%ma = sqrt (ma_2)
q%mb = sqrt (mb_2)
q%m1 = sqrt (m1_2)
q%m2 = sqrt (m2_2)
q%m3 = sqrt (m3_2)
q%s = dot (k1k2, k1k2)
q%s2 = dot (p2p3, p2p3)
q%t1 = dot (k1p1, k1p1)
q%phi = atan2 (p%p(1,2), p%p(1,1))
if (q%phi < 0) then
    q%phi = q%phi + 2*PI
end if
p3_23 = boost_momentum (p%p(3,:), p2p3)
q%cos_theta3 = p3_23(3) / sqrt (dot_product (p3_23(1:3), p3_23(1:3)))
q%phi3 = atan2 (p3_23(2), p3_23(1))
if (q%phi3 < 0) then
    q%phi3 = q%phi3 + 2*PI
end if
q%jacobian = 1.0 / ((2*PI)**5 * 32 * q%s2) &
    * sqrt (lambda (q%s2, m2_2, m3_2) / lambda (q%s, ma_2, mb_2))
end function invariants_from_p

```

229a \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 228f 229b \rangle

```

pure function invariants_to_p (p) result (q)
type(LIPS3_m5i2a3), intent(in) :: p
type(LIPS3) :: q
q = two_to_three (p%s, p%t1, p%s2, p%phi, p%cos_theta3, p%phi3)
q%jacobian = q%jacobian * p%jacobian
end function invariants_to_p

```

229b \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 229a 230 \rangle

```

pure function invariants_from_x (x, s, ma, mb, m1, m2, m3) result (p)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), intent(in) :: s, ma, mb, m1, m2, m3
  type(LIPS3_m5i2a3) :: p
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  p%ma = ma
  p%mb = mb
  p%m1 = m1
  p%m2 = m2
  p%m3 = m3
  p%s = s
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  p%s2 = s2_max * x(1) + s2_min * (1 - x(1))
  t1_min = p%ma**2 + p%m1**2 &
    - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
      + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
        * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
    - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
      - sqrt (lambda (p%s, p%ma**2, p%mb**2) &
        * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  p%t1 = t1_max * x(2) + t1_min * (1 - x(2))
  p%phi = 2*PI * x(3)
  p%cos_theta3 = 2 * x(4) - 1
  p%phi3 = 2*PI * x(5)
  p%jacobian = 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_from_x

```

230 \langle Implementation of cross-section procedures 224a $\rangle + \equiv$ (222a) \langle 229b 231b \rangle

```

pure function invariants_to_x (p) result (x)
  type(LIPS3_m5i2a3), intent(in) :: p
  type(x5) :: x
  real(kind=default) :: s2_min, s2_max, t1_min, t1_max
  s2_min = (p%m2 + p%m3)**2
  s2_max = (sqrt (p%s) - p%m1)**2
  t1_min = p%ma**2 + p%m1**2 &
    - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
      + sqrt (lambda (p%s, p%ma**2, p%mb**2) &
        * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
  t1_max = p%ma**2 + p%m1**2 &
    - ((p%s + p%ma**2 - p%mb**2) * (p%s - p%s2 + p%m1**2) &
      - sqrt (lambda (p%s, p%ma**2, p%mb**2) &

```

```

        * lambda (p%s, p%s2, p%m1**2))) / (2*p%s)
x%x(1) = (p%s2 - s2_min) / (s2_max - s2_min)
x%x(2) = (p%t1 - t1_min) / (t1_max - t1_min)
x%x(3) = p%phi / (2*PI)
x%x(4) = (p%cos_theta3 + 1) / 2
x%x(5) = p%phi3 / (2*PI)
x%jacobian = p%jacobian * 8*PI**2 * (s2_max - s2_min) * (t1_max - t1_min)
end function invariants_to_x

```

231a *<Declaration of cross_section procedures 223d>+≡ (222a) <228e 232b>*
public :: sigma, sigma_raw, sigma_massless

231b *<Implementation of cross_section procedures 224a>+≡ (222a) <230 231c>*
function sigma (x, weights, channel, grids) result (xs)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in), optional :: weights
 integer, intent(in), optional :: channel
 type(vamp_grid), dimension(:), intent(in), optional :: grids
 real(kind=default) :: xs
 real(kind=default), dimension(2,0:3) :: k
 type(LIPS3) :: p
 k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 if (present (channel)) then
 p = phase_space (x, channel)
 else
 p = phase_space (x, 0)
 end if
 if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
 xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
 * jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
 !!! * p%jacobian
 else
 xs = 0.0
 end if
end function sigma

231c *<Implementation of cross_section procedures 224a>+≡ (222a) <231b 232a>*
function sigma_raw (k1, k2, p1, p2, q) result (xs)
 real(kind=default), dimension(0:), intent(in) :: k1, k2, p1, p2, q
 real(kind=default) :: xs
 if (cuts (k1, k2, p1, p2, q)) then
 xs = xsect (k1, k2, p1, p2, q)
 end if
end function sigma_raw


```

else
  xs = 0.0
end if
end function sigma_raw

```

232a \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 231c 232c \rangle

```

function sigma_massless (x, weights, channel, grids) result (xs)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: xs
  real(kind=default), dimension(2,0:3) :: k
  type(LIPS3) :: p
  k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
  k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  p = phase_space_massless (x, 0)
  if (cuts (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))) then
    xs = xsect (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
      * p%jacobian
  else
    xs = 0.0
  end if
end function sigma_massless

```

232b \langle Declaration of cross_section procedures 223d $\rangle + \equiv$ (222a) \langle 231a 234a \rangle

```

public :: w

```



232c \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 232a 233 \rangle

```

function w (x, weights, channel, grids) result (w_x)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default), dimension(:), intent(in), optional :: weights
  integer, intent(in), optional :: channel
  type(vamp_grid), dimension(:), intent(in), optional :: grids
  real(kind=default) :: w_x
  real(kind=default), dimension(size(weights)) :: g_x

```

```

real(kind=default), dimension(2,0:3) :: k
type(LIPS3) :: p
integer :: ch
if (present (channel)) then
    ch = channel
else
    ch = 0
end if
k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
p = phase_space (x, abs (ch))
g_x(1) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:))
g_x(2) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(2,:), p%p(1,:), p%p(3,:))
g_x(3) = 1.0_double / jacobian (k(1,:), k(2,:), p%p(3,:), p%p(2,:), p%p(1,:))
if (ch > 0) then
    w_x = sigma_raw (k(1,:), k(2,:), p%p(1,:), p%p(2,:), p%p(3,:)) &
        / sum (weights * g_x)
else if (ch < 0) then
    w_x = g_x(-ch) / sum (weights * g_x)
else
    w_x = -1
end if
end function w

```

233 \langle Implementation of cross-section procedures 224a $\rangle + \equiv$ (222a) \langle 232c 234c \rangle

```

function sigma_rambo (x, weights, channel, grids) result (xs)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), dimension(:), intent(in), optional :: weights
    integer, intent(in), optional :: channel
    type(vamp_grid), dimension(:), intent(in), optional :: grids
    real(kind=default) :: xs
    real(kind=default), dimension(2,0:3) :: k
    real(kind=default), dimension(3,0:3) :: p
    k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
    k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    p = massless_isotropic_decay (sum (k(:,0)), reshape (x, (/ 3, 4 /)))
    if (cuts (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:))) then
        xs = xsect (k(1,:), k(2,:), p(1,:), p(2,:), p(3,:)) &
            * phase_space_volume (size (p, dim = 1), sum (k(:,0)))
    else
        xs = 0.0
    end if
end function sigma_rambo

```

234a *<Declaration of cross_section procedures 223d>+≡ (222a) <232b 234b>*
public :: sigma_rambo

234b *<Declaration of cross_section procedures 223d>+≡ (222a) <234a 235a>*
public :: check_kinematics
private :: print_LIPS3_m5i2a3

234c *<Implementation of cross_section procedures 224a>+≡ (222a) <233 234d>*
subroutine check_kinematics (rng)
type(tao_random_state), intent(inout) :: rng
real(kind=default), dimension(5) :: x
real(kind=default), dimension(0:3) :: k1, k2
type(x5) :: x1, x2
type(LIPS3) :: p1, p2
type(LIPS3_m5i2a3) :: q, q1, q2
k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
call tao_random_number (rng, x)
q = invariants_from_x (x, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
p1 = invariants_to_p (q)
q1 = invariants_from_p (p1, k1, k2)
p2 = phase_space (x, 1)
q2 = invariants_from_p (p2, k1, k2)
x1 = invariants_to_x (q1)
x2 = invariants_to_x (q2)
print *, p1%jacobian, p2%jacobian, x1%jacobian, x2%jacobian
call print_lips3_m5i2a3 (q)
call print_lips3_m5i2a3 (q1)
call print_lips3_m5i2a3 (q2)
end subroutine check_kinematics

234d *<Implementation of cross_section procedures 224a>+≡ (222a) <234c 235b>*
subroutine print_LIPS3_m5i2a3 (p)
type(LIPS3_m5i2a3), intent(in) :: p
print "(1x,5('m',a1,'=',e9.2,' '))", &
'a', p%ma, 'b', p%mb, '1', p%m1, '2', p%m2, '3', p%m3
print "(1x,'s=',e9.2,' s2=',e9.2,' t1=',e9.2)", &
p%s, p%s2, p%t1
print "(1x,'phi=',e9.2,' cos(th3)=',e9.2,' phi2=',e9.2)", &
p%phi, p%cos_theta3, p%phi3
print "(1x,'j=',e9.2)", &
p%jacobian
end subroutine print_LIPS3_m5i2a3

235a *<Declaration of cross_section procedures 223d>+≡ (222a) <234b 238a>*

```

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

```

235b *<Implementation of cross_section procedures 224a>+≡ (222a) <234d 235c>*

```

pure function phi12 (x1, dummy) result (x2)
  real(kind=default), dimension(:), intent(in) :: x1
  integer, intent(in) :: dummy
  real(kind=default), dimension(size(x1)) :: x2
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x52
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
  p1 = invariants_to_p (q1)
  p2%p(1,:) = p1%p(2,:)
  p2%p(2,:) = p1%p(1,:)
  p2%p(3,:) = p1%p(3,:)
  if (dummy < 0) then
    q2 = invariants_from_p (p2, k2, k1)
  else
    q2 = invariants_from_p (p2, k1, k2)
  end if
  x52 = invariants_to_x (q2)
  x2 = x52%x
end function phi12

```

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

```

pure function phi21 (x2, dummy) result (x1)
  real(kind=default), dimension(:), intent(in) :: x2
  integer, intent(in) :: dummy
  real(kind=default), dimension(size(x2)) :: x1
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x51
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
  p2 = invariants_to_p (q2)
  p1%p(1,:) = p2%p(2,:)
  p1%p(2,:) = p2%p(1,:)

```

```

p1%p(3,:) = p2%p(3,:)
if (dummy < 0) then
    q1 = invariants_from_p (p1, k2, k1)
else
    q1 = invariants_from_p (p1, k1, k2)
end if
x51 = invariants_to_x (q1)
x1 = x51%x
end function phi21

```

236a \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 235c 236b \rangle

```

pure function phi1 (x1) result (p1)
    real(kind=default), dimension(:), intent(in) :: x1
    type(LIPS3) :: p1
    type(LIPS3_m5i2a3) :: q1
    q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
    p1 = invariants_to_p (q1)
end function phi1

```

236b \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 236a 236c \rangle

```

pure function phi2 (x2) result (p2)
    real(kind=default), dimension(:), intent(in) :: x2
    type(LIPS3) :: p2
    type(LIPS3_m5i2a3) :: q2
    q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
    p2 = invariants_to_p (q2)
end function phi2

```

236c \langle Implementation of cross_section procedures 224a $\rangle + \equiv$ (222a) \langle 236b 237a \rangle

```

pure function g12 (x1) result (g)
    real(kind=default), dimension(:), intent(in) :: x1
    real(kind=default) :: g
    type(LIPS3) :: p1, p2
    type(LIPS3_m5i2a3) :: q1, q2
    type(x5) :: x52
    real(kind=default), dimension(0:3) :: k1, k2
    k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
    k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
    q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
    p1 = invariants_to_p (q1)
    p2%p(1,:) = p1%p(2,:)
    p2%p(2,:) = p1%p(1,:)

```

```

p2%p(3,:) = p1%p(3,:)
q2 = invariants_from_p (p2, k2, k1)
x52 = invariants_to_x (q2)
g = x52%jacobian / p1%jacobian
end function g12

```

237a *<Implementation of cross_section procedures 224a>+≡ (222a) <236c 237b>*

```

pure function g21 (x2) result (g)
  real(kind=default), dimension(:), intent(in) :: x2
  real(kind=default) :: g
  type(LIPS3) :: p1, p2
  type(LIPS3_m5i2a3) :: q1, q2
  type(x5) :: x51
  real(kind=default), dimension(0:3) :: k1, k2
  k1 = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
  k2 = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
  q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
  p2 = invariants_to_p (q2)
  p1%p(1,:) = p2%p(2,:)
  p1%p(2,:) = p2%p(1,:)
  p1%p(3,:) = p2%p(3,:)
  q1 = invariants_from_p (p1, k2, k1)
  x51 = invariants_to_x (q1)
  g = x51%jacobian / p2%jacobian
end function g21

```

237b *<Implementation of cross_section procedures 224a>+≡ (222a) <237a 237c>*

```

pure function g1 (x1) result (g)
  real(kind=default), dimension(:), intent(in) :: x1
  real(kind=default) :: g
  type(LIPS3) :: p1
  type(LIPS3_m5i2a3) :: q1
  q1 = invariants_from_x (x1, S_0, MA_0, MB_0, M1_0, M2_0, M3_0)
  p1 = invariants_to_p (q1)
  g = 1 / p1%jacobian
end function g1

```

237c *<Implementation of cross_section procedures 224a>+≡ (222a) <237b 238b>*

```

pure function g2 (x2) result (g)
  real(kind=default), dimension(:), intent(in) :: x2
  real(kind=default) :: g
  type(LIPS3) :: p2

```

```

type(LIPS3_m5i2a3) :: q2
q2 = invariants_from_x (x2, S_0, MA_0, MB_0, M2_0, M1_0, M3_0)
p2 = invariants_to_p (q2)
g = 1 / p2%jacobian
end function g2

```

238a *<Declaration of cross_section procedures 223d>+≡* (222a) <235a
public :: wx

238b *<Implementation of cross_section procedures 224a>+≡* (222a) <237c
function wx (x, weights, channel, grids) result (w_x)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), dimension(:), intent(in) :: weights
 integer, intent(in) :: channel
 type(vamp_grid), dimension(:), intent(in) :: grids
 real(kind=default) :: w_x
 real(kind=default), dimension(size(weights)) :: g_x, p_q
 real(kind=default), dimension(size(x)) :: x1, x2
 real(kind=default), dimension(2,0:3) :: k
 type(LIPS3) :: q
 k(1,:) = (/ 100.0_double, 0.0_double, 0.0_double, 100.0_double /)
 k(2,:) = (/ 100.0_double, 0.0_double, 0.0_double, -100.0_double /)
 select case (abs (channel))
 case (1)
 x1 = x
 x2 = phi12 (x, 0)
 q = phi1 (x1)
 case (2)
 x1 = phi21 (x, 0)
 x2 = x
 q = phi2 (x2)
 end select
 p_q(1) = vamp_probability (grids(1), x1)
 p_q(2) = vamp_probability (grids(2), x2)
 g_x(1) = p_q(1) * g1 (x1)
 g_x(2) = p_q(2) * g2 (x2)
 g_x = g_x / p_q(abs(channel))
 if (channel > 0) then
 w_x = sigma_raw (k(1,:), k(2,:), q%p(1,:), q%p(2,:), q%p(3,:)) &
 / dot_product (weights, g_x)
 else if (channel < 0) then
 w_x = vamp_probability (grids(-channel), x) / dot_product (weights, g_x)
 else
 w_x = 0
 end if
end function wx

```

        end if
    end function wx

```

```

239  <application.f90 222a>+≡                                     <222a
    program application
        use kinds
        use utils
        use vampi
        use mpi90
        use linalg
        use exceptions
        use kinematics, only: phase_space_volume
        use cross_section !NODEP!
        use tao_random_numbers
        implicit none
        type(vamp_grid) :: gr
        type(vamp_grids) :: grs
        real(kind=default), dimension(:,:), allocatable :: region
        real(kind=default) :: integral, standard_dev, chi_squared
        real(kind=default) :: &
            single_integral, single_standard_dev, &
            rambo_integral, rambo_standard_dev
        real(kind=default), dimension(2) :: weight_vector
        integer, dimension(2) :: calls, iterations
        type(vamp_history), dimension(100) :: history
        type(vamp_history), dimension(100,size(weight_vector)) :: histories
        type(exception) :: exc
        type( tao_random_state ) :: rng
        real(kind=default), dimension(5) :: x
        real(kind=default) :: jac
        integer :: i
        integer :: num_proc, proc_id, ticks, ticks0, ticks_per_second, command
        character(len=72) :: command_line
        integer, parameter :: &
            CMD_SINGLE = 1, &
            CMD_MULTI = 2, &
            CMD_ROTATING = 3, &
            CMD_RAMBO = 4, &
            CMD_COMPARE = 5, &
            CMD_MASSLESS = 6, &
            CMD_ERROR = 0
        call mpi90_init ()
        call mpi90_size (num_proc)

```



```

call mpi90_rank (proc_id)
call system_clock (ticks0)
call tao_random_create (rng, 0)
call tao_random_seed (rng, ticks0 + proc_id)
!!! call tao_random_seed (rng, proc_id)
call vamp_create_history (history, verbose = .true.)
call vamp_create_history (histories, verbose = .true.)
iterations = (/ 3, 4 /)
calls = (/ 10000, 100000 /)
if (proc_id == 0) then
  read *, command_line
  if (command_line == "single") then
    command = CMD_SINGLE
  else if (command_line == "multi") then
    command = CMD_MULTI
  else if (command_line == "rotating") then
    command = CMD_ROTATING
  else if (command_line == "rambo") then
    command = CMD_RAMBO
  else if (command_line == "compare") then
    command = CMD_COMPARE
  else if (command_line == "massless") then
    command = CMD_MASSLESS
  else
    command = CMD_ERROR
  end if
end if
call mpi90_broadcast (command, 0)
call system_clock (ticks0)
select case (command)
case (CMD_SINGLE)
  Application in single channel mode 242a
case (CMD_MASSLESS)
  Application in massless single channel mode 242b
case (CMD_MULTI)
  Application in multi channel mode 243
case (CMD_ROTATING)
  allocate (region(2,5))
  region(1,:) = 0.0
  region(2,:) = 1.0
  if (proc_id == 0) then
    print *, "rotating N/A yet ..."
  end if

```

```

case (CMD_RAMBO)
  <Application in Rambo mode 244>
case (CMD_COMPARE)
  <Application in single channel mode 242a>
  single_integral = integral
  single_standard_dev = standard_dev
  <Application in Rambo mode 244>
  if (proc_id == 0) then
    rambo_integral = integral
    rambo_standard_dev = standard_dev
    integral = &
      (single_integral / single_standard_dev**2 &
       + rambo_integral / rambo_standard_dev**2) &
      / (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    standard_dev = 1.0_double &
      / sqrt (1.0_double / single_standard_dev**2 &
       + 1.0_double / rambo_standard_dev**2)
    chi_squared = &
      ((single_integral - integral)**2 / single_standard_dev**2) &
      + ((rambo_integral - integral)**2 / rambo_standard_dev**2)
    print *, "S&R:   ", integral, standard_dev, chi_squared
  end if
case default
  if (proc_id == 0) then
    print *, "???: ", command
    !!! TO BE REMOVED !!!
    call check_kinematics (rng)
    allocate (region(2,5))
    region(1,:) = 0
    region(2,:) = 1
    do i = 1, 10
      call tao_random_number (rng, x)
      call vamp_jacobian (phi12, 0, x, region, jac)
      print *, "12:  ", jac, 1 / g12 (x), jac * g12 (x) - 1
      call vamp_jacobian (phi21, 0, x, region, jac)
      print *, "21:  ", jac, 1 / g21 (x), jac * g21 (x) - 1
      print *, "1:   ", real(x)
      print *, "2:   ", real(phi12(phi21(x,0),0))
      print *, "2':  ", real(phi12(phi21(x,-1),-1))
      print *, "3:   ", real(phi21(phi12(x,0),0))
      print *, "3':  ", real(phi21(phi12(x,-1),-1))
      print *, "2-1: ", real(phi12(phi21(x,0),0) - x)
    end do
  end if
end case

```

```

        print *, "3-1: ", real(phi21(phi12(x,0),0) - x)
        print *, "a:   ", real(phi12(x,0))
        print *, "a':  ", real(phi12(x,-1))
        print *, "b:   ", real(phi21(x,0))
        print *, "b':  ", real(phi21(x,-1))
    end do
    deallocate (region)
    ! do i = 2, 5
    !     print *, i, phase_space_volume (i, 200.0_double)
    ! end do
end if
end select
if (proc_id == 0) then
    call system_clock (ticks, ticks_per_second)
    print "(1X,A,F8.2,A)", &
        "time = ", real (ticks - ticks0) / ticks_per_second, " secs"
end if
call mpi90_finalize ()
end program application
242a  <Application in single channel mode 242a>≡ (239)
    allocate (region(2,5))
    region(1,:) = 0.0
    region(2,:) = 1.0
    call vamp_create_grid (gr, region, calls(1))
    call clear_exception (exc)
    call vamp_sample_grid &
        (rng, gr, sigma, iterations(1), history = history, exc = exc)
    call handle_exception (exc)
    call vamp_discard_integral (gr, calls(2))
    call vamp_sample_grid &
        (rng, gr, sigma, iterations(2), &
         integral, standard_dev, chi_squared, &
         history = history(iterations(1)+1:), exc = exc)
    call handle_exception (exc)
    call vamp_print_history (history, "single")
    if (proc_id == 0) then
        print *, "SINGLE: ", integral, standard_dev, chi_squared
    end if
    call vamp_write_grid (gr, "application.grid")
    call vamp_delete_grid (gr)
    deallocate (region)
242b  <Application in massless single channel mode 242b>≡ (239)
    allocate (region(2,5))

```

```

region(1,:) = 0.0
region(2,:) = 1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
    (rng, gr, sigma_massless, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
    (rng, gr, sigma_massless, iterations(2), &
     integral, standard_dev, chi_squared, &
     history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "single")
if (proc_id == 0) then
    print *, "M=0:   ", integral, standard_dev, chi_squared
end if
call vamp_write_grid (gr, "application.grid")
call vamp_delete_grid (gr)
deallocate (region)

```

243 *Application in multi channel mode 243* ≡ (239)

```

allocate (region(2,5))
region(1,:) = 0.0
region(2,:) = 1.0
weight_vector = 1.0
if (proc_id == 0) then
    read *, weight_vector
end if
call mpi90_broadcast (weight_vector, 0)
weight_vector = weight_vector / sum (weight_vector)
call vamp_create_grids (grs, region, calls(1), weight_vector)
do i = 1, 3
    call clear_exception (exc)
    call vamp_sample_grids &
        (rng, grs, wx, iterations(1), &
         history = history(1+(i-1)*iterations(1):), &
         histories = histories(1+(i-1)*iterations(1):,:), exc = exc)
    call handle_exception (exc)
    call vamp_refine_weights (grs)
end do
call vamp_discard_integrals (grs, calls(2))
call vamp_sample_grids &
    (rng, grs, wx, iterations(2), &

```

```

        integral, standard_dev, chi_squared, &
        history = history(3*iterations(1)+1:), &
        histories = histories(3*iterations(1)+1:,:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "multi")
call vamp_print_history (histories, "multi")
if (proc_id == 0) then
    print *, "MULTI: ", integral, standard_dev, chi_squared
end if
call vamp_write_grids (grs, "application.grids")
call vamp_delete_grids (grs)
deallocate (region)

```

244 *Application in Rambo mode 244*≡

(239)

```

allocate (region(2,12))
region(1,:) = 0.0
region(2,:) = 1.0
call vamp_create_grid (gr, region, calls(1))
call clear_exception (exc)
call vamp_sample_grid &
    (rng, gr, sigma_rambo, iterations(1), history = history, exc = exc)
call handle_exception (exc)
call vamp_discard_integral (gr, calls(2))
call vamp_sample_grid &
    (rng, gr, sigma_rambo, iterations(2), &
    integral, standard_dev, chi_squared, &
    history = history(iterations(1)+1:), exc = exc)
call handle_exception (exc)
call vamp_print_history (history, "rambo")
if (proc_id == 0) then
    print *, "RAMBO: ", integral, standard_dev, chi_squared
end if
call vamp_delete_grid (gr)
deallocate (region)

```

—A—

CONSTANTS

A.1 Kinds

This borders on overkill, but it is the most portable way to get double precision in standard Fortran without relying on `kind (1.0D0)`. Currently, it is possible to change `double` to any other supported real kind. The MPI interface is a potential trouble source for such things, however.

```
245a <vamp_kinds.f90 245a>≡
      ! vamp_kinds.f90 --
      <Copyleft notice 1>
      module kinds
        implicit none
        integer, parameter, private :: single = &
          & selected_real_kind (precision(1.0), range(1.0))
        integer, parameter, private :: double = &
          & selected_real_kind (precision(1.0_single) + 1, range(1.0_single) + 1)
        integer, parameter, private :: extended = &
          & selected_real_kind (precision (1.0_double) + 1, range (1.0_double))
        integer, parameter, public :: default = double
        character(len=*), public, parameter :: KINDS_RCS_ID = &
          "$Id: kinds.nw 314 2010-04-17 20:32:33Z ohl $"
      end module kinds
```

A.2 Mathematical and Physical Constants

```
245b <constants.f90 245b>≡
      ! constants.f90 --
      <Copyleft notice 1>
```

```
module constants
  use kinds
  implicit none
  private
  real(kind=default), public, parameter :: &
    PI = 3.1415926535897932384626433832795028841972_default
  character(len=*), public, parameter :: CONSTANTS_RCS_ID = &
    "$Id: constants.nw 314 2010-04-17 20:32:33Z ohl $"
end module constants
```

—B—

ERRORS AND EXCEPTIONS

Fortran95 does not allow *any* I/O in pure and elemental procedures, not even output to the unit *. A stop statement is verboten as well. Therefore we have to use condition codes

```
247a <exceptions.f90 247a>≡
! exceptions.f90 --
<Copyleft notice 1>
module exceptions
  use kinds
  implicit none
  private
  <Declaration of exceptions procedures 248b>
  <Interfaces of exceptions procedures (never defined)>
  <Variables in exceptions 247c>
  <Declaration of exceptions types 247b>
  character(len=*), public, parameter :: EXCEPTIONS_RCS_ID = &
    "$Id: exceptions.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    <Implementation of exceptions procedures 248c>
  end module exceptions

247b <Declaration of exceptions types 247b>≡ (247a)
  type, public :: exception
    integer :: level = EXC_NONE
    character(len=NAME_LENGTH) :: message = ""
    character(len=NAME_LENGTH) :: origin = ""
  end type exception

247c <Variables in exceptions 247c>≡ (247a) 248a>
  integer, public, parameter :: &
    EXC_NONE = 0, &
    EXC_INFO = 1, &
    EXC_WARN = 2, &
```



```

    EXC_ERROR = 3, &
    EXC_FATAL = 4

```

248a *<Variables in exceptions 247c>+≡* (247a) *<247c*

```

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

```

248b *<Declaration of exceptions procedures 248b>≡* (247a) 248d*>*

```

    public :: handle_exception

```

248c *<Implementation of exceptions procedures 248c>≡* (247a) 248e*>*

```

    subroutine handle_exception (exc)
        type(exception), intent(inout) :: exc
        character(len=10) :: name
        if (exc%level > 0) then
            select case (exc%level)
                case (EXC_NONE)
                    name = "(none)"
                case (EXC_INFO)
                    name = "info"
                case (EXC_WARN)
                    name = "warning"
                case (EXC_ERROR)
                    name = "error"
                case (EXC_FATAL)
                    name = "fatal"
                case default
                    name = "invalid"
            end select
            print *, trim (exc%origin), ": ", trim(name), ": ", trim (exc%message)
            if (exc%level >= EXC_FATAL) then
                print *, "terminated."
                stop
            end if
        end if
    end subroutine handle_exception

```

248d *<Declaration of exceptions procedures 248b>+≡* (247a) *<248b*

```

    public :: raise_exception, clear_exception, gather_exceptions

```

Raise an exception, but don't overwrite the messages in `exc` if it holds a more severe exception. This way we can accumulate error codes across procedure calls. We have `exc` optional to simplify life for the calling procedures, which might have it optional themselves.

248e *<Implementation of exceptions procedures 248c>+≡* (247a) *<248c 249a>*

```

    elemental subroutine raise_exception (exc, level, origin, message)

```

```

type(exception), intent(inout), optional :: exc
integer, intent(in), optional :: level
character(len=*), intent(in), optional :: origin, message
integer :: local_level
if (present (exc)) then
  if (present (level)) then
    local_level = level
  else
    local_level = EXC_DEFAULT
  end if
  if (exc%level < local_level) then
    exc%level = local_level
    if (present (origin)) then
      exc%origin = origin
    else
      exc%origin = "[vamp]"
    end if
    if (present (message)) then
      exc%message = message
    else
      exc%message = "[vamp]"
    end if
  end if
end if
end subroutine raise_exception

```

249a *⟨Implementation of exceptions procedures 248c⟩+≡* (247a) *◁248e 249b▷*

```

elemental subroutine clear_exception (exc)
  type(exception), intent(inout) :: exc
  exc%level = 0
  exc%message = ""
  exc%origin = ""
end subroutine clear_exception

```

249b *⟨Implementation of exceptions procedures 248c⟩+≡* (247a) *◁249a*

```

pure subroutine gather_exceptions (exc, excs)
  type(exception), intent(inout) :: exc
  type(exception), dimension(:), intent(in) :: excs
  integer :: i
  i = sum (maxloc (excs%level))
  if (exc%level < excs(i)%level) then
    call raise_exception (exc, excs(i)%level, excs(i)%origin, &
                        excs(i)%message)
  end if
end subroutine gather_exceptions

```

Here's how to use `gather_exceptions`. `elemental_procedure`

250 *<Idioms 101c>+≡*

<101c

```
call clear_exception (excs)
call elemental_procedure_1 (y, x, excs)
call elemental_procedure_2 (b, a, excs)
if (any (excs%level > 0)) then
  call gather_exceptions (exc, excs)
  return
end if
```

—C—

THE ART OF RANDOM NUMBERS

Volume two of Donald E. Knuth’ *The Art of Computer Programming* [16] has always been celebrated as a prime reference for random number generation. Recently, the third edition has been published and it contains a gem of a *portable* random number generator. It generates 30-bit integers with the following desirable properties

- they pass all the tests from George Marsaglia’s “diehard” suite of tests for random number generators [24] (but see [16] for a caveat regarding the “birthday-spacing” test)
- they can be generated with portable signed 32-bit arithmetic (Fortran can’t do unsigned arithmetic)
- it is faster than other lagged Fibonacci generators
- it can create at least $2^{30} - 2$ independent sequences

We implement the improved versions available as FORTRAN77 code from

<http://www-cs-faculty.stanford.edu/~uno/programs.html#rng>

that contain a streamlined seeding algorithm with better independence of substreams.

C.1 Application Program Interface

A function returning single reals and integers. Note that the static version without the `tao_random_state` argument does not require initialization. It will behave as if call `tao_random_seed(0)` had been executed. On the other hand, the parallelizable version with the explicit `tao_random_state` will fail if none of the `tao_random_create` have been called for the state. (This is a deficiency of Fortran90 that can be fixed in Fortran95).

251 *<API documentation 251>*≡ 252a>

```
call tao_random_number (r)
call tao_random_number (s, r)
```

The state of the random number generator comes in two varieties: buffered and raw. The former is much more efficient, but it can be beneficial to flush the buffers and to pass only the raw state in order to save of interprocess communication (IPC) costs.

252a *<API documentation 251>*+≡ <251 252b>

```
type(tao_random_state) :: s
type(tao_random_raw_state) :: rs
```

Subroutines filling arrays of reals and integers:

252b *<API documentation 251>*+≡ <252a 252c>

```
call tao_random_number (a, num = n)
call tao_random_number (s, a, num = n)
```

Subroutine for changing the seed:

252c *<API documentation 251>*+≡ <252b 252d>

```
call tao_random_seed (seed = seed)
call tao_random_seed (s, seed = seed)
```

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

252d *<API documentation 251>*+≡ <252c 252e>

```
call tao_random_luxury ()
call tao_random_luxury (s)
```

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

252e *<API documentation 251>*+≡ <252d 252f>

```
call tao_random_luxury (n)
call tao_random_luxury (s, n)
```

With a floating point argument, use that fraction of each fill of the buffer:

252f *<API documentation 251>*+≡ <252e 252g>

```
call tao_random_luxury (x)
call tao_random_luxury (s, x)
```

Create a **tao_random_state**

252g *<API documentation 251>*+≡ <252f 252h>

```
call tao_random_create (s, seed, buffer_size = buffer_size)
call tao_random_create (s, raw_state, buffer_size = buffer_size)
call tao_random_create (s, state)
```

Create a **tao_random_raw_state**

252h *<API documentation 251>*+≡ <252g 253a>

```
call tao_random_create (rs, seed)
call tao_random_create (rs, raw_state)
call tao_random_create (rs, state)
```

Destroy a `tao_random_state` or `tao_random_raw_state`

253a *<API documentation 251>+≡* *<252h 253b>*

```
call tao_random_destroy (s)
```

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

253b *<API documentation 251>+≡* *<253a 253c>*

```
call tao_random_copy (lhs, rhs)
lhs = rhs
```

253c *<API documentation 251>+≡* *<253b 253d>*

```
call tao_random_flush (s)
```

253d *<API documentation 251>+≡* *<253c 253e>*

```
call tao_random_read (s, unit)
call tao_random_write (s, unit)
```

253e *<API documentation 251>+≡* *<253d 253f>*

```
call tao_random_test (name = name)
```

Here is a sample application of random number states:

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

```
subroutine threads (args, y, state)
  real, dimension(:), intent(in) :: args
  real, dimension(:), intent(out) :: y
  type(tao_random_state) :: state
  integer :: seed
  type(tao_random_raw_state), dimension(size(y)) :: states
  integer :: s
  call tao_random_number (state, seed)
  call tao_random_create (states, (/ (s, s=seed,size(y)-1) /))
  y = thread (args, states)
end function thread
```

In this example, we could equivalently pass an integer seed, instead of `raw_state`. But in more complicated cases it can be beneficial to have the option of reusing `raw_state` in the calling routine.

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

```
elemental function thread (arg, raw_state) result (y)
  real, dimension, intent(in) :: arg
  type(tao_random_raw_state) :: raw_state
  real :: y
  type(tao_random_state) :: state
  real :: r
  call tao_random_create (state, raw_state)
do
  ...
```

```

        call tao_random_number (state, r)
        ...
    end do
end function thread

```

C.2 Low Level Routines

Here the low level routines are *much* more interesting than the high level routines. The latter contain a lot of duplication (made necessary by Fortran’s lack of parametric polymorphism) and consist mostly of bookkeeping. We wil therefore start with the former.

C.2.1 Generation of 30-bit Random Numbers

The generator is a subtractive lagged Fibonacci

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

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

254a \langle Parameters in tao_random_numbers 254a $\rangle \equiv$ (273c 274a) 254d \triangleright
integer, parameter, private :: K = 100, L = 37

Other good choices for K and L are (cf. [16], table 1 in section 3.2.2, p. 29)

254b \langle Parameters in tao_random_numbers (alternatives) 254b $\rangle \equiv$
integer, parameter, private :: K = 55, L = 24
integer, parameter, private :: K = 89, L = 38
integer, parameter, private :: K = 100, L = 37
integer, parameter, private :: K = 127, L = 30
integer, parameter, private :: K = 258, L = 83
integer, parameter, private :: K = 378, L = 107
integer, parameter, private :: K = 607, L = 273

A modulus of 2^{30} is the largest we can handle in *portable* (i.e. *signed*) 32-bit arithmetic

254c \langle Variables in 30-bit tao_random_numbers 254c $\rangle \equiv$ (273c) 256a \triangleright
integer(kind=tao_i32), parameter, private :: M = 2**30

generate fills the array a_1, \dots, a_n with random integers $0 \leq a_i < 2^{30}$. We *must* have at least $n \geq K$. Higher values don’t change the results, but make **generate** more efficient (about a factor of two, asymptotically). For $K = 100$, DEK recommends $n \geq 1000$. Best results are obtained using the first 100 random numbers out of 1009. Let’s therefore use 1009 as a default buffer size. The user can call **tao_random_luxury** (100) him/herself:

254d \langle Parameters in `tao_random_numbers` 254a $\rangle + \equiv$ (273c 274a) \triangleleft 254a
integer, parameter, private :: `DEFAULT_BUFFER_SIZE` = 1009

Since users are not expected to call `generate` directly, we do *not* check for $n \geq K$ and assume that the caller knows what (s)he's doing ...

255a \langle Implementation of 30-bit `tao_random_numbers` 255a $\rangle \equiv$ (273c) 256d \triangleright
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 255c \rangle
end subroutine `generate`

255b \langle Declaration of `tao_random_numbers` 255b $\rangle \equiv$ (273c 274a) 258g \triangleright
private :: `generate`

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

255c \langle Load a and refresh state 255c $\rangle \equiv$ (255a) 255d \triangleright
a(1:K) = state(1:K)

The remaining $n - K$ random numbers can be gotten directly from the recursion (C.1). Note that Fortran90's `modulo` intrinsic does the right thing, since it guarantees (unlike Fortran77's `mod`) that $0 \leq \text{modulo}(a, m) < a$ if $m > 0$).

255d \langle Load a and refresh state 255c $\rangle + \equiv$ (255a) \triangleleft 255c 255e \triangleright
do j = K+1, n
a(j) = modulo (a(j-K) - a(j-L), M)
end do

Do the recursion (C.1) K more times to prepare `state(1:K)` for the next invocation of `generate`.

255e \langle Load a and refresh state 255c $\rangle + \equiv$ (255a) \triangleleft 255d \triangleright
state(1:L) = modulo (a(n+1-K:n+L-K) - a(n+1-L:n), M)
do j = L+1, K
state(j) = modulo (a(n+j-K) - state(j-L), M)
end do

C.2.2 Initialization of 30-bit Random Numbers

The non-trivial and most beautiful part is the algorithm to initialize the random number generator state `state` with the first K numbers. I haven't studied algebra over finite fields in sufficient depth to consider the mathematics behind it straightforward. The commentary below is rather verbose and reflects my understanding of DEK's rather terse remarks (solution to exercise 3.6-9 [16]).

255f \langle Implementation of `tao_random_numbers` 255f $\rangle \equiv$ (273c 274a) 256b \triangleright


```

subroutine seed_static (seed)
  integer, optional, intent(in) :: seed
  call seed_stateless (s_state, seed)
  s_virginal = .false.
  s_last = size (s_buffer)
end subroutine seed_static

```

The static version of `tao_random_raw_state`:

256a *<Variables in 30-bit tao_random_numbers 254c>+≡ (273c) <254c 275b>*

```

integer(kind=tao_i32), dimension(K), save, private :: s_state
logical, save, private :: s_virginal = .true.

```

256b *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <255f 256c>*

```

elemental subroutine seed_raw_state (s, seed)
  type(tao_random_raw_state), intent(inout) :: s
  integer, optional, intent(in) :: seed
  call seed_stateless (s%x, seed)
end subroutine seed_raw_state

```

256c *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <256b 262b>*

```

elemental subroutine seed_state (s, seed)
  type(tao_random_state), intent(inout) :: s
  integer, optional, intent(in) :: seed
  call seed_raw_state (s%state, seed)
  s%last = size (s%buffer)
end subroutine seed_state

```

This incarnation of the procedure is pure.

256d *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <255a 267b>*

```

pure subroutine seed_stateless (state, seed)
  integer(kind=tao_i32), dimension(:), intent(out) :: state
  integer, optional, intent(in) :: seed
  <Parameters local to tao_random_seed 257a>
  integer :: seed_value, j, s, t
  integer(kind=tao_i32), dimension(2*K-1) :: x
  <Set up seed_value from seed or DEFAULT_SEED 257c>
  <Bootstrap the x buffer 257d>
  <Set up s and t 257f>
  do
    <p(z) → p(z)2 (modulo zK + zL + 1) 257g>
    <p(z) → zp(z) (modulo zK + zL + 1) 258b>
    <Shift s or t and exit if t ≤ 0 258c>
  end do
  <Fill state from x 258d>
  <Warm up state 258e>
end subroutine seed_stateless

```

Any default will do

257a \langle Parameters local to tao_random_seed 257a $\rangle \equiv$ (256d 259e) 257b \triangleright
integer, parameter :: DEFAULT_SEED = 0

These must not be changed:

257b \langle Parameters local to tao_random_seed 257a $\rangle + \equiv$ (256d 259e) \triangleleft 257a
integer, parameter :: MAX_SEED = 2**30 - 3
integer, parameter :: TT = 70

257c \langle Set up seed_value from seed or DEFAULT_SEED 257c $\rangle \equiv$ (256d 259e)
if (present (seed)) then
seed_value = modulo (seed, MAX_SEED + 1)
else
seed_value = DEFAULT_SEED
end if

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

257d \langle Bootstrap the x buffer 257d $\rangle \equiv$ (256d) 257e \triangleright
s = seed_value - modulo (seed_value, 2) + 2
do j = 1, K
x(j) = s
s = 2*s
if (s >= M) then
s = s - M + 2
end if
end do
x(K+1:2*K-1) = 0

Make x_2 (and only x_2) odd:

257e \langle Bootstrap the x buffer 257d $\rangle + \equiv$ (256d) \triangleleft 257d
x(2) = x(2) + 1

257f \langle Set up s and t 257f $\rangle \equiv$ (256d 259e)
s = seed_value
t = TT - 1

Consider the polynomial

$$p(z) = \sum_{n=1}^K x_n z^{n-1} = x_K z^{K-1} + \dots + x_2 z + x_1 \quad (\text{C.2})$$

We have $p(z)^2 = p(z^2) \pmod{2}$ because cross terms have an even coefficient and $x_n^2 = x_n \pmod{2}$. Therefore we can square the polynomial by shifting the coefficients. The coefficients for $n > K$ will be reduced.

257g $\langle p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1} \rangle \equiv$ (256d) 258a \triangleright
x(3:2*K-1:2) = x(2:K)
x(2:2*K-2:2) = 0

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

```

258a  <p(z) → p(z)2 (modulo  $z^K + z^L + 1$ ) 257g>+≡ (256d) <257g
      do j = 2*K-1, K+1, -1
        x(j-(K-L)) = modulo (x(j-(K-L))-x(j), M)
        x(j-K)=modulo (x(j-K)-x(j), M)
      end do

258b  <p(z) → zp(z) (modulo  $z^K + z^L + 1$ ) 258b>≡ (256d)
      if (modulo (s, 2) == 1) then
        x(2:K+1) = x(1:K)
        x(1) = x(K+1)
        x(L+1) = modulo (x(L+1) - x(K+1), M)
      end if

258c  <Shift s or t and exit if t ≤ 0 258c>≡ (256d 259e)
      if (s /= 0) then
        s = s / 2
      else
        t = t - 1
      end if
      if (t <= 0) then
        exit
      end if

258d  <Fill state from x 258d>≡ (256d 259e)
      state(1:K-L) = x(L+1:K)
      state(K-L+1:K) = x(1:L)

258e  <Warm up state 258e>≡ (256d 259e)
      do j = 1, 10
        call generate (x, state)
      end do

258f  <Interfaces of tao_random_numbers 258f>≡ (273c 274a) 261e>
      interface tao_random_seed
        module procedure <Specific procedures for tao_random_seed 258h>
      end interface

258g  <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <255b 260a>
      private :: <Specific procedures for tao_random_seed 258h>

258h  <Specific procedures for tao_random_seed 258h>≡ (258)
      seed_static, seed_state, seed_raw_state

```

C.2.3 Generation of 52-bit Random Numbers

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

259a *<Variables in 52-bit tao_random_numbers 259a>*≡ (274a) 259b>
`real(kind=tao_r64), parameter, private :: M = 1.0_tao_r64`

The state of the internal routines

259b *<Variables in 52-bit tao_random_numbers 259a>*+≡ (274a) <259a 276a>
`real(kind=tao_r64), dimension(K), save, private :: s_state`
`logical, save, private :: s_virginal = .true.`

259c *<Implementation of 52-bit tao_random_numbers 259c>*≡ (274a) 259e>
`pure subroutine generate (a, state)`
`real(kind=tao_r64), dimension(:), intent(inout) :: a`
`real(kind=tao_r64), dimension(:), intent(inout) :: state`
`integer :: j, n`
`n = size (a)`
<Load 52-bit a and refresh state 259d>
`end subroutine generate`

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

259d *<Load 52-bit a and refresh state 259d>*≡ (259c)
`a(1:K) = state(1:K)`
`do j = K+1, n`
`a(j) = modulo (a(j-K) + a(j-L), M)`
`end do`
`state(1:L) = modulo (a(n+1-K:n+L-K) + a(n+1-L:n), M)`
`do j = L+1, K`
`state(j) = modulo (a(n+j-K) + state(j-L), M)`
`end do`

C.2.4 Initialization of 52-bit Random Numbers

This incarnation of the procedure is pure.

259e *<Implementation of 52-bit tao_random_numbers 259c>*+≡ (274a) <259c 267f>
`pure subroutine seed_stateless (state, seed)`
`real(kind=tao_r64), dimension(:), intent(out) :: state`
`integer, optional, intent(in) :: seed`
<Parameters local to tao_random_seed 257a>
<Variables local to 52-bit tao_random_seed 260b>
<Set up seed_value from seed or DEFAULT_SEED 257c>
<Bootstrap the 52-bit x buffer 260d>
<Set up s and t 257f>

```

do
  <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  260f>
  <52-bit  $p(z) \rightarrow zp(z) \pmod{z^K + z^L + 1}$  260h>
  <Shift s or t and exit if  $t \leq 0$  258c>
end do
<Fill state from x 258d>
<Warm up state 258e>
end subroutine seed_stateless

260a <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <258g 261f>
private :: seed_stateless

260b <Variables local to 52-bit tao_random_seed 260b>≡ (259e) 260c>
real(kind=tao_r64), parameter :: ULP = 2.0_tao_r64**(-52)

260c <Variables local to 52-bit tao_random_seed 260b>+≡ (259e) <260b>
real(kind=tao_r64), dimension(2*K-1) :: x
real(kind=tao_r64) :: ss
integer :: seed_value, t, s, j

260d <Bootstrap the 52-bit x buffer 260d>≡ (259e) 260e>
ss = 2*ULP * (seed_value + 2)
do j = 1, K
  x(j) = ss
  ss = 2*ss
  if (ss >= 1) then
    ss = ss - 1 + 2*ULP
  end if
end do
x(K+1:2*K-1) = 0.0

260e <Bootstrap the 52-bit x buffer 260d>+≡ (259e) <260d>
x(2) = x(2) + ULP

260f <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  260f>≡ (259e) 260g>
x(3:2*K-1:2) = x(2:K)
x(2:2*K-2:2) = 0

This works because 2*K-1 is odd

260g <52-bit  $p(z) \rightarrow p(z)^2 \pmod{z^K + z^L + 1}$  260f>+≡ (259e) <260f>
do j = 2*K-1, K+1, -1
  x(j-(K-L)) = modulo (x(j-(K-L)) + x(j), M)
  x(j-K) = modulo (x(j-K) + x(j), M)
end do

260h <52-bit  $p(z) \rightarrow zp(z) \pmod{z^K + z^L + 1}$  260h>≡ (259e)
if (modulo (s, 2) == 1) THEN
  x(2:K+1) = x(1:K)

```

```

    x(1) = x(K+1)
    x(L+1) = modulo (x(L+1) + x(K+1), M)
end if

```

C.3 The State

- 261a \langle Declaration of 30-bit tao_random_numbers types 261a $\rangle \equiv$ (273c) 261b \triangleright
- ```

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

```
- 261b  $\langle$ Declaration of 30-bit tao\_random\_numbers types 261a $\rangle + \equiv$  (273c)  $\triangleleft$ 261a
- ```

type, public :: tao_random_state
private
type(tao_random_raw_state) :: state
integer(kind=tao_i32), dimension(:), pointer :: buffer => null ()
integer :: buffer_end, last
end type tao_random_state

```
- 261c \langle Declaration of 52-bit tao_random_numbers types 261c $\rangle \equiv$ (274a) 261d \triangleright
- ```

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

```
- 261d  $\langle$ Declaration of 52-bit tao\_random\_numbers types 261c $\rangle + \equiv$  (274a)  $\triangleleft$ 261c
- ```

type, public :: tao_random_state
private
type(tao_random_raw_state) :: state
real(kind=tao_r64), dimension(:), pointer :: buffer => null ()
integer :: buffer_end, last
end type tao_random_state

```

C.3.1 Creation

- 261e \langle Interfaces of tao_random_numbers 258f $\rangle + \equiv$ (273c 274a) \triangleleft 258f 263d \triangleright
- ```

interface tao_random_create
module procedure \langle Specific procedures for tao_random_create 262a \rangle
end interface

```
- 261f  $\langle$ Declaration of tao\_random\_numbers 255b $\rangle + \equiv$  (273c 274a)  $\triangleleft$ 260a 263e $\triangleright$
- ```

private ::  $\langle$ Specific procedures for tao_random_create 262a $\rangle$ 

```

262a \langle Specific procedures for tao_random_create 262a $\rangle \equiv$ (261)

```
create_state_from_seed, create_raw_state_from_seed, &
create_state_from_state, create_raw_state_from_state, &
create_state_from_raw_state, create_raw_state_from_raw_st
```

There are no procedures for copying the state of the static generator to or from an explicit `tao_random_state`. Users needing this functionality can be expected to handle explicit states anyway. Since the direction of the copying can not be obvious from the type of the argument, such functions would spoil the simplicity of the generic procedure interface.

262b \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273c 274a) \triangleleft 256c 262c \triangleright

```
elemental subroutine create_state_from_seed (s, seed, buffer_size)
  type(tao_random_state), intent(out) :: s
  integer, intent(in) :: seed
  integer, intent(in), optional :: buffer_size
  call create_raw_state_from_seed (s%state, seed)
  if (present (buffer_size)) then
    s%buffer_end = max (buffer_size, K)
  else
    s%buffer_end = DEFAULT_BUFFER_SIZE
  end if
  allocate (s%buffer(s%buffer_end))
  call tao_random_flush (s)
end subroutine create_state_from_seed
```

262c \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273c 274a) \triangleleft 262b 262d \triangleright

```
elemental subroutine create_state_from_state (s, state)
  type(tao_random_state), intent(out) :: s
  type(tao_random_state), intent(in) :: state
  call create_raw_state_from_raw_st (s%state, state%state)
  allocate (s%buffer(size(state%buffer)))
  call tao_random_copy (s, state)
end subroutine create_state_from_state
```

262d \langle Implementation of tao_random_numbers 255f $\rangle + \equiv$ (273c 274a) \triangleleft 262c 263a \triangleright

```
elemental subroutine create_state_from_raw_state &
  (s, raw_state, buffer_size)
  type(tao_random_state), intent(out) :: s
  type(tao_random_raw_state), intent(in) :: raw_state
  integer, intent(in), optional :: buffer_size
  call create_raw_state_from_raw_st (s%state, raw_state)
  if (present (buffer_size)) then
    s%buffer_end = max (buffer_size, K)
  else
    s%buffer_end = DEFAULT_BUFFER_SIZE
```

```

        end if
        allocate (s%buffer(s%buffer_end))
        call tao_random_flush (s)
    end subroutine create_state_from_raw_state
263a <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <262d 263b>
    elemental subroutine create_raw_state_from_seed (s, seed)
        type(tao_random_raw_state), intent(out) :: s
        integer, intent(in) :: seed
        call seed_raw_state (s, seed)
    end subroutine create_raw_state_from_seed
263b <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <263a 263c>
    elemental subroutine create_raw_state_from_state (s, state)
        type(tao_random_raw_state), intent(out) :: s
        type(tao_random_state), intent(in) :: state
        call copy_state_to_raw_state (s, state)
    end subroutine create_raw_state_from_state
263c <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <263b 263f>
    elemental subroutine create_raw_state_from_raw_st (s, raw_state)
        type(tao_random_raw_state), intent(out) :: s
        type(tao_random_raw_state), intent(in) :: raw_state
        call copy_raw_state (s, raw_state)
    end subroutine create_raw_state_from_raw_st

```

C.3.2 Destruction

```

263d <Interfaces of tao_random_numbers 258f>+≡ (273c 274a) <261e 264a>
    interface tao_random_destroy
        module procedure destroy_state, destroy_raw_state
    end interface
263e <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <261f 264c>
    private :: destroy_state, destroy_raw_state
263f <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <263c 263g>
    elemental subroutine destroy_state (s)
        type(tao_random_state), intent(inout) :: s
        deallocate (s%buffer)
    end subroutine destroy_state

```

Currently, this is a no-op, but we might need a non-trivial destruction method in the future

```

263g <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <263f 264e>
    elemental subroutine destroy_raw_state (s)

```



```

    type(tao_random_raw_state), intent(inout) :: s
end subroutine destroy_raw_state

```

C.3.3 Copying

- 264a *⟨Interfaces of tao_random_numbers 258f⟩+≡ (273c 274a) <263d 264b>*
- ```

 interface tao_random_copy
 module procedure ⟨Specific procedures for tao_random_copy 264d⟩
 end interface

```
- 264b *⟨Interfaces of tao\_random\_numbers 258f⟩+≡ (273c 274a) <264a 265d>*
- ```

    interface assignment(=)
        module procedure ⟨Specific procedures for tao_random_copy 264d⟩
    end interface

```
- 264c *⟨Declaration of tao_random_numbers 255b⟩+≡ (273c 274a) <263e 265e>*
- ```

 public :: assignment(=)
 private :: ⟨Specific procedures for tao_random_copy 264d⟩

```
- 264d *⟨Specific procedures for tao\_random\_copy 264d⟩≡ (264)*
- ```

    copy_state, copy_raw_state, &
    copy_raw_state_to_state, copy_state_to_raw_state

```
- 264e *⟨Implementation of tao_random_numbers 255f⟩+≡ (273c 274a) <263g 264f>*
- ```

 elemental subroutine copy_state (lhs, rhs)
 type(tao_random_state), intent(inout) :: lhs
 type(tao_random_state), intent(in) :: rhs
 call copy_raw_state (lhs%state, rhs%state)
 if (size (lhs%buffer) /= size (rhs%buffer)) then
 deallocate (lhs%buffer)
 allocate (lhs%buffer(size(rhs%buffer)))
 end if
 lhs%buffer = rhs%buffer
 lhs%buffer_end = rhs%buffer_end
 lhs%last = rhs%last
 end subroutine copy_state

```
- 264f *⟨Implementation of tao\_random\_numbers 255f⟩+≡ (273c 274a) <264e 265a>*
- ```

    elemental subroutine copy_raw_state (lhs, rhs)
        type(tao_random_raw_state), intent(out) :: lhs
        type(tao_random_raw_state), intent(in) :: rhs
        lhs%x = rhs%x
    end subroutine copy_raw_state

```

265a *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <264f 265b>*
 elemental subroutine copy_raw_state_to_state (lhs, rhs)
 type(tao_random_state), intent(inout) :: lhs
 type(tao_random_raw_state), intent(in) :: rhs
 call copy_raw_state (lhs%state, rhs)
 call tao_random_flush (lhs)
 end subroutine copy_raw_state_to_state

265b *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <265a 265c>*
 elemental subroutine copy_state_to_raw_state (lhs, rhs)
 type(tao_random_raw_state), intent(out) :: lhs
 type(tao_random_state), intent(in) :: rhs
 call copy_raw_state (lhs, rhs%state)
 end subroutine copy_state_to_raw_state

C.3.4 Flushing

265c *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <265b 266b>*
 elemental subroutine tao_random_flush (s)
 type(tao_random_state), intent(inout) :: s
 s%last = size (s%buffer)
 end subroutine tao_random_flush

C.3.5 Input and Output

265d *<Interfaces of tao_random_numbers 258f>+≡ (273c 274a) <264b 265f>*
 interface tao_random_write
 module procedure &
 write_state_unit, write_state_name, &
 write_raw_state_unit, write_raw_state_name
 end interface

265e *<Declaration of tao_random_numbers 255b>+≡ (273c 274a) <264c 266a>*
 private :: write_state_unit, write_state_name
 private :: write_raw_state_unit, write_raw_state_name

265f *<Interfaces of tao_random_numbers 258f>+≡ (273c 274a) <265d 270a>*
 interface tao_random_read
 module procedure &
 read_state_unit, read_state_name, &
 read_raw_state_unit, read_raw_state_name
 end interface

266a *<Declaration of tao_random_numbers 255b>+≡ (273c 274a) <265e 269b>*
 private :: read_state_unit, read_state_name
 private :: read_raw_state_unit, read_raw_state_name

266b *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <265c 266c>*
 subroutine write_state_unit (s, unit)
 type(tao_random_state), intent(in) :: s
 integer, intent(in) :: unit
 write (unit = unit, fmt = *) "BEGIN TAO_RANDOM_STATE"
 call write_raw_state_unit (s%state, unit)
 write (unit = unit, fmt = "(2(1x,a16,1x,i10/),1x,a16,1x,i10)") &
 "BUFFER_SIZE", size (s%buffer), &
 "BUFFER_END", s%buffer_end, &
 "LAST", s%last
 write (unit = unit, fmt = *) "BEGIN BUFFER"
 call write_state_array (s%buffer, unit)
 write (unit = unit, fmt = *) "END BUFFER"
 write (unit = unit, fmt = *) "END TAO_RANDOM_STATE"
 end subroutine write_state_unit

266c *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <266b 266d>*
 subroutine read_state_unit (s, unit)
 type(tao_random_state), intent(inout) :: s
 integer, intent(in) :: unit
 integer :: buffer_size
 read (unit = unit, fmt = *)
 call read_raw_state_unit (s%state, unit)
 read (unit = unit, fmt = "(2(1x,16x,1x,i10/),1x,16x,1x,i10)") &
 buffer_size, s%buffer_end, s%last
 read (unit = unit, fmt = *)
 if (buffer_size /= size (s%buffer)) then
 deallocate (s%buffer)
 allocate (s%buffer(buffer_size))
 end if
 call read_state_array (s%buffer, unit)
 read (unit = unit, fmt = *)
 read (unit = unit, fmt = *)
 end subroutine read_state_unit

266d *<Implementation of tao_random_numbers 255f>+≡ (273c 274a) <266c 267a>*
 subroutine write_raw_state_unit (s, unit)
 type(tao_random_raw_state), intent(in) :: s
 integer, intent(in) :: unit
 write (unit = unit, fmt = *) "BEGIN TAO_RANDOM_RAW_STATE"
 call write_state_array (s%x, unit)

```

        write (unit = unit, fmt = *) "END TAO_RANDOM_RAW_STATE"
    end subroutine write_raw_state_unit
267a  <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <266d 268d>
    subroutine read_raw_state_unit (s, unit)
        type(tao_random_raw_state), intent(inout) :: s
        integer, intent(in) :: unit
        read (unit = unit, fmt = *)
        call read_state_array (s%x, unit)
        read (unit = unit, fmt = *)
    end subroutine read_raw_state_unit
267b  <Implementation of 30-bit tao_random_numbers 255a>+≡      (273c) <256d 267d>
    subroutine write_state_array (a, unit)
        integer(kind=tao_i32), dimension(:), intent(in) :: a
        integer, intent(in) :: unit
        integer :: i
        do i = 1, size (a)
            write (unit = unit, fmt = "(1x,i10,1x,i10)") i, a(i)
        end do
    end subroutine write_state_array
267c  <Declaration of 30-bit tao_random_numbers 267c>≡      (273c) 267e>
    private :: write_state_array
267d  <Implementation of 30-bit tao_random_numbers 255a>+≡      (273c) <267b 270c>
    subroutine read_state_array (a, unit)
        integer(kind=tao_i32), dimension(:), intent(inout) :: a
        integer, intent(in) :: unit
        integer :: i, idum
        do i = 1, size (a)
            read (unit = unit, fmt = *) idum, a(i)
        end do
    end subroutine read_state_array
267e  <Declaration of 30-bit tao_random_numbers 267c>+≡      (273c) <267c 281a>
    private :: read_state_array

```

Reading and writing 52-bit floating point numbers accurately is beyond most Fortran runtime libraries. Their job is simplified considerably if we rescale by 2^{52} before writing. Then the temptation to truncate will not be as overwhelming as before ...

```

267f  <Implementation of 52-bit tao_random_numbers 259c>+≡      (274a) <259e 268b>
    subroutine write_state_array (a, unit)
        real(kind=tao_r64), dimension(:), intent(in) :: a
        integer, intent(in) :: unit
        integer :: i

```

```

do i = 1, size (a)
    write (unit = unit, fmt = "(1x,i10,1x,f30.0)") i, 2.0_tao_r64**52 * a(i)
end do
end subroutine write_state_array

268a <Declaration of 52-bit tao_random_numbers 268a>≡ (274a) 268c>
private :: write_state_array

268b <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <267f 272a>
subroutine read_state_array (a, unit)
    real(kind=tao_r64), dimension(:), intent(inout) :: a
    integer, intent(in) :: unit
    real(kind=tao_r64) :: x
    integer :: i, idum
do i = 1, size (a)
    read (unit = unit, fmt = *) idum, x
    a(i) = 2.0_tao_r64**(-52) * x
end do
end subroutine read_state_array

268c <Declaration of 52-bit tao_random_numbers 268a>+≡ (274a) <268a 281e>
private :: read_state_array

268d <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <267a 269c>
subroutine find_free_unit (u, iostat)
    integer, intent(out) :: u
    integer, intent(out), optional :: iostat
    logical :: exists, is_open
    integer :: i, status
do i = MIN_UNIT, MAX_UNIT
    inquire (unit = i, exist = exists, opened = is_open, &
        iostat = status)
    if (status == 0) then
        if (exists .and. .not. is_open) then
            u = i
            if (present (iostat)) then
                iostat = 0
            end if
            return
        end if
    end if
end do
if (present (iostat)) then
    iostat = -1
end if
u = -1

```

```

end subroutine find_free_unit

269a  <Variables in tao_random_numbers 269a>≡ (273c 274a)
      integer, parameter, private :: MIN_UNIT = 11, MAX_UNIT = 99

269b  <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <266a 270b>
      private :: find_free_unit

269c  <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <268d 269d>
      subroutine write_state_name (s, name)
        type(tao_random_state), intent(in) :: s
        character(len=*), intent(in) :: name
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", file = name)
        call write_state_unit (s, unit)
        close (unit = unit)
      end subroutine write_state_name

269d  <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <269c 269e>
      subroutine write_raw_state_name (s, name)
        type(tao_random_raw_state), intent(in) :: s
        character(len=*), intent(in) :: name
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "write", status = "replace", file = name)
        call write_raw_state_unit (s, unit)
        close (unit = unit)
      end subroutine write_raw_state_name

269e  <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <269d 269f>
      subroutine read_state_name (s, name)
        type(tao_random_state), intent(inout) :: s
        character(len=*), intent(in) :: name
        integer :: unit
        call find_free_unit (unit)
        open (unit = unit, action = "read", status = "old", file = name)
        call read_state_unit (s, unit)
        close (unit = unit)
      end subroutine read_state_name

269f  <Implementation of tao_random_numbers 255f>+≡ (273c 274a) <269e 281g>
      subroutine read_raw_state_name (s, name)
        type(tao_random_raw_state), intent(inout) :: s
        character(len=*), intent(in) :: name
        integer :: unit

```

```

call find_free_unit (unit)
open (unit = unit, action = "read", status = "old", file = name)
call read_raw_state_unit (s, unit)
close (unit = unit)
end subroutine read_raw_state_name

```

C.3.6 Marshaling and Unmarshaling

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

```

270a <Interfaces of tao_random_numbers 258f>+≡ (273c 274a) <265f
interface tao_random_marshall_size
  module procedure marshal_state_size, marshal_raw_state_size
end interface
interface tao_random_marshall
  module procedure marshal_state, marshal_raw_state
end interface
interface tao_random_unmarshal
  module procedure unmarshal_state, unmarshal_raw_state
end interface

270b <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <269b 274b>
public :: tao_random_marshall
private :: marshal_state, marshal_raw_state
public :: tao_random_marshall_size
private :: marshal_state_size, marshal_raw_state_size
public :: tao_random_unmarshal
private :: unmarshal_state, unmarshal_raw_state

270c <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <267d 271a>
pure subroutine marshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  integer :: buf_size
  buf_size = size (s%buffer)
  ibuf(1) = s%buffer_end
  ibuf(2) = s%last
  ibuf(3) = buf_size
  ibuf(4:3+buf_size) = s%buffer
  call marshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
end subroutine marshal_state

```

271a *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <270c 271b>*

```

pure subroutine marshal_state_size (s, iwords, dwords)
  type(tao_random_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  call marshal_raw_state_size (s%state, iwords, dwords)
  iwords = iwords + 3 + size (s%buffer)
end subroutine marshal_state_size

```

271b *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271a 271c>*

```

pure subroutine unmarshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  s%buffer_end = ibuf(1)
  s%last = ibuf(2)
  buf_size = ibuf(3)
  s%buffer = ibuf(4:3+buf_size)
  call unmarshal_raw_state (s%state, ibuf(4+buf_size:), dbuf)
end subroutine unmarshal_state

```

271c *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271b 271d>*

```

pure subroutine marshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  ibuf(1) = size (s%x)
  ibuf(2:1+size(s%x)) = s%x
end subroutine marshal_raw_state

```

271d *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271c 271e>*

```

pure subroutine marshal_raw_state_size (s, iwords, dwords)
  type(tao_random_raw_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  iwords = 1 + size (s%x)
  dwords = 0
end subroutine marshal_raw_state_size

```

271e *<Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271d 274c>*

```

pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  buf_size = ibuf(1)
  s%x = ibuf(2:1+buf_size)

```



```

end subroutine unmarshal_raw_state

272a <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <268b 272b>
pure subroutine marshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  integer :: buf_size
  buf_size = size (s%buffer)
  ibuf(1) = s%buffer_end
  ibuf(2) = s%last
  ibuf(3) = buf_size
  dbuf(1:buf_size) = s%buffer
  call marshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine marshal_state

272b <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <272a 272c>
pure subroutine marshal_state_size (s, iwords, dwords)
  type(tao_random_state), intent(in) :: s
  integer, intent(out) :: iwords, dwords
  call marshal_raw_state_size (s%state, iwords, dwords)
  iwords = iwords + 3
  dwords = dwords + size(s%buffer)
end subroutine marshal_state_size

272c <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <272b 272d>
pure subroutine unmarshal_state (s, ibuf, dbuf)
  type(tao_random_state), intent(inout) :: s
  integer, dimension(:), intent(in) :: ibuf
  real(kind=tao_r64), dimension(:), intent(in) :: dbuf
  integer :: buf_size
  s%buffer_end = ibuf(1)
  s%last = ibuf(2)
  buf_size = ibuf(3)
  s%buffer = dbuf(1:buf_size)
  call unmarshal_raw_state (s%state, ibuf(4:), dbuf(buf_size+1:))
end subroutine unmarshal_state

272d <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <272c 273a>
pure subroutine marshal_raw_state (s, ibuf, dbuf)
  type(tao_random_raw_state), intent(in) :: s
  integer, dimension(:), intent(inout) :: ibuf
  real(kind=tao_r64), dimension(:), intent(inout) :: dbuf
  ibuf(1) = size (s%x)
  dbuf(1:size(s%x)) = s%x
end subroutine marshal_raw_state

```

273a *<Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <272d 273b>*
 pure subroutine marshal_raw_state_size (s, iwords, dwords)
 type(tao_random_raw_state), intent(in) :: s
 integer, intent(out) :: iwords, dwords
 iwords = 1
 dwords = size (s%x)
 end subroutine marshal_raw_state_size

273b *<Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <273a 275e>*
 pure subroutine unmarshal_raw_state (s, ibuf, dbuf)
 type(tao_random_raw_state), intent(inout) :: s
 integer, dimension(:), intent(in) :: ibuf
 real(kind=tao_r64), dimension(:), intent(in) :: dbuf
 integer :: buf_size
 buf_size = ibuf(1)
 s%x = dbuf(1:buf_size)
 end subroutine unmarshal_raw_state

C.4 High Level Routines

273c *<tao_random_numbers.f90 273c>≡*
 ! tao_random_numbers.f90 --
<Copyleft notice 1>
 module tao_random_numbers
 use kinds
 implicit none
 integer, parameter, private :: tao_i32 = selected_int_kind (9)
 integer, parameter, private :: tao_r64 = selected_real_kind (15)
<Declaration of tao_random_numbers 255b>
<Declaration of 30-bit tao_random_numbers 267c>
<Interfaces of tao_random_numbers 258f>
<Interfaces of 30-bit tao_random_numbers 280e>
<Parameters in tao_random_numbers 254a>
<Variables in tao_random_numbers 269a>
<Variables in 30-bit tao_random_numbers 254c>
<Declaration of 30-bit tao_random_numbers types 261a>
 character(len=*), public, parameter :: TAO_RANDOM_NUMBERS_RCS_ID = &
 "\$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl \$"
 contains
<Implementation of tao_random_numbers 255f>
<Implementation of 30-bit tao_random_numbers 255a>
 end module tao_random_numbers

```

274a <tao52_random_numbers.f90 274a>≡
! tao52_random_numbers.f90 --
<Copyleft notice 1>
module tao52_random_numbers
  use kinds
  implicit none
  integer, parameter, private :: tao_i32 = selected_int_kind (9)
  integer, parameter, private :: tao_r64 = selected_real_kind (15)
  <Declaration of tao_random_numbers 255b>
  <Declaration of 52-bit tao_random_numbers 268a>
  <Interfaces of tao_random_numbers 258f>
  <Interfaces of 52-bit tao_random_numbers 281c>
  <Parameters in tao_random_numbers 254a>
  <Variables in tao_random_numbers 269a>
  <Variables in 52-bit tao_random_numbers 259a>
  <Declaration of 52-bit tao_random_numbers types 261c>
  character(len=*), public, parameter :: TAO52_RANDOM_NUMBERS_RCS_ID = &
    "$Id: tao_random_numbers.nw 314 2010-04-17 20:32:33Z ohl $"
  contains
    <Implementation of tao_random_numbers 255f>
    <Implementation of 52-bit tao_random_numbers 259c>
end module tao52_random_numbers

```

Ten functions are exported

```

274b <Declaration of tao_random_numbers 255b>+≡ (273c 274a) <270b>
public :: tao_random_number
public :: tao_random_seed
public :: tao_random_create
public :: tao_random_destroy
public :: tao_random_copy
public :: tao_random_read
public :: tao_random_write
public :: tao_random_flush
! public :: tao_random_luxury
public :: tao_random_test

```

C.4.1 Single Random Numbers

A random integer r with $0 \leq r < 2^{30} = 1073741824$:

```

274c <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <271e 275d>
  pure subroutine integer_stateless &
    (state, buffer, buffer_end, last, r)
    integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer

```

```

integer, intent(in) :: buffer_end
integer, intent(inout) :: last
integer, intent(out) :: r
integer, parameter :: NORM = 1
<Body of tao_random.* 275a>
end subroutine integer_stateless

```

275a <Body of tao_random.* 275a>≡ (274 275)
 <Step last and reload buffer iff necessary 275c>
 r = NORM * buffer(last)

The low level routine **generate** will fill an array a_1, \dots, a_n , which will be consumed and refilled like an input buffer. We need at least $n \geq K$ for the call to **generate**.

275b <Variables in 30-bit tao_random_numbers 254c>+≡ (273c) <256a
 integer(kind=tao_i32), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
 integer, save, private :: s_buffer_end = size(s_buffer)
 integer, save, private :: s_last = size(s_buffer)

Increment the index **last** and reload the array buffer, iff this buffer is exhausted. Throughout these routines, **last** will point to random number that has just been consumed. For the array filling routines below, this is simpler than pointing to the next waiting number.

275c <Step last and reload buffer iff necessary 275c>≡ (275a)
 last = last + 1
 if (last > buffer_end) then
 call generate(buffer, state)
 last = 1
 end if

A random real $r \in [0, 1)$. This is almost identical to **tao_random_integer**, but we duplicate the code to avoid the function call overhead for speed.

275d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <274c 276b>
 pure subroutine real_stateless(state, buffer, buffer_end, last, r)
 integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
 integer, intent(in) :: buffer_end
 integer, intent(inout) :: last
 real(kind=default), intent(out) :: r
 real(kind=default), parameter :: NORM = 1.0_default / M
 <Body of tao_random.* 275a>
 end subroutine real_stateless

A random real $r \in [0, 1)$.

275e <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <273b 278a>
 pure subroutine real_stateless(state, buffer, buffer_end, last, r)
 real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer

```

integer, intent(in) :: buffer_end
integer, intent(inout) :: last
real(kind=default), intent(out) :: r
integer, parameter :: NORM = 1
<Body of tao_random.* 275a>
end subroutine real_stateless

```

The low level routine `generate` will fill an array a_1, \dots, a_N , which will be consumed and refilled like an input buffer.

276a <Variables in 52-bit tao_random_numbers 259a>+≡ (274a) <259b

```

real(kind=tao_r64), dimension(DEFAULT_BUFFER_SIZE), save, private :: s_buffer
integer, save, private :: s_buffer_end = size (s_buffer)
integer, save, private :: s_last = size (s_buffer)

```

C.4.2 Arrays of Random Numbers

Fill the array j_1, \dots, j_ν with random integers $0 \leq j_i < 2^{30} = 1073741824$. This has to be done such that the underlying array length in `generate` is transparent to the user. At the same time we want to avoid the overhead of calling `tao_random_real` ν times.

276b <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <275d 277e>

```

pure subroutine integer_array_stateless &
  (state, buffer, buffer_end, last, v, num)
integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
integer, intent(in) :: buffer_end
integer, intent(inout) :: last
integer, dimension(:), intent(out) :: v
integer, optional, intent(in) :: num
integer, parameter :: NORM = 1
<Body of tao_random.*_array 276c>
end subroutine integer_array_stateless

```

276c <Body of tao_random.*_array 276c>≡ (276–78)

```

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

```

277a *⟨Set nu to num or size(v) 277a⟩*≡ (276c)

```

    if (present (num)) then
        nu = num
    else
        nu = size (v)
    end if

```

`last` is used as an offset into the buffer `buffer`, as usual. `done` is an offset into the target. We still have to process all `nu` numbers. The first chunk can only use what's left in the buffer.

277b *⟨Prepare array buffer and done, todo, chunk 277b⟩*≡ (276c)

```

    if (last >= buffer_end) then
        call generate (buffer, state)
        last = 0
    end if
    done = 0
    todo = nu
    chunk = min (todo, buffer_end - last)

```

This logic is a bit weird, but after the first chunk, `todo` will either vanish (in which case we're done) or we have consumed all of the buffer and must reload. In any case we can pretend that the next chunk can use the whole buffer.

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

```

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

```

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

```

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

```

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

```

pure subroutine real_array_stateless &
    (state, buffer, buffer_end, last, v, num)
    integer(kind=tao_i32), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    real(kind=default), parameter :: NORM = 1.0_default / M

```

```

    <Body of tao_random.*_array 276c>
end subroutine real_array_stateless

```

Fill the array v_1, \dots, v_ν with uniform deviates $v_i \in [0, 1)$.

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

```

pure subroutine real_array_stateless &
    (state, buffer, buffer_end, last, v, num)
    real(kind=tao_r64), dimension(:), intent(inout) :: state, buffer
    integer, intent(in) :: buffer_end
    integer, intent(inout) :: last
    real(kind=default), dimension(:), intent(out) :: v
    integer, optional, intent(in) :: num
    integer, parameter :: NORM = 1
    <Body of tao_random.*_array 276c>
end subroutine real_array_stateless

```

C.4.3 Procedures With Explicit tao_random_state

Unfortunately, this is very boring, but Fortran's lack of parametric polymorphism forces this duplication on us:

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

```

elemental subroutine integer_state (s, r)
    type(tao_random_state), intent(inout) :: s
    integer, intent(out) :: r
    call integer_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine integer_state

```

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

```

elemental subroutine real_state (s, r)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(out) :: r
    call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine real_state

```

278d <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <278a 279b>

```

elemental subroutine real_state (s, r)
    type(tao_random_state), intent(inout) :: s
    real(kind=default), intent(out) :: r
    call real_stateless (s%state%x, s%buffer, s%buffer_end, s%last, r)
end subroutine real_state

```

278e <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278c 279a>

```

pure subroutine integer_array_state (s, v, num)
    type(tao_random_state), intent(inout) :: s
    integer, dimension(:), intent(out) :: v

```

```

integer, optional, intent(in) :: num
call integer_array_stateless &
    (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine integer_array_state

279a <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <278e 279d>
pure subroutine real_array_state (s, v, num)
type(tao_random_state), intent(inout) :: s
real(kind=default), dimension(:), intent(out) :: v
integer, optional, intent(in) :: num
call real_array_stateless &
    (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine real_array_state

279b <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <278d 280a>
pure subroutine real_array_state (s, v, num)
type(tao_random_state), intent(inout) :: s
real(kind=default), dimension(:), intent(out) :: v
integer, optional, intent(in) :: num
call real_array_stateless &
    (s%state%x, s%buffer, s%buffer_end, s%last, v, num)
end subroutine real_array_state

```

C.4.4 Static Procedures

First make sure that `tao_random_seed` has been called to initialize the generator state:

```

279c <Initialize a virginal random number generator 279c>≡ (279 280 282)
if (s_virginal) then
    call tao_random_seed ()
end if

279d <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <279a 279e>
subroutine integer_static (r)
integer, intent(out) :: r
<Initialize a virginal random number generator 279c>
call integer_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine integer_static

279e <Implementation of 30-bit tao_random_numbers 255a>+≡ (273c) <279d 280b>
subroutine real_static (r)
real(kind=default), intent(out) :: r
<Initialize a virginal random number generator 279c>
call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)
end subroutine real_static

```


280a \langle Implementation of 52-bit tao_random_numbers 259c $\rangle + \equiv$ (274a) \triangleleft 279b 280d \triangleright
`subroutine real_static (r)`
`real(kind=default), intent(out) :: r`
 \langle Initialize a virginal random number generator 279c \rangle
`call real_stateless (s_state, s_buffer, s_buffer_end, s_last, r)`
`end subroutine real_static`

280b \langle Implementation of 30-bit tao_random_numbers 255a $\rangle + \equiv$ (273c) \triangleleft 279e 280c \triangleright
`subroutine integer_array_static (v, num)`
`integer, dimension(:), intent(out) :: v`
`integer, optional, intent(in) :: num`
 \langle Initialize a virginal random number generator 279c \rangle
`call integer_array_stateless &`
`(s_state, s_buffer, s_buffer_end, s_last, v, num)`
`end subroutine integer_array_static`

280c \langle Implementation of 30-bit tao_random_numbers 255a $\rangle + \equiv$ (273c) \triangleleft 280b 283b \triangleright
`subroutine real_array_static (v, num)`
`real(kind=default), dimension(:), intent(out) :: v`
`integer, optional, intent(in) :: num`
 \langle Initialize a virginal random number generator 279c \rangle
`call real_array_stateless &`
`(s_state, s_buffer, s_buffer_end, s_last, v, num)`
`end subroutine real_array_static`

280d \langle Implementation of 52-bit tao_random_numbers 259c $\rangle + \equiv$ (274a) \triangleleft 280a 285b \triangleright
`subroutine real_array_static (v, num)`
`real(kind=default), dimension(:), intent(out) :: v`
`integer, optional, intent(in) :: num`
 \langle Initialize a virginal random number generator 279c \rangle
`call real_array_stateless &`
`(s_state, s_buffer, s_buffer_end, s_last, v, num)`
`end subroutine real_array_static`

C.4.5 Generic Procedures

280e \langle Interfaces of 30-bit tao_random_numbers 280e $\rangle \equiv$ (273c)
`interface tao_random_number`
`module procedure \langle Specific procedures for 30-bit tao_random_number 280f \rangle`
`end interface`

280f \langle Specific procedures for 30-bit tao_random_number 280f $\rangle \equiv$ (280e 281b)
`integer_static, integer_state, &`
`integer_array_static, integer_array_state, &`
`real_static, real_state, real_array_static, real_array_state`

These are not exported

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

Thes are not exported

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

C.4.6 *Luxury*

- 281g *<Implementation of tao_random_numbers 255f>+≡* (273c 274a) *<269f 281h>*
`pure subroutine luxury_stateless &`
`(buffer_size, buffer_end, last, consumption)`
`integer, intent(in) :: buffer_size`
`integer, intent(inout) :: buffer_end`
`integer, intent(inout) :: last`
`integer, intent(in) :: consumption`
`if (consumption >= 1 .and. consumption <= buffer_size) then`
`buffer_end = consumption`
`last = min (last, buffer_end)`
`else`
`!!! print *, "tao_random_luxury: ", "invalid consumption ", &`
`!!! consumption, ", not in [1,", buffer_size, "]."`
`buffer_end = buffer_size`
`end if`
`end subroutine luxury_stateless`
- 281h *<Implementation of tao_random_numbers 255f>+≡* (273c 274a) *<281g 282a>*
`elemental subroutine luxury_state (s)`
`type(tao_random_state), intent(inout) :: s`

```

        call luxury_state_integer (s, size (s%buffer))
    end subroutine luxury_state

282a  <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <281h 282b>
        elemental subroutine luxury_state_integer (s, consumption)
            type(tao_random_state), intent(inout) :: s
            integer, intent(in) :: consumption
            call luxury_stateless (size (s%buffer), s%buffer_end, s%last, consumption)
        end subroutine luxury_state_integer

282b  <Implementation of tao_random_numbers 255f>+≡      (273c 274a) <282a 282c>
        elemental subroutine luxury_state_real (s, consumption)
            type(tao_random_state), intent(inout) :: s
            real(kind=default), intent(in) :: consumption
            call luxury_state_integer (s, int (consumption * size (s%buffer)))
        end subroutine luxury_state_real

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

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

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

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

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

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

```

283a \langle Specific procedures for tao_random_luxury 283a $\rangle \equiv$ (282)
 luxury_static, luxury_state, &
 luxury_static_integer, luxury_state_integer, &
 luxury_static_real, luxury_state_real

C.5 Testing

C.5.1 30-bit

283b \langle Implementation of 30-bit tao_random_numbers 255a $\rangle + \equiv$ (273c) \triangleleft 280c
 subroutine tao_random_test (name)
 character(len=*), optional, intent(in) :: name
 character (len = *), parameter :: &
 OK = "(1x,i10,' is ok. ')", &
 NOT_OK = "(1x,i10,' is not ok, (expected ',i10,')!')"
 \langle Parameters in tao_random_test 283c \rangle
 integer, parameter :: &
 A_2027082 = 995235265
 integer, dimension(N) :: a
 type(tao_random_state) :: s, t
 integer, dimension(:), allocatable :: ibuf
 real(kind=tao_r64), dimension(:), allocatable :: dbuf
 integer :: i, ibuf_size, dbuf_size
 print *, TAO_RANDOM_NUMBERS_RCS_ID
 print *, "testing the 30-bit tao_random_numbers ..."
 \langle Perform simple tests of tao_random_numbers 283d \rangle
 \langle Perform more tests of tao_random_numbers 284c \rangle
 end subroutine tao_random_test

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

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

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

⟨Test a(1) = A_2027082 284a⟩

284a *⟨Test a(1) = A_2027082 284a⟩≡* (283–85)
 if (a(1) == A_2027082) then
 print OK, a(1)
 else
 print NOT_OK, a(1), A_2027082
 stop 1
 end if

Deja vu all over again, but 2027081 is factored the other way around this time

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

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

284c *⟨Perform more tests of tao_random_numbers 284c⟩≡* (283b 285b) 284d>
 print *, "testing the stateless stuff ..."
 call tao_random_create (s, SEED)
 do i = 1, N_SHORT
 call tao_random_number (s, a, M)
 end do
 call tao_random_create (t, s)
 do i = 1, N+1 - N_SHORT
 call tao_random_number (s, a, M)
 end do
⟨Test a(1) = A_2027082 284a⟩

and restart the saved generator

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

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

284e *⟨Perform more tests of tao_random_numbers 284c⟩+≡* (283b 285b) <284d 285a>
 if (present (name)) then
 print *, "testing I/O ..."
 call tao_random_seed (s, SEED)
 do i = 1, N_SHORT
 call tao_random_number (s, a, M)

```

end do
call tao_random_write (s, name)
do i = 1, N+1 - N_SHORT
    call tao_random_number (s, a, M)
end do
<Test a(1) = A_2027082 284a>
call tao_random_read (s, name)
do i = 1, N+1 - N_SHORT
    call tao_random_number (s, a, M)
end do
<Test a(1) = A_2027082 284a>
end if

```

And finally using marshaling/unmarshaling:

```

285a <Perform more tests of tao_random_numbers 284c>+≡ (283b 285b) <284e
    print *, "testing marshaling/unmarshaling ..."
    call tao_random_seed (s, SEED)
    do i = 1, N_SHORT
        call tao_random_number (s, a, M)
    end do
    call tao_random_marshall_size (s, ibuf_size, dbuf_size)
    allocate (ibuf(ibuf_size), dbuf(dbuf_size))
    call tao_random_marshall (s, ibuf, dbuf)
    do i = 1, N+1 - N_SHORT
        call tao_random_number (s, a, M)
    end do
    <Test a(1) = A_2027082 284a>
    call tao_random_unmarshal (s, ibuf, dbuf)
    do i = 1, N+1 - N_SHORT
        call tao_random_number (s, a, M)
    end do
    <Test a(1) = A_2027082 284a>

```

C.5.2 52-bit

DEK's "official" test expects $x_{1009 \cdot 2009 + 1} = x_{2027082} = 0.36410514377569680455$:

```

285b <Implementation of 52-bit tao_random_numbers 259c>+≡ (274a) <280d
    subroutine tao_random_test (name)
        character(len=*), optional, intent(in) :: name
        character(len=*), parameter :: &
            OK = "(1x,f22.20,' is ok.')" , &
            NOT_OK = "(1x,f22.20,' is not ok, (A_2027082 ',f22.20,')!')'"
        <Parameters in tao_random_test 283c>

```

```

real(kind=default), parameter :: &
    A_2027082 = 0.36410514377569680455_tao_r64
real(kind=default), dimension(N) :: a
type(tao_random_state) :: s, t
integer, dimension(:), allocatable :: ibuf
real(kind=tao_r64), dimension(:), allocatable :: dbuf
integer :: i, ibuf_size, dbuf_size
print *, TAO52_RANDOM_NUMBERS_RCS_ID
print *, "testing the 52-bit tao_random_numbers ..."
  <Perform simple tests of tao_random_numbers 283d>
  <Perform more tests of tao_random_numbers 284c>
end subroutine tao_random_test

```

C.5.3 Test Program

```

286 <tao_test.f90 286>≡
    program tao_test
        use tao_random_numbers, only: test30 => tao_random_test
        use tao52_random_numbers, only: test52 => tao_random_test
        implicit none
        call test30 ("tmp.tao")
        call test52 ("tmp.tao")
        stop 0
    end program tao_test

```

—D—

SPECIAL FUNCTIONS

```

287a  <specfun.f90 287a>≡
      ! specfun.f90 --
      <Copyleft notice 1>
      module specfun
        use kinds
        ! use constants
        implicit none
        private
        <Declaration of specfun procedures 287b>
        character(len=*), public, parameter :: SPECFUN_RCS_ID = &
          "$Id: specfun.nw 314 2010-04-17 20:32:33Z ohl $"
        !WK:
        real(kind=default), public, parameter :: &
          PI = 3.1415926535897932384626433832795028841972_default
        contains
        <Implementation of specfun procedures 288c>
      end module specfun

```

The algorithm is stolen from the FORTRAN version in routine C303 of the CERN library [25]. It has an accuracy which is approximately one digit less than machine precision.

```

287b  <Declaration of specfun procedures 287b>≡ (287a)
      public :: gamma

```

The so-called reflection formula is used for negative arguments:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x} \quad (\text{D.1})$$

Here's the identity transformation that pulls the argument of Γ into [3, 4]:

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

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

```

f = 1
if (u < 3) then
  do i = 1, int (4 - u)
    f = f / u
    u = u + 1
  end do
else
  do i = 1, int (u - 3)
    u = u - 1
    f = f * u
  end do
end if

```

A Chebyshev approximation for $\Gamma(x)$ is used after mapping $x \in [3, 4]$ linearly to $h \in [-1, 1]$. The series is evaluted by Clenshaw's recurrence formula:

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

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

```

alpha = 2*g
b1 = 0
b2 = 0
do i = 15, 0, -1
  b0 = c(i) + alpha * b1 - b2
  b2 = b1
  b1 = b0
end do
g = f * (b0 - g * b2)

```

Note that we're assuming that $c(0)$ is in fact $c_0/2$. This is for compatibility with the CERN library routines.

288c \langle Implementation of specfun procedures 288c $\rangle \equiv$ (287a)

```

pure function gamma (x) result (g)
  real(kind=default), intent(in) :: x
  real(kind=default) :: g
  integer :: i
  real(kind=default) :: u, f, alpha, b0, b1, b2
  real(kind=default), dimension(0:15), parameter :: &
    c =  $\langle c_0/2, c_1, c_2, \dots, c_{15}$  for  $\Gamma(x)$  289a  $\rangle$ 
  u = x
  if (u <= 0.0) then

```

```

        if (u == int (u)) then
            g = huge (g)
            return
        else
            u = 1 - u
        end if
    endif
    <Pull u into the intervall [3,4] 288a>
    g = 2*u - 7
    <Clenshaw's recurrence formula 288b>
    if (x < 0) then
        g = PI / (sin (PI * x) * g)
    end if
end function gamma
289a <c0/2, c1, c2, ..., c15 for  $\Gamma(x)$  289a>≡ (288c)
    (/ 3.65738772508338244_default, &
       1.95754345666126827_default, &
       0.33829711382616039_default, &
       0.04208951276557549_default, &
       0.00428765048212909_default, &
       0.00036521216929462_default, &
       0.00002740064222642_default, &
       0.00000181240233365_default, &
       0.00000010965775866_default, &
       0.00000000598718405_default, &
       0.00000000030769081_default, &
       0.00000000001431793_default, &
       0.00000000000065109_default, &
       0.0000000000002596_default, &
       0.0000000000000111_default, &
       0.0000000000000004_default /)

```

D.1 Test

```

289b <stest.f90 289b>≡ (290c)
    ! stest.f90 --
    <Copyleft notice 1>
    module stest_functions
        use kinds
        use constants
        use specfun

```

```

private
  <Declaration of stest_functions procedures 290a>
contains
  <Implementation of stest_functions procedures 290b>
end module stest_functions

```

290a <Declaration of stest_functions procedures 290a>≡ (289b)

```

public :: gauss_multiplication

```

Gauss' multiplication fomula can serve as a non-trivial test

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma(x + k/n) \quad (\text{D.4})$$

290b <Implementation of stest_functions procedures 290b>≡ (289b)

```

pure function gauss_multiplication (x, n) result (delta)
  real(kind=default), intent(in) :: x
  integer, intent(in) :: n
  real(kind=default) :: delta
  real(kind=default) :: gxn
  integer :: k
  gxn = (2*PI)**(0.5_double*(1-n)) * n**(n*x-0.5_double)
  do k = 0, n - 1
    gxn = gxn * gamma (x + real (k, kind=default) / n)
  end do
  delta = abs ((gamma (n*x) - gxn) / gamma (n*x))
end function gauss_multiplication

```

290c <stest.f90 289b>+≡ <289b

```

program stest
  use kinds
  use specfun
  use stest_functions !NODEP!
  implicit none
  integer :: i, steps
  real(kind=default) :: x, g, xmin, xmax
  xmin = -4.5
  xmax = 4.5
  steps = 100 ! 9
  do i = 0, steps
    x = xmin + ((xmax - xmin) / real (steps)) * i
    print "(f6.3,4(1x,e9.2))", x, &
      gauss_multiplication (x, 2), &
      gauss_multiplication (x, 3), &
      gauss_multiplication (x, 4), &

```

```
        gauss_multiplication (x, 5)
    end do
end program stest
```

—E—

STATISTICS

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

292b $\langle \text{Declaration of vamp_stat procedures 292b} \rangle \equiv$ (292a) 293c \triangleright
`public :: average, standard_deviation, value_spread`

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

292c $\langle \text{Implementation of vamp_stat procedures 292c} \rangle \equiv$ (292a) 293a \triangleright
`pure function average (x) result (a)`
`real(kind=default), dimension(:), intent(in) :: x`
`real(kind=default) :: a`
`integer :: n`
`n = size (x)`
`if (n == 0) then`
`a = 0.0`
`else`
`a = sum (x) / n`
`end if`
`end function average`

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

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

```

pure function standard_deviation (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  integer :: n
  n = size (x)
  if (n < 2) then
    s = huge (s)
  else
    s = sqrt (max ((sum (x**2) / n - (average (x))**2) / (n - 1), &
                  0.0_default))
  end if
end function standard_deviation

```

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

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

```

pure function value_spread (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  s = maxval(x) - minval(x)
end function value_spread

```

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

```

public :: standard_deviation_percent, value_spread_percent

```

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

```

pure function standard_deviation_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x
  real(kind=default) :: s
  real(kind=default) :: abs_avg
  abs_avg = abs (average (x))
  if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
  else
    s = 100.0 * standard_deviation (x) / abs_avg
  end if
end function standard_deviation_percent

```

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

```

pure function value_spread_percent (x) result (s)
  real(kind=default), dimension(:), intent(in) :: x

```

```

real(kind=default) :: s
real(kind=default) :: abs_avg
abs_avg = abs (average (x))
if (abs_avg <= tiny (abs_avg)) then
    s = huge (s)
else
    s = 100.0 * value_spread (x) / abs_avg
end if
end function value_spread_percent

```

—F—

HISTOGRAMMING

⚡ Merged WK's improvements for WHIZARD. TODO *after* merging:

1. bins3 is a bad undescriptive name
2. bins3 should be added to `histogram2`
3. `write_histogram2_unit` for symmetry.

⚡ There's almost no sanity checking. If you call one of these functions on a histogram that has not been initialized, you loose. — *Big time.*

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

295b <Declaration of histograms types 295b>≡ (295a) 296a>
type, public :: histogram
  private
  integer :: n_bins
  real(kind=default) :: x_min, x_max
```



```

        real(kind=default), dimension(:), pointer :: bins => null ()
        real(kind=default), dimension(:), pointer :: bins2 => null ()
        real(kind=default), dimension(:), pointer :: bins3 => null ()
    end type histogram
296a  <Declaration of histograms types 295b>+≡ (295a) <295b
    type, public :: histogram2
        private
        integer, dimension(2) :: n_bins
        real(kind=default), dimension(2) :: x_min, x_max
        real(kind=default), dimension(:,:), pointer :: bins => null ()
        real(kind=default), dimension(:,:), pointer :: bins2 => null ()
    end type histogram2
296b  <Declaration of histograms procedures 296b>≡ (295a) 296d>
    public :: create_histogram
    public :: fill_histogram
    public :: delete_histogram
    public :: write_histogram
296c  <Interfaces of histograms procedures 296c>≡ (295a) 301b>
    interface create_histogram
        module procedure create_histogram1, create_histogram2
    end interface
    interface fill_histogram
        module procedure fill_histogram1, fill_histogram2s, fill_histogram2v
    end interface
    interface delete_histogram
        module procedure delete_histogram1, delete_histogram2
    end interface
    interface write_histogram
        module procedure write_histogram1, write_histogram2
        module procedure write_histogram1_unit
    end interface
296d  <Declaration of histograms procedures 296b>+≡ (295a) <296b 300a>
    private :: create_histogram1, create_histogram2
    private :: fill_histogram1, fill_histogram2s, fill_histogram2v
    private :: delete_histogram1, delete_histogram2
    private :: write_histogram1, write_histogram2
296e  <Variables in histograms 296e>≡ (295a)
    integer, parameter, private :: N_BINS_DEFAULT = 10
296f  <Implementation of histograms procedures 296f>≡ (295a) 297a>
    elemental subroutine create_histogram1 (h, x_min, x_max, nb)
        type(histogram), intent(out) :: h

```

```

real(kind=default), intent(in) :: x_min, x_max
integer, intent(in), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins+1), h%bins2(0:h%n_bins+1))
h%bins = 0
h%bins2 = 0
allocate (h%bins3(0:h%n_bins+1))
h%bins3 = 0
end subroutine create_histogram1

```

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

```

pure subroutine create_histogram2 (h, x_min, x_max, nb)
type(histogram2), intent(out) :: h
real(kind=default), dimension(:), intent(in) :: x_min, x_max
integer, intent(in), dimension(:), optional :: nb
if (present (nb)) then
    h%n_bins = nb
else
    h%n_bins = N_BINS_DEFAULT
end if
h%x_min = x_min
h%x_max = x_max
allocate (h%bins(0:h%n_bins(1)+1,0:h%n_bins(1)+1), &
          h%bins2(0:h%n_bins(2)+1,0:h%n_bins(2)+1))
h%bins = 0
h%bins2 = 0
end subroutine create_histogram2

```

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

```

elemental subroutine fill_histogram1 (h, x, weight, excess)
type(histogram), intent(inout) :: h
real(kind=default), intent(in) :: x
real(kind=default), intent(in), optional :: weight
real(kind=default), intent(in), optional :: excess
integer :: i
if (x < h%x_min) then
    i = 0
else if (x > h%x_max) then
    i = h%n_bins + 1

```

```

else
    i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
!WK! i = min (max (i, 0), h%n_bins + 1)
end if
if (present (weight)) then
    h%bins(i) = h%bins(i) + weight
    h%bins2(i) = h%bins2(i) + weight*weight
else
    h%bins(i) = h%bins(i) + 1
    h%bins2(i) = h%bins2(i) + 1
end if
if (present (excess)) h%bins3(i) = h%bins3(i) + excess
end subroutine fill_histogram1

```

298a *<Implementation of histograms procedures 296f>+≡ (295a) <297b 298b>*
 elemental subroutine fill_histogram2s (h, x1, x2, weight)
 type(histogram2), intent(inout) :: h
 real(kind=default), intent(in) :: x1, x2
 real(kind=default), intent(in), optional :: weight
 call fill_histogram2v (h, (/ x1, x2 /), weight)
 end subroutine fill_histogram2s

298b *<Implementation of histograms procedures 296f>+≡ (295a) <298a 298c>*
 pure subroutine fill_histogram2v (h, x, weight)
 type(histogram2), intent(inout) :: h
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), intent(in), optional :: weight
 integer, dimension(2) :: i
 i = 1 + h%n_bins * (x - h%x_min) / (h%x_max - h%x_min)
 i = min (max (i, 0), h%n_bins + 1)
 if (present (weight)) then
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + weight
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + weight*weight
 else
 h%bins(i(1),i(2)) = h%bins(i(1),i(2)) + 1
 h%bins2(i(1),i(2)) = h%bins2(i(1),i(2)) + 1
 end if
 end subroutine fill_histogram2v

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

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

299b *<Implementation of histograms procedures 296f>+≡* (295a) <299a 300b>
 subroutine write_histogram1 (h, name, over)
 type(histogram), intent(in) :: h
 character(len=*), intent(in), optional :: name
 logical, intent(in), optional :: over
 integer :: i, iounit
 if (present (name)) then
 call find_free_unit (iounit)
 if (iounit > 0) then
 open (unit = iounit, action = "write", status = "replace", &
 file = name)
 if (present (over)) then
 if (over) then
 write (unit = iounit, fmt = *) &
 "underflow", h%bins(0), sqrt (h%bins2(0))
 end if
 end if
 do i = 1, h%n_bins
 write (unit = iounit, fmt = *) &
 midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
 end do
 if (present (over)) then
 if (over) then
 write (unit = iounit, fmt = *) &
 "overflow", h%bins(h%n_bins+1), &
 sqrt (h%bins2(h%n_bins+1))
 end if
 end if
 close (unit = iounit)
 else
 print *, "write_histogram: Can't find a free unit!"
 end if
 else
 if (present (over)) then
 if (over) then
 print *, "underflow", h%bins(0), sqrt (h%bins2(0))
 end if
 end if
 end if

```

do i = 1, h%n_bins
  print *, midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
end do
if (present (over)) then
  if (over) then
    print *, "overflow", h%bins(h%n_bins+1), &
      sqrt (h%bins2(h%n_bins+1))
  end if
end if
end if
end subroutine write_histogram1

```

300a *<Declaration of histograms procedures 296b>+≡ (295a) <296d 301a>*
 !WK! public :: write_histogram1_unit



I don't like the format statement with the line number. Use a character constant instead (after we have merged with WHIZARD's branch).

300b *<Implementation of histograms procedures 296f>+≡ (295a) <299b 301d>*
 subroutine write_histogram1_unit (h, iounit, over, show_excess)
 type(histogram), intent(in) :: h
 integer, intent(in) :: iounit
 logical, intent(in), optional :: over, show_excess
 integer :: i
 logical :: show_exc
 show_exc = .false.; if (present(show_excess)) show_exc = show_excess
 if (present (over)) then
 if (over) then
 if (show_exc) then
 write (unit = iounit, fmt = 1) &
 "underflow", h%bins(0), sqrt (h%bins2(0)), h%bins3(0)
 else
 write (unit = iounit, fmt = 1) &
 "underflow", h%bins(0), sqrt (h%bins2(0))
 end if
 end if
 end if
 do i = 1, h%n_bins
 if (show_exc) then
 write (unit = iounit, fmt = 1) &
 midpoint (h, i), h%bins(i), sqrt (h%bins2(i)), h%bins3(i)
 else
 write (unit = iounit, fmt = 1) &
 midpoint (h, i), h%bins(i), sqrt (h%bins2(i))
 end if
 end do

```

        end if
    end do
    if (present (over)) then
        if (over) then
            if (show_exc) then
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1)), &
                    h%bins3(h%n_bins+1)
            else
                write (unit = iounit, fmt = 1) &
                    "overflow", h%bins(h%n_bins+1), &
                    sqrt (h%bins2(h%n_bins+1))
            end if
        end if
    end if
    1 format (1x,4(G16.9,2x))
end subroutine write_histogram1_unit

```

- 301a *<Declaration of histograms procedures 296b>+≡* (295a) *<300a 301c>*
 private :: midpoint
- 301b *<Interfaces of histograms procedures 296c>+≡* (295a) *<296c*
 interface midpoint
 module procedure midpoint1, midpoint2
end interface
- 301c *<Declaration of histograms procedures 296b>+≡* (295a) *<301a*
 private :: midpoint1, midpoint2
- 301d *<Implementation of histograms procedures 296f>+≡* (295a) *<300b 301e>*
 elemental function midpoint1 (h, bin) result (x)
 type(histogram), intent(in) :: h
 integer, intent(in) :: bin
 real(kind=default) :: x
 x = h%x_min + (h%x_max - h%x_min) * (bin - 0.5) / h%n_bins
end function midpoint1
- 301e *<Implementation of histograms procedures 296f>+≡* (295a) *<301d 302>*
 elemental function midpoint2 (h, bin, d) result (x)
 type(histogram2), intent(in) :: h
 integer, intent(in) :: bin, d
 real(kind=default) :: x
 x = h%x_min(d) + (h%x_max(d) - h%x_min(d)) * (bin - 0.5) / h%n_bins(d)
end function midpoint2

302 *Implementation of histograms procedures 296f* +≡ (295a) <301e

```

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

```

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

```

G.1 Memory Management

```

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

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

```

```

        create_integer_array2_pointer, &
        create_real_array2_pointer
    end interface
306a  <Body of create_*_array_pointer 306a>≡ (306c 307a)
    if (associated (lhs)) then
        if (size (lhs) /= n) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb:n+lb-1))
            else
                allocate (lhs(n))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb:n+lb-1))
        else
            allocate (lhs(n))
        end if
    end if
    lhs = 0
306b  <Body of create_*_array2_pointer 306b>≡ (307)
    if (associated (lhs)) then
        if (any (ubound (lhs) /= n)) then
            deallocate (lhs)
            if (present (lb)) then
                allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
            else
                allocate (lhs(n(1),n(2)))
            end if
        end if
    else
        if (present (lb)) then
            allocate (lhs(lb(1):n(1)+lb(1)-1,lb(2):n(2)+lb(2)-1))
        else
            allocate (lhs(n(1),n(2)))
        end if
    end if
    lhs = 0
306c  <Implementation of utils procedures 306c>≡ (305a) 307a>
    pure subroutine create_integer_array_pointer (lhs, n, lb)
        integer, dimension(:), pointer :: lhs

```

```

integer, intent(in) :: n
integer, intent(in), optional :: lb
<Body of create_*.array_pointer 306a>
end subroutine create_integer_array_pointer

307a <Implementation of utils procedures 306c>+≡ (305a) <306c 307b>
pure subroutine create_real_array_pointer (lhs, n, lb)
real(kind=default), dimension(:), pointer :: lhs
integer, intent(in) :: n
integer, intent(in), optional :: lb
<Body of create_*.array_pointer 306a>
end subroutine create_real_array_pointer

307b <Implementation of utils procedures 306c>+≡ (305a) <307a 307c>
pure subroutine create_integer_array2_pointer (lhs, n, lb)
integer, dimension(:,:), pointer :: lhs
integer, dimension(:), intent(in) :: n
integer, dimension(:), intent(in), optional :: lb
<Body of create_*.array2_pointer 306b>
end subroutine create_integer_array2_pointer

307c <Implementation of utils procedures 306c>+≡ (305a) <307b 308a>
pure subroutine create_real_array2_pointer (lhs, n, lb)
real(kind=default), dimension(:,:), pointer :: lhs
integer, dimension(:), intent(in) :: n
integer, dimension(:), intent(in), optional :: lb
<Body of create_*.array2_pointer 306b>
end subroutine create_real_array2_pointer

Copy an allocatable array component of a derived type, reshaping the target
if necessary. The target can be disassociated, but its association must not
be undefined.

307d <Declaration of utils procedures 305b>+≡ (305a) <305b 308e>
public :: copy_array_pointer
private :: copy_integer_array_pointer
private :: copy_real_array_pointer
private :: copy_integer_array2_pointer
private :: copy_real_array2_pointer

307e <Interfaces of utils procedures 305c>+≡ (305a) <305c 309a>
interface copy_array_pointer
module procedure &
    copy_integer_array_pointer, &
    copy_real_array_pointer, &
    copy_integer_array2_pointer, &
    copy_real_array2_pointer

```

```

end interface

308a <Implementation of utils procedures 306c>+≡ (305a) <307c 308b>
pure subroutine copy_integer_array_pointer (lhs, rhs, lb)
  integer, dimension(:), pointer :: lhs
  integer, dimension(:), intent(in) :: rhs
  integer, intent(in), optional :: lb
  call create_integer_array_pointer (lhs, size (rhs), lb)
  lhs = rhs
end subroutine copy_integer_array_pointer

308b <Implementation of utils procedures 306c>+≡ (305a) <308a 308c>
pure subroutine copy_real_array_pointer (lhs, rhs, lb)
  real(kind=default), dimension(:), pointer :: lhs
  real(kind=default), dimension(:), intent(in) :: rhs
  integer, intent(in), optional :: lb
  call create_real_array_pointer (lhs, size (rhs), lb)
  lhs = rhs
end subroutine copy_real_array_pointer

308c <Implementation of utils procedures 306c>+≡ (305a) <308b 308d>
pure subroutine copy_integer_array2_pointer (lhs, rhs, lb)
  integer, dimension(:, :), pointer :: lhs
  integer, dimension(:, :), intent(in) :: rhs
  integer, dimension(:), intent(in), optional :: lb
  call create_integer_array2_pointer &
    (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
  lhs = rhs
end subroutine copy_integer_array2_pointer

308d <Implementation of utils procedures 306c>+≡ (305a) <308c 309b>
pure subroutine copy_real_array2_pointer (lhs, rhs, lb)
  real(kind=default), dimension(:, :), pointer :: lhs
  real(kind=default), dimension(:, :), intent(in) :: rhs
  integer, dimension(:), intent(in), optional :: lb
  call create_real_array2_pointer &
    (lhs, (/ size (rhs, dim=1), size (rhs, dim=2) /), lb)
  lhs = rhs
end subroutine copy_real_array2_pointer

```

G.2 Sorting

```

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

```

309a *<Interfaces of utils procedures 305c>+≡* (305a) *<307e 311a>*

```
interface swap
  module procedure swap_integer, swap_real
end interface
```

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

```
elemental subroutine swap_integer (a, b)
  integer, intent(inout) :: a, b
  integer :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_integer
```

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

```
elemental subroutine swap_real (a, b)
  real(kind=default), intent(inout) :: a, b
  real(kind=default) :: tmp
  tmp = a
  a = b
  b = tmp
end subroutine swap_real
```

Straight insertion:

309d *<Implementation of utils procedures 306c>+≡* (305a) *<309c 310b>*

```
pure subroutine sort_real (key, reverse)
  real(kind=default), dimension(:), intent(inout) :: key
  logical, intent(in), optional :: reverse
  logical :: rev
  integer :: i, j
  <Set rev to reverse or .false. 309e>
  do i = 1, size (key) - 1
    <Set j to minloc(key) 310a>
    if (j /= i) then
      call swap (key(i), key(j))
    end if
  end do
end subroutine sort_real
```

309e *<Set rev to reverse or .false. 309e>≡* (309 310)

```
if (present (reverse)) then
  rev = reverse
else
  rev = .false.
end if
```

```

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

310b  <Implementation of utils procedures 306c>+≡ (305a) <309d 310c>
      pure subroutine sort_real_and_real_array (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        real(kind=default), dimension(:, :), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 309e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 310a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(:, i), table(:, j))
          end if
        end do
      end subroutine sort_real_and_real_array

310c  <Implementation of utils procedures 306c>+≡ (305a) <310b 311c>
      pure subroutine sort_real_and_integer (key, table, reverse)
        real(kind=default), dimension(:), intent(inout) :: key
        integer, dimension(:), intent(inout) :: table
        logical, intent(in), optional :: reverse
        logical :: rev
        integer :: i, j
        <Set rev to reverse or .false. 309e>
        do i = 1, size (key) - 1
          <Set j to minloc(key) 310a>
          if (j /= i) then
            call swap (key(i), key(j))
            call swap (table(i), table(j))
          end if
        end do
      end subroutine sort_real_and_integer

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

```

311a \langle Interfaces of utils procedures 305c $\rangle + \equiv$ (305a) \triangleleft 309a \triangleright

```

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

```

G.3 Mathematics

311b \langle Declaration of utils procedures 305b $\rangle + \equiv$ (305a) \triangleleft 310d 311d \triangleright

```

public :: outer_product

```

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

311c \langle Implementation of utils procedures 306c $\rangle + \equiv$ (305a) \triangleleft 310c 311e \triangleright

```

pure function outer_product (x, y) result (xy)
  real(kind=default), dimension(:), intent(in) :: x, y
  real(kind=default), dimension(size(x),size(y)) :: xy
  xy = spread (x, dim=2, ncopies=size(y)) &
    * spread (y, dim=1, ncopies=size(x))
end function outer_product

```

Greatest common divisor and least common multiple

311d \langle Declaration of utils procedures 305b $\rangle + \equiv$ (305a) \triangleleft 311b 313a \triangleright

```

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

```

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

311e \langle Implementation of utils procedures 306c $\rangle + \equiv$ (305a) \triangleleft 311c 311f \triangleright

```

pure recursive function gcd_internal (m, n) result (gcd_m_n)
  integer, intent(in) :: m, n
  integer :: gcd_m_n
  if (n <= 0) then
    gcd_m_n = m
  else
    gcd_m_n = gcd_internal (n, modulo (m, n))
  end if
end function gcd_internal

```

Wrap an elemental procedure around the recursive procedure:

311f \langle Implementation of utils procedures 306c $\rangle + \equiv$ (305a) \triangleleft 311e 312a \triangleright

```

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 $\text{gcd}(m, n) \text{lcm}(m, n) = mn$:

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

```

elemental function lcm (m, n) result (lcm_m_n)
  integer, intent(in) :: m, n
  integer :: lcm_m_n
  lcm_m_n = (m * n) / gcd (m, n)
end function lcm

```

A very simple minded factorization procedure, that is not fool proof at all. It maintains $n == \text{product}(\text{factors}(1:i))$, however, and will work in all cases of practical relevance.

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

```

pure subroutine factorize (n, factors, i)
  integer, intent(in) :: n
  integer, dimension(:), intent(out) :: factors
  integer, intent(out) :: i
  integer :: nn, p
  nn = n
  i = 0
  do p = 1, size (PRIMES)
    try: do
      if (modulo (nn, PRIMES(p)) == 0) then
        i = i + 1
        factors(i) = PRIMES(p)
        nn = nn / PRIMES(p)
        if (i >= size (factors)) then
          factors(i) = nn
          return
        end if
      else
        exit try
      end if
    end do try
    if (nn == 1) then
      return
    end if
  end do
end subroutine factorize

```

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

```

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

```

G.4 I/O

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

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

313c *<Implementation of utils procedures 306c>+≡* (305a) <312b
 subroutine find_free_unit (u, iostat)
 integer, intent(out) :: u
 integer, intent(out), optional :: iostat
 logical :: exists, is_open
 integer :: **i**, status
 do **i** = **MIN_UNIT**, **MAX_UNIT**
 inquire (**unit** = **i**, exist = exists, opened = is_open, &
 iostat = status)
 if (status == 0) then
 if (exists .and. .not. is_open) then
 u = **i**
 if (present (iostat)) then
 iostat = 0
 end if
 return
 end if
 end if
 end do
 if (present (iostat)) then
 iostat = -1
 end if
 u = -1
 end **subroutine find_free_unit**

—H— LINEAR ALGEBRA

```

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

```

H.1 LU Decomposition

```

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

```

$$A = LU \tag{H.1a}$$

In more detail

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \dots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix} \tag{H.1b}$$

Rewriting (H.1) in block matrix notation

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

we can solve it easily

$$u_{11} = a_{11} \quad (\text{H.3a})$$

$$u_{1\cdot} = a_{1\cdot} \quad (\text{H.3b})$$

$$l_{\cdot 1} = \frac{a_{\cdot 1}}{a_{11}} \quad (\text{H.3c})$$

$$LU = A - \frac{a_{\cdot 1} \otimes a_{1\cdot}}{a_{11}} \quad (\text{H.3d})$$

and (H.3c) and (H.3d) define a simple iterative algorithm if we work from the outside in. It just remains to add pivoting.

315 *<Implementation of linalg procedures 315>* (314a) 317b>
 pure subroutine lu_decompose (a, pivots, eps, l, u)
 real(kind=default), dimension(:,:), intent(inout) :: a
 integer, dimension(:), intent(out), optional :: pivots
 real(kind=default), intent(out), optional :: eps
 real(kind=default), dimension(:,:), intent(out), optional :: l, u
 real(kind=default), dimension(size(a,dim=1)) :: vv
 integer, dimension(size(a,dim=1)) :: p
 integer :: j, pivot
 <eps = 1 316a>
 vv = maxval (abs (a), dim=2)
 if (any (vv == 0.0)) then
 a = 0.0
 <pivots = 0 and eps = 0 316c>
 return
 end if
 vv = 1.0 / vv
 do j = 1, size (a, dim=1)
 pivot = j - 1 + sum (maxloc (vv(j:) * abs (a(j:,j))))
 if (j /= pivot) then
 call swap (a(pivot,:), a(j,:))
 <eps = - eps 316b>
 vv(pivot) = vv(j)
 end if
 p(j) = pivot
 if (a(j,j) == 0.0) then
 a(j,j) = tiny (a(j,j))

```

        end if
        a(j+1:,j) = a(j+1:,j) / a(j,j)
        a(j+1:,j+1:) &
            = a(j+1:,j+1:) - outer_product (a(j+1:,j), a(j,j+1:))
    end do
    <Return optional arguments in lu_decompose 316d>
end subroutine lu_decompose

316a <eps = 1 316a>≡ (315)
    if (present (eps)) then
        eps = 1.0
    end if

316b <eps = - eps 316b>≡ (315)
    if (present (eps)) then
        eps = - eps
    end if

316c <pivots = 0 and eps = 0 316c>≡ (315)
    if (present (pivots)) then
        pivots = 0
    end if
    if (present (eps)) then
        eps = 0
    end if

316d <Return optional arguments in lu_decompose 316d>≡ (315)
    if (present (pivots)) then
        pivots = p
    end if
    if (present (l)) then
        do j = 1, size (a, dim=1)
            l(1:j-1,j) = 0.0
            l(j,j) = 1.0
            l(j+1:,j) = a(j+1:,j)
        end do
        do j = size (a, dim=1), 1, -1
            call swap (l(j,:), l(p(j),:))
        end do
    end if
    if (present (u)) then
        do j = 1, size (a, dim=1)
            u(1:j,j) = a(1:j,j)
            u(j+1:,j) = 0.0
        end do
    end if
end if

```

H.2 Determinant

317a \langle Declaration of `linalg` procedures 314b $\rangle + \equiv$ (314a) \langle 314b 318a \rangle
`public :: determinant`

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

317b \langle Implementation of `linalg` procedures 315 $\rangle + \equiv$ (314a) \langle 315 318b \rangle
`pure subroutine determinant (a, det)`
`real(kind=default), dimension(:, :), intent(in) :: a`
`real(kind=default), intent(out) :: det`
`real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: lu`
`integer :: i`
`lu = a`
`call lu_decompose (lu, eps = det)`
`do i = 1, size (a, dim = 1)`
`det = det * lu(i,i)`
`end do`
`end subroutine determinant`

H.3 Diagonalization

The code is an implementation of the algorithm presented in [17, 18], but independent from the code presented in [19] to avoid legal problems.

A Jacobi rotation around the angle ϕ in row p and column q

$$P(\phi; p, q) = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & \cos \phi & \cdots & \sin \phi \\ & & \vdots & 1 & \vdots \\ & & -\sin \phi & \cdots & \cos \phi \\ & & & & \ddots \\ & & & & & 1 \end{pmatrix} \quad (\text{H.4})$$

results in

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

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

318b \langle Implementation of linalg procedures 315 $\rangle + \equiv$ (314a) \langle 317b 321b \rangle
pure subroutine diagonalize_real_symmetric (a, eval, evec, num_rot)
real(kind=default), dimension(:, :), intent(in) :: a
real(kind=default), dimension(:), intent(out) :: eval
real(kind=default), dimension(:, :), intent(out) :: evec
integer, intent(out), optional :: num_rot
real(kind=default), dimension(size(a,dim=1),size(a,dim=2)) :: aa
real(kind=default) :: off_diagonal_norm, threshold, &
c, g, h, s, t, tau, cot_2phi
logical, dimension(size(eval),size(eval)) :: upper_triangle
integer, dimension(size(eval)) :: one_to_ndim
integer :: p, q, ndim, j, sweep
integer, parameter :: MAX_SWEEPS = 50
ndim = size (eval)
one_to_ndim = (/ (j, j=1,ndim) /)
upper_triangle = &
spread (one_to_ndim, dim=1, ncopies=ndim) &
> spread (one_to_ndim, dim=2, ncopies=ndim)
aa = a
call unit (evec)
 \langle Initialize num_rot 321e \rangle
sweeps: do sweep = 1, MAX_SWEEPS
off_diagonal_norm = sum (abs (aa), mask=upper_triangle)
if (off_diagonal_norm == 0.0) then
eval = diag (aa)
return
end if
if (sweep < 4) then
threshold = 0.2 * off_diagonal_norm / ndim**2
else

```

        threshold = 0.0
    end if
    do p = 1, ndim - 1
        do q = p + 1, ndim
            ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  319⟩
        end do
    end do
end do sweeps
if (present (num_rot)) then
    num_rot = -1
end if
!!! print *, "linalg::diagonalize_real_symmetric: exceeded sweep count"
end subroutine diagonalize_real_symmetric
319 ⟨Perform the Jacobi rotation resulting in  $A'_{pq} = 0$  319⟩ ≡ (318b)
    g = 100 * abs (aa (p,q))
    if ((sweep > 4) &
        .and. (g <= min (spacing (aa(p,p)), spacing (aa(q,q)))) then
        aa(p,q) = 0.0
    else if (abs (aa(p,q)) > threshold) then
        ⟨Determine  $\phi$  for the Jacobi rotation  $P(\phi; p, q)$  with  $A'_{pq} = 0$  320a⟩
        ⟨ $A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q)$  320c⟩
        ⟨ $V' = V \cdot P(\phi; p, q)$  321d⟩
        ⟨Update num_rot 321f⟩
    end if
end if

```

We want

$$A'_{pq} = (c^2 - s^2)A_{pq} + sc(A_{pp} - A_{qq}) = 0 \quad (\text{H.6})$$

and therefore

$$\cot 2\phi = \frac{1 - \tan^2 \phi}{2 \tan \phi} = \frac{\cos^2 \phi - \sin^2 \phi}{2 \sin \phi \cos \phi} = \frac{A_{pp} - A_{qq}}{2A_{pq}} \quad (\text{H.7})$$

i.e. with $t = \tan \phi = s/c$

$$t^2 + 2t \cot 2\phi - 1 = 0 \quad (\text{H.8})$$

This quadratic equation has the roots

$$t = -\cot 2\phi \pm \sqrt{1 + \cot^2 2\phi} = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| \pm \epsilon(\cot 2\phi)\sqrt{1 + \cot^2 2\phi}} \quad (\text{H.9})$$

and the smaller in magnitude of these is

$$t = \frac{\epsilon(\cot 2\phi)}{|\cot 2\phi| + \sqrt{1 + \cot^2 2\phi}} \quad (\text{H.10})$$

and since $|t| \leq 1$, it corresponds to $|\phi| \leq \pi/4$. For very large $\cot 2\phi$ we will use

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

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

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

```

h = aa(q,q) - aa(p,p)
if (g <= spacing (h)) then
  t = aa(p,q) / h
else
  cot_2phi = 0.5 * h / aa(p,q)
  t = sign (1.0_default, cot_2phi) &
    / (abs (cot_2phi) + sqrt (1.0 + cot_2phi**2))
end if

```

Trivia

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

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

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

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

```

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

```

$$\begin{aligned}
A'_{pp} &= c^2 A_{pp} + s^2 A_{qq} - 2sc A_{pq} = A_{pp} - t A_{pq} \\
A'_{qq} &= s^2 A_{pp} + c^2 A_{qq} + 2sc A_{pq} = A_{qq} + t A_{pq} \\
A'_{pq} &= (c^2 - s^2) A_{pq} + sc (A_{pp} - A_{qq})
\end{aligned} \quad (\text{H.14})$$

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

```

aa(p,p) = aa(p,p) - t * aa(p,q)
aa(q,q) = aa(q,q) + t * aa(p,q)
aa(p,q) = 0.0

```

$$\begin{aligned}
r \neq p < q \neq r : A'_{rp} &= c A_{rp} - s A_{rq} \\
A'_{rq} &= s A_{rp} + c A_{rq}
\end{aligned} \quad (\text{H.15})$$

Here's how we cover the upper triangular region using array notation:

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

321a $\langle A' = P^T(\phi; p, q) \cdot A \cdot P(\phi; p, q) \text{ 320c} \rangle + \equiv$ (319) $\langle \text{320c}$
`call jacobi_rotation (s, tau, aa(1:p-1,p), aa(1:p-1,q))`
`call jacobi_rotation (s, tau, aa(p,p+1:q-1), aa(p+1:q-1,q))`
`call jacobi_rotation (s, tau, aa(p,q+1:ndim), aa(q,q+1:ndim))`

Using (H.13c), we can write the rotation as a perturbation:

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

321b $\langle \text{Implementation of linalg procedures 315} \rangle + \equiv$ (314a) $\langle \text{318b 322a} \rangle$
`pure subroutine jacobi_rotation (s, tau, vp, vq)`
`real(kind=default), intent(in) :: s, tau`
`real(kind=default), dimension(:), intent(inout) :: vp, vq`
`real(kind=default), dimension(size(vp)) :: vp_tmp`
`vp_tmp = vp`
`vp = vp - s * (vq + tau * vp)`
`vq = vq + s * (vp_tmp - tau * vq)`
`end subroutine jacobi_rotation`

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

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

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

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

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

```

pure subroutine unit (u)
  real(kind=default), dimension(:,,:), intent(out) :: u
  integer :: i
  u = 0.0
  do i = 1, min (size (u, dim = 1), size (u, dim = 2))
    u(i,i) = 1.0
  end do
end subroutine unit

```

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

```

pure function diag (a) result (d)
  real(kind=default), dimension(:,,:), intent(in) :: a
  real(kind=default), dimension(min(size(a,dim=1),size(a,dim=2))) :: d
  integer :: i
  do i = 1, min (size (a, dim = 1), size (a, dim = 2))
    d(i) = a(i,i)
  end do
end function diag

```

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

```

public :: unit, diag

```

H.4 Test

322d *<la_sample.f90 322d>≡*

```

! la_sample.f90 --
<Copyleft notice 1>
program la_sample
  use kinds
  use utils
  use tao_random_numbers
  use linalg
  implicit none
  integer, parameter :: N = 200
  real(kind=default), dimension(N,N) :: a, evec, a0, l, u, NAG_bug
  real(kind=default), dimension(N) :: b, eval
  real(kind=default) :: d
  integer :: i
  call system_clock (i)
  call tao_random_seed (i)
  print *, i
  do i = 1, N

```

```

        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

```
324 <products.f90 324>≡
! products.f90 --
<Copyleft notice 1>
module products
  use kinds
  implicit none
  private
  public :: dot, sp, spc
  character(len=*), public, parameter :: PRODUCTS_RCS_ID = &
    "$Id: products.nw 314 2010-04-17 20:32:33Z ohl $"
contains
  pure function dot (p, q) result (pq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    real(kind=default) :: pq
    pq = p(0)*q(0) - dot_product (p(1:), q(1:))
  end function dot
  pure function sp (p, q) result (sppq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: sppq
    sppq = cmplx (p(2), p(3), kind=default) * sqrt ((q(0)-q(1))/(p(0)-p(1))) &
      - cmplx (q(2), q(3), kind=default) * sqrt ((p(0)-p(1))/(q(0)-q(1)))
  end function sp
  pure function spc (p, q) result (spcpq)
    real(kind=default), dimension(0:), intent(in) :: p, q
    complex(kind=default) :: spcpq
    spcpq = conjg (sp (p, q))
  end function spc
end module products
```

—J—

KINEMATICS

```

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

```

J.1 Lorentz Transformations

```

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

325c  <Interfaces of kinematics procedures 325c>≡                (325a) 327f>
      interface boost_velocity
        module procedure boost_one_velocity, boost_many_velocity
      end interface

```

```

interface boost_momentum
  module procedure boost_one_momentum, boost_many_momentum
end interface

```

Boost a four vector p to the inertial frame moving with the velocity β :

$$p'_0 = \gamma (p_0 - \vec{\beta} \vec{p}) \quad (\text{J.1a})$$

$$\vec{p}' = \gamma (\vec{p}_{\parallel} - \vec{\beta} p_0) + \vec{p}_{\perp} \quad (\text{J.1b})$$

with $\gamma = 1/\sqrt{1 - \vec{\beta}^2}$, $\vec{p}_{\parallel} = \vec{\beta}(\vec{\beta} \vec{p})/\vec{\beta}^2$ 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

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

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

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

```

pure function boost_one_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(0:3) :: p_prime
  real(kind=default), dimension(1:3) :: b
  real(kind=default) :: gamma, b_dot_p
  gamma = 1.0 / sqrt (1.0 - dot_product (beta, beta))
  b = gamma * beta
  b_dot_p = dot_product (b, p(1:3))
  p_prime(0) = gamma * p(0) - b_dot_p
  p_prime(1:3) = p(1:3) + (b_dot_p / (1.0 + gamma) - p(0)) * b
end function boost_one_velocity

```

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

```

pure function boost_many_velocity (p, beta) result (p_prime)
  real(kind=default), dimension(:,0:), intent(in) :: p
  real(kind=default), dimension(1:), intent(in) :: beta
  real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
  integer :: i
  do i = 1, size (p, dim=1)
    p_prime(i,:) = boost_one_velocity (p(i,:), beta)
  end do
end function boost_many_velocity

```

Boost a four vector p to the rest frame of the four vector q . The velocity is $\vec{\beta} = \vec{q}/|q_0|$:

327a \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 326b 327b \rangle
 pure function **boost_one_momentum** (p, q) result (p_prime)
 real(kind=default), dimension(0:), intent(in) :: p, q
 real(kind=default), dimension(0:3) :: p_prime
 p_prime = **boost_velocity** (p, q(1:3) / abs (q(0)))
 end function **boost_one_momentum**

327b \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 327a 327c \rangle
 pure function **boost_many_momentum** (p, q) result (p_prime)
 real(kind=default), dimension(:,0:), intent(in) :: p
 real(kind=default), dimension(0:), intent(in) :: q
 real(kind=default), dimension(size(p,dim=1),0:3) :: p_prime
 p_prime = **boost_many_velocity** (p, q(1:3) / abs (q(0)))
 end function **boost_many_momentum**

J.2 Massive Phase Space

$$\lambda(a, b, c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca = (a - b - c)^2 - 4bc \quad (\text{J.3})$$

and permutations

327c \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 327b 328a \rangle
 pure function **lambda** (a, b, c) result (lam)
 real(kind=default), intent(in) :: a, b, c
 real(kind=default) :: lam
 lam = a**2 + b**2 + c**2 - 2*(a*b + b*c + c*a)
 end function **lambda**

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

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

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

327g \langle Declaration of kinematics types 327g $\rangle \equiv$ (325a)
 type, public :: **LIPS3**
 real(kind=default), dimension(3,0:3) :: p
 real(kind=default) :: **jacobian**
 end type **LIPS3**

$$dLIPS_3 = \int \frac{d^3\vec{p}_1}{(2\pi)^3 2E_1} \frac{d^3\vec{p}_2}{(2\pi)^3 2E_2} \frac{d^3\vec{p}_3}{(2\pi)^3 2E_3} (2\pi)^4 \delta^4(p_1 + p_2 + p_3 - p_a - p_b) \quad (J.4)$$

The jacobian is given by

$$dLIPS_3 = \frac{1}{(2\pi)^5} \int d\phi dt_1 ds_2 d\Omega_3^{[23]} \frac{1}{32\sqrt{ss_2}} \frac{|p_3^{[23]}|}{|p_a^{[ab]}|} \quad (J.5)$$

where $\vec{p}_i^{[jk]}$ denotes the momentum of particle i in the center of mass system of particles j and k .

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

```

pure function two_to_three_massive &
  (s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3) result (p)
  real(kind=default), intent(in) :: &
    s, t1, s2, phi, cos_theta3, phi3, ma, mb, m1, m2, m3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: Ea, pa_abs, E1, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (lambda (s, ma**2, mb**2) / (4 * s))
  Ea = sqrt (ma**2 + pa_abs**2)
  p1_abs = sqrt (lambda (s, m1**2, s2) / (4 * s))
  E1 = sqrt (m1**2 + p1_abs**2)
  p3_abs = sqrt (lambda (s2, m2**2, m3**2) / (4 * s2))
  p%jacobian = &
    1.0 / (2*PI)**5 * (p3_abs / pa_abs) / (32 * sqrt (s * s2))
  cos_theta = (t1 - ma**2 - m1**2 + 2*Ea*E1) / (2*pa_abs*p1_abs)
  p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
  p%p(1,0) = on_shell (p%p(1,:), m1)
  p23(1:3) = - p%p(1,1:3)
  p23(0) = on_shell (p23, sqrt (s2))
  p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3, m3, m2)
end function two_to_three_massive

```

A specialized version for massless particles can be faster, because the kinematics is simpler:

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

```

pure function two_to_three_massless (s, t1, s2, phi, cos_theta3, phi3) &
  result (p)
  real(kind=default), intent(in) :: s, t1, s2, phi, cos_theta3, phi3
  type(LIPS3) :: p
  real(kind=default), dimension(0:3) :: p23
  real(kind=default) :: pa_abs, p1_abs, p3_abs, cos_theta
  pa_abs = sqrt (s) / 2
  p1_abs = (s - s2) / (2 * sqrt (s))

```

```

    p3_abs = sqrt (s2) / 2
    p%jacobian = 1.0 / ((2*PI)**5 * 32 * s)
    cos_theta = 1 + t1 / (2*pa_abs*p1_abs)
    p%p(1,0) = p1_abs
    p%p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
    p23(1:3) = - p%p(1,1:3)
    p23(0) = on_shell (p23, sqrt (s2))
    p%p(3:2:-1,:) = one_to_two (p23, cos_theta3, phi3)
end function two_to_three_massless

329a <Declaration of kinematics procedures 325b>+≡ (325a) <327e 330a>
    public :: one_to_two
    private :: one_to_two_massive, one_to_two_massless

329b <Interfaces of kinematics procedures 325c>+≡ (325a) <327f
    interface one_to_two
        module procedure one_to_two_massive, one_to_two_massless
    end interface

329c <Implementation of kinematics procedures 326a>+≡ (325a) <328b 329d>
    pure function one_to_two_massive (p12, cos_theta, phi, m1, m2) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi, m1, m2
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: s, p1_abs
        s = dot (p12, p12)
        p1_abs = sqrt (lambda (s, m1**2, m2**2) / (4 * s))
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,1:3) = - p(1,1:3)
        p(1,0) = on_shell (p(1,:), m1)
        p(2,0) = on_shell (p(2,:), m2)
        p = boost_momentum (p, - p12)
    end function one_to_two_massive

329d <Implementation of kinematics procedures 326a>+≡ (325a) <329c 330b>
    pure function one_to_two_massless (p12, cos_theta, phi) result (p)
        real(kind=default), dimension(0:), intent(in) :: p12
        real(kind=default), intent(in) :: cos_theta, phi
        real(kind=default), dimension(2,0:3) :: p
        real(kind=default) :: p1_abs
        p1_abs = sqrt (dot (p12, p12)) / 2
        p(1,0) = p1_abs
        p(1,1:3) = polar_to_cartesian (p1_abs, cos_theta, phi)
        p(2,0) = p1_abs
        p(2,1:3) = - p(1,1:3)
        p = boost_momentum (p, - p12)

```

```

end function one_to_two_massless

330a <Declaration of kinematics procedures 325b>+≡ (325a) <329a 333c>
public :: polar_to_cartesian, on_shell

330b <Implementation of kinematics procedures 326a>+≡ (325a) <329d 330c>
pure function polar_to_cartesian (v_abs, cos_theta, phi) result (v)
  real(kind=default), intent(in) :: v_abs, cos_theta, phi
  real(kind=default), dimension(3) :: v
  real(kind=default) :: sin_phi, cos_phi, sin_theta
  sin_theta = sqrt (1.0 - cos_theta**2)
  cos_phi = cos (phi)
  sin_phi = sin (phi)
  v = (/ sin_theta * cos_phi, sin_theta * sin_phi, cos_theta /) * v_abs
end function polar_to_cartesian

330c <Implementation of kinematics procedures 326a>+≡ (325a) <330b 333d>
pure function on_shell (p, m) result (E)
  real(kind=default), dimension(0:), intent(in) :: p
  real(kind=default), intent(in) :: m
  real(kind=default) :: E
  E = sqrt (m**2 + dot_product (p(1:3), p(1:3)))
end function on_shell

```

J.3 Massive 3-Particle Phase Space Revisited

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

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

```

330d <kinematics.f90 325a>+≡ <325a>
module phase_space
  use kinds
  use constants
  use kinematics !NODEP!
  use tao_random_numbers
  implicit none
  private

```

```

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

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

331a <Declaration of phase_space types 331a>≡ (330d) 331b>
type, public :: LIPS3_unit
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_unit

331b <Declaration of phase_space types 331a>+≡ (330d) <331a 331c>
type, public :: LIPS3_unit_massless
    real(kind=default), dimension(5) :: x
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_unit_massless

LIPS3_s2_t1_angles : (s2, t1, ϕ, cos θ3, ϕ3) (J.9)

331c <Declaration of phase_space types 331a>+≡ (330d) <331b 331d>
type, public :: LIPS3_s2_t1_angles
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default), dimension(2) :: mass_in
    real(kind=default), dimension(3) :: mass_out
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles

331d <Declaration of phase_space types 331a>+≡ (330d) <331c 331e>
type, public :: LIPS3_s2_t1_angles_massless
    real(kind=default) :: s2, t1, phi, cos_theta3, phi3
    real(kind=default) :: s
    real(kind=default) :: jacobian
end type LIPS3_s2_t1_angles_massless

LIPS3_momenta : (p1, p2, p3) (J.10)

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

```

```

type, public :: LIPS3_momenta
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default), dimension(2) :: mass_in
  real(kind=default), dimension(3) :: mass_out
  real(kind=default) :: jacobian
end type LIPS3_momenta

332a <Declaration of phase_space types 331a>+≡ (330d) <331e>
type, public :: LIPS3_momenta_massless
  real(kind=default), dimension(0:3,3) :: p
  real(kind=default) :: s
  real(kind=default) :: jacobian
end type LIPS3_momenta_massless

332b <Declaration of phase_space procedures 332b>≡ (330d) 332f>
public :: random_LIPS3
private :: random_LIPS3_unit, random_LIPS3_unit_massless

332c <Interfaces of phase_space procedures 332c>≡ (330d)
interface random_LIPS3
  module procedure random_LIPS3_unit, random_LIPS3_unit_massless
end interface

332d <Implementation of phase_space procedures 332d>≡ (330d) 332e>
pure subroutine random_LIPS3_unit (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit

332e <Implementation of phase_space procedures 332d>+≡ (330d) <332d 333a>
pure subroutine random_LIPS3_unit_massless (rng, lips)
  type(tao_random_state), intent(inout) :: rng
  type(LIPS3_unit_massless), intent(inout) :: lips
  call tao_random_number (rng, lips%x)
  lips%jacobian = 1
end subroutine random_LIPS3_unit_massless

332f <Declaration of phase_space procedures 332b>+≡ (330d) <332b>
private :: LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0

332g <(Unused) Interfaces of phase_space procedures 332g>≡
interface assignment(=)
  module procedure &
    LIPS3_unit_to_s2_t1_angles, LIPS3_unit_to_s2_t1_angles_m0
end interface

```

333a \langle Implementation of phase_space procedures 332d $\rangle + \equiv$ (330d) \langle 332e 333b \rangle
 pure subroutine LIPS3_unit_to_s2_t1_angles (s2_t1_angles, unit)
 type(LIPS3_s2_t1_angles), intent(out) :: s2_t1_angles
 type(LIPS3_unit), intent(in) :: unit
 end subroutine LIPS3_unit_to_s2_t1_angles

333b \langle Implementation of phase_space procedures 332d $\rangle + \equiv$ (330d) \langle 333a
 pure subroutine LIPS3_unit_to_s2_t1_angles_m0 (s2_t1_angles, unit)
 type(LIPS3_s2_t1_angles_massless), intent(out) :: s2_t1_angles
 type(LIPS3_unit_massless), intent(in) :: unit
 end subroutine LIPS3_unit_to_s2_t1_angles_m0

J.4 Massless n -Particle Phase Space: RAMBO

333c \langle Declaration of kinematics procedures 325b $\rangle + \equiv$ (325a) \langle 330a 334b \rangle
 public :: massless_isotropic_decay

The massless RAMBO algorithm [26]:

333d \langle Implementation of kinematics procedures 326a $\rangle + \equiv$ (325a) \langle 330c 334c \rangle
 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
 \langle Generate isotropic null vectors 333e \rangle
 \langle Boost and rescale the vectors 334a \rangle
 end function massless_isotropic_decay

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

333e \langle Generate isotropic null vectors 333e $\rangle \equiv$ (333d)
 do k = 1, size (p, dim = 1)
 q(k,0) = - log (ran(k,1) * ran(k,2))
 cos_theta = 2 * ran(k,3) - 1
 sin_theta = sqrt (1 - cos_theta**2)
 phi = 2 * PI * ran(k,4)
 q(k,1) = q(k,0) * sin_theta * cos (phi)
 q(k,2) = q(k,0) * sin_theta * sin (phi)
 q(k,3) = q(k,0) * cos_theta
 enddo

The proof that the Jacobian of the transformation vanishes can be found in [26]. The transformation is really a Lorentz boost (as can be seen easily).

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

```
qsum = sum (q, dim = 1)
qabs = sqrt (dot (qsum, qsum))
x = roots / qabs
do k = 1, size (p, dim = 1)
  r = dot (q(k,:), qsum) / qabs
  z = (q(k,0) + r) / (qsum(0) + qabs)
  p(k,1:3) = x * (q(k,1:3) - qsum(1:3) * z)
  p(k,0) = x * r
enddo
```

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

```
public :: phase_space_volume
```

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

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

```
pure function phase_space_volume (n, roots) result (volume)
  integer, intent(in) :: n
  real (kind=default), intent(in) :: roots
  real (kind=default) :: volume
  real (kind=default) :: nd
  nd = n
  volume = (nd - 1) / (8*PI * (gamma (nd))**2) * (roots / (4*PI))**(2*n-4)
end function phase_space_volume
```

J.5 Tests

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

```
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!

335 \langle Trivial ktest.f90 335 $\rangle \equiv$

```

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

```

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

```

K.1 Angular Spherical Coordinates

$$\begin{aligned}
 x_n &= r \cos \theta_{n-2} \\
 x_{n-1} &= r \sin \theta_{n-2} \cos \theta_{n-3} \\
 &\dots \\
 x_3 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \cos \theta_1 \\
 x_2 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \cos \phi \\
 x_1 &= r \sin \theta_{n-2} \sin \theta_{n-3} \cdots \sin \theta_1 \sin \phi
 \end{aligned} \tag{K.1}$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} (\sin \theta_i)^i \tag{K.2}$$

We can minimize the number of multiplications by computing the products

$$P_j = \prod_{i=j}^{n-2} \sin \theta_i \quad (\text{K.3})$$

Then

$$\begin{aligned} x_n &= r \cos \theta_{n-2} \\ x_{n-1} &= r P_{n-2} \cos \theta_{n-3} \\ &\dots \\ x_3 &= r P_2 \cos \theta_1 \\ x_2 &= r P_1 \cos \phi \\ x_1 &= r P_1 \sin \phi \end{aligned} \quad (\text{K.4})$$

and

$$J = r^{n-1} \prod_{i=1}^{n-2} P_i \quad (\text{K.5})$$

Note that $\theta_i \in [0, \pi]$ and $\phi \in [0, 2\pi]$ or $\phi \in [-\pi, \pi]$. Therefore $\sin \theta_i \geq 0$ and

$$\sin \theta_i = \sqrt{1 - \cos^2 \theta_i} \quad (\text{K.6})$$

which is not true for ϕ . Since `sqrt` is typically much faster than `sin` and `cos`, we use (K.6) where ever possible.

```

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

338b <Implementation of coordinates procedures 338b>≡ (337) 339a>
      pure subroutine spherical_to_cartesian_2 (r, phi, theta, x, jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(:), intent(out), optional :: x
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default), dimension(size(theta)) :: cos_theta
        real(kind=default), dimension(size(theta)+1) :: product_sin_theta
        integer :: n, i
        n = size (theta) + 2
        cos_theta = cos (theta)
        product_sin_theta(n-1) = 1.0_default
        do i = n - 2, 1, -1
          product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
        end do

```

```

if (present (x)) then
  x(1) = r * product_sin_theta(1) * sin (phi)
  x(2) = r * product_sin_theta(1) * cos (phi)
  x(3:) = r * product_sin_theta(2:n-1) * cos_theta
end if
if (present (jacobian)) then
  jacobian = r**(n-1) * product (product_sin_theta)
end if
end subroutine spherical_to_cartesian_2

```



Note that call inside of a function breaks F-compatibility. Here it would be easy to fix, but the inverse can not be coded as a function, unless a type for spherical coordinates is introduced, where `theta` could not be assumed shape ...

- 339a *<Implementation of coordinates procedures 338b>+≡ (337) <338b 339b>*
 pure function `spherical_to_cartesian` (r, phi, theta) result (x)
 real(kind=default), intent(in) :: r, phi
 real(kind=default), dimension(:), intent(in) :: theta
 real(kind=default), dimension(size(theta)+2) :: x
 call `spherical_to_cartesian_2` (r, phi, theta, x = x)
 end function `spherical_to_cartesian`
- 339b *<Implementation of coordinates procedures 338b>+≡ (337) <339a 339d>*
 pure function `spherical_to_cartesian_j` (r, phi, theta) &
 result (jacobian)
 real(kind=default), intent(in) :: r, phi
 real(kind=default), dimension(:), intent(in) :: theta
 real(kind=default) :: jacobian
 call `spherical_to_cartesian_2` (r, phi, theta, jacobian = jacobian)
 end function `spherical_to_cartesian_j`
- 339c *<Declaration of coordinates procedures 338a>+≡ (337) <338a 341c>*
 public :: `cartesian_to_spherical_2`, &
 `cartesian_to_spherical`, `cartesian_to_spherical_j`
- 339d *<Implementation of coordinates procedures 338b>+≡ (337) <339b 341a>*
 pure subroutine `cartesian_to_spherical_2` (x, r, phi, theta, jacobian)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default), intent(out), optional :: r, phi
 real(kind=default), dimension(:), intent(out), optional :: theta
 real(kind=default), intent(out), optional :: jacobian
 real(kind=default) :: local_r
 real(kind=default), dimension(size(x)-2) :: cos_theta
 real(kind=default), dimension(size(x)-1) :: product_sin_theta

```

integer :: n, i
n = size (x)
local_r = sqrt (dot_product (x, x))
if (local_r == 0) then
  if (present (r)) then
    r = 0
  end if
  if (present (phi)) then
    phi = 0
  end if
  if (present (theta)) then
    theta = 0
  end if
  if (present (jacobian)) then
    jacobian = 1
  end if
else
  product_sin_theta(n-1) = 1
  do i = n, 3, -1
    if (product_sin_theta(i-1) == 0) then
      cos_theta(i-2) = 0
    else
      cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
    end if
    product_sin_theta(i-2) = &
      product_sin_theta(i-1) * sqrt (1 - cos_theta(i-2)**2)
  end do
  if (present (r)) then
    r = local_r
  end if
  if (present (phi)) then
    ! Set phi = 0 for vanishing vector
    if (x(1) == 0 .and. x(2)==0) then
      phi = 0
    else
      phi = atan2 (x(1), x(2))
    end if
  end if
  if (present (theta)) then
    theta = acos (cos_theta)
  end if
  if (present (jacobian)) then
    jacobian = local_r**(1-n) / product (product_sin_theta)
  end if
end if

```

```

        end if
    end if
end subroutine cartesian_to_spherical_2
341a  <Implementation of coordinates procedures 338b>+≡ (337) <339d 341b>
pure subroutine cartesian_to_spherical (x, r, phi, theta)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default), intent(out) :: r, phi
    real(kind=default), dimension(:), intent(out) :: theta
    call cartesian_to_spherical_2 (x, r, phi, theta)
end subroutine cartesian_to_spherical
341b  <Implementation of coordinates procedures 338b>+≡ (337) <341a 341d>
pure function cartesian_to_spherical_j (x) result (jacobian)
    real(kind=default), dimension(:), intent(in) :: x
    real(kind=default) :: jacobian
    call cartesian_to_spherical_2 (x, jacobian = jacobian)
end function cartesian_to_spherical_j

```

K.2 Trigonometric Spherical Coordinates

```

341c  <Declaration of coordinates procedures 338a>+≡ (337) <339c 342c>
public :: spherical_cos_to_cartesian_2, &
        spherical_cos_to_cartesian, spherical_cos_to_cartesian_j

```

Using the cosine, we have to drop P_1 from the Jacobian

```

341d  <Implementation of coordinates procedures 338b>+≡ (337) <341b 342a>
pure subroutine spherical_cos_to_cartesian_2 (r, phi, cos_theta, x, jacobian)
    real(kind=default), intent(in) :: r, phi
    real(kind=default), dimension(:), intent(in) :: cos_theta
    real(kind=default), dimension(:), intent(out), optional :: x
    real(kind=default), intent(out), optional :: jacobian
    real(kind=default), dimension(size(cos_theta)+1) :: product_sin_theta
    integer :: n, i
    n = size (cos_theta) + 2
    product_sin_theta(n-1) = 1.0_default
    do i = n - 2, 1, -1
        product_sin_theta(i) = &
            product_sin_theta(i+1) * sqrt (1 - cos_theta(i)**2)
    end do
    if (present (x)) then
        x(1) = r * product_sin_theta(1) * sin (phi)
        x(2) = r * product_sin_theta(1) * cos (phi)
        x(3:) = r * product_sin_theta(2:n-1) * cos_theta
    end if
end subroutine spherical_cos_to_cartesian_2

```

```

        end if
        if (present (jacobian)) then
            jacobian = r**(n-1) * product (product_sin_theta(2:))
        end if
    end subroutine spherical_cos_to_cartesian_2
342a  <Implementation of coordinates procedures 338b>+≡ (337) <341d 342b>
    pure function spherical_cos_to_cartesian (r, phi, theta) result (x)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default), dimension(size(theta)+2) :: x
        call spherical_cos_to_cartesian_2 (r, phi, theta, x = x)
    end function spherical_cos_to_cartesian
342b  <Implementation of coordinates procedures 338b>+≡ (337) <342a 342d>
    pure function spherical_cos_to_cartesian_j (r, phi, theta) &
        result (jacobian)
        real(kind=default), intent(in) :: r, phi
        real(kind=default), dimension(:), intent(in) :: theta
        real(kind=default) :: jacobian
        call spherical_cos_to_cartesian_2 (r, phi, theta, jacobian = jacobian)
    end function spherical_cos_to_cartesian_j
342c  <Declaration of coordinates procedures 338a>+≡ (337) <341c 344b>
    public :: cartesian_to_spherical_cos_2, &
        cartesian_to_spherical_cos, cartesian_to_spherical_cos_j
342d  <Implementation of coordinates procedures 338b>+≡ (337) <342b 343>
    pure subroutine cartesian_to_spherical_cos_2 (x, r, phi, cos_theta, jacobian)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out), optional :: r, phi
        real(kind=default), dimension(:), intent(out), optional :: cos_theta
        real(kind=default), intent(out), optional :: jacobian
        real(kind=default) :: local_r
        real(kind=default), dimension(size(x)-2) :: local_cos_theta
        real(kind=default), dimension(size(x)-1) :: product_sin_theta
        integer :: n, i
        n = size (x)
        local_r = sqrt (dot_product (x, x))
        if (local_r == 0) then
            if (present (r)) then
                r = 0
            end if
            if (present (phi)) then
                phi = 0
            end if
        end if
    end subroutine

```

```

    if (present (cos_theta)) then
        cos_theta = 0
    end if
    if (present (jacobian)) then
        jacobian = 1
    end if
else
    product_sin_theta(n-1) = 1
    do i = n, 3, -1
        if (product_sin_theta(i-1) == 0) then
            local_cos_theta(i-2) = 0
        else
            local_cos_theta(i-2) = x(i) / product_sin_theta(i-1) / local_r
        end if
        product_sin_theta(i-2) = &
            product_sin_theta(i-1) * sqrt (1 - local_cos_theta(i-2)**2)
    end do
    if (present (r)) then
        r = local_r
    end if
    if (present (phi)) then
        ! Set phi = 0 for vanishing vector
        if (x(1) == 0 .and. x(2)==0) then
            phi = 0
        else
            phi = atan2 (x(1), x(2))
        end if
    end if
    if (present (cos_theta)) then
        cos_theta = local_cos_theta
    end if
    if (present (jacobian)) then
        jacobian = local_r**(1-n) / product (product_sin_theta(2:))
    end if
end if
end subroutine cartesian_to_spherical_cos_2
343  <Implementation of coordinates procedures 338b>+≡ (337) <342d 344a>
    pure subroutine cartesian_to_spherical_cos (x, r, phi, cos_theta)
        real(kind=default), dimension(:), intent(in) :: x
        real(kind=default), intent(out) :: r, phi
        real(kind=default), dimension(:), intent(out), optional :: cos_theta
        call cartesian_to_spherical_cos_2 (x, r, phi, cos_theta)
    end subroutine cartesian_to_spherical_cos

```


344a \langle Implementation of coordinates procedures 338b $\rangle + \equiv$ (337) \triangleleft 343 344c \triangleright
 pure function cartesian_to_spherical_cos_j (x) result (jacobian)
 real(kind=default), dimension(:), intent(in) :: x
 real(kind=default) :: jacobian
 call cartesian_to_spherical_cos_2 (x, jacobian = jacobian)
 end function cartesian_to_spherical_cos_j

K.3 Surface of a Sphere

344b \langle Declaration of coordinates procedures 338a $\rangle + \equiv$ (337) \triangleleft 342c
 public :: surface

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

344c \langle Implementation of coordinates procedures 338b $\rangle + \equiv$ (337) \triangleleft 344a
 pure function surface (n) result (vol)
 integer, intent(in) :: n
 real(kind=default) :: vol
 real(kind=default) :: n_by_2
 n_by_2 = 0.5_default * n
 vol = 2 * PI**n_by_2 / gamma (n_by_2)
 end function surface

—L—

IDIOMATIC FORTRAN90 INTERFACE FOR MPI

```

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

```

L.1 Basics

```

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

```

```

346a  <Implementation of mpi90 procedures 346a>≡ (345a) 346d>
      subroutine mpi90_init (error)
        integer, intent(out), optional :: error
        integer :: local_error
        character(len=*), parameter :: FN = "mpi90_init"
        external mpi_init
        call mpi_init (local_error)
        <Handle local_error (no mpi90_abort) 346b>
      end subroutine mpi90_init

346b  <Handle local_error (no mpi90_abort) 346b>≡ (346)
      if (present (error)) then
        error = local_error
      else
        if (local_error /= MPI_SUCCESS) then
          call mpi90_print_error (local_error, FN)
          stop
        end if
      end if

346c  <Handle local_error 346c>≡ (346-49 351c 353d 354b 356a)
      if (present (error)) then
        error = local_error
      else
        if (local_error /= MPI_SUCCESS) then
          call mpi90_print_error (local_error, FN)
          call mpi90_abort (local_error)
          stop
        end if
      end if

346d  <Implementation of mpi90 procedures 346a>+≡ (345a) <346a 346e>
      subroutine mpi90_finalize (error)
        integer, intent(out), optional :: error
        integer :: local_error
        character(len=*), parameter :: FN = "mpi90_finalize"
        external mpi_finalize
        call mpi_finalize (local_error)
        <Handle local_error 346c>
      end subroutine mpi90_finalize

346e  <Implementation of mpi90 procedures 346a>+≡ (345a) <346d 347a>
      subroutine mpi90_abort (code, domain, error)
        integer, intent(in), optional :: code, domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_abort"

```

```

integer :: local_domain, local_code, local_error
external mpi_abort
if (present (code)) then
    local_code = code
else
    local_code = MPI_ERR_UNKNOWN
end if
<Set default for domain 347b>
call mpi_abort (local_domain, local_code, local_error)
<Handle local_error (no mpi90_abort) 346b>
end subroutine mpi90_abort
347a <Implementation of mpi90 procedures 346a>+≡ (345a) <346e 347c>
subroutine mpi90_print_error (error, msg)
integer, intent(in) :: error
character(len=*), optional :: msg
character(len=*), parameter :: FN = "mpi90_print_error"
integer :: msg_len, local_error
external mpi_error_string
call mpi_error_string (error, msg, msg_len, local_error)
if (local_error /= MPI_SUCCESS) then
    print *, "PANIC: even MPI_ERROR_STRING() failed!!!"
    call mpi90_abort (local_error)
else if (present (msg)) then
    print *, trim (msg), ": ", trim (msg(msg_len+1:))
else
    print *, "mpi90: ", trim (msg(msg_len+1:))
end if
end subroutine mpi90_print_error
347b <Set default for domain 347b>≡ (346-50 356a) 354f>
if (present (domain)) then
    local_domain = domain
else
    local_domain = MPI_COMM_WORLD
end if
347c <Implementation of mpi90 procedures 346a>+≡ (345a) <347a 348a>
subroutine mpi90_size (sz, domain, error)
integer, intent(out) :: sz
integer, intent(in), optional :: domain
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_size"
integer :: local_domain, local_error
external mpi_comm_size

```

```

    <Set default for domain 347b>
    call mpi_comm_size (local_domain, sz, local_error)
    <Handle local_error 346c>
end subroutine mpi90_size
348a <Implementation of mpi90 procedures 346a>+≡ (345a) <347c 348d>
    subroutine mpi90_rank (rank, domain, error)
        integer, intent(out) :: rank
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_rank"
        integer :: local_domain, local_error
        external mpi_comm_rank
        <Set default for domain 347b>
        call mpi_comm_rank (local_domain, rank, local_error)
        <Handle local_error 346c>
    end subroutine mpi90_rank

```

L.2 Point to Point

```

348b <Declaration of mpi90 procedures 345b>+≡ (345a) <345b 351d>
    public :: mpi90_send
    public :: mpi90_receive
    public :: mpi90_receive_pointer

348c <Interfaces of mpi90 procedures 348c>≡ (345a) 350d>
    interface mpi90_send
        module procedure &
            mpi90_send_integer, mpi90_send_double, &
            mpi90_send_integer_array, mpi90_send_double_array, &
            mpi90_send_integer_array2, mpi90_send_double_array2
    end interface

348d <Implementation of mpi90 procedures 346a>+≡ (345a) <348a 348e>
    subroutine mpi90_send_integer (value, target, tag, domain, error)
        integer, intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        call mpi90_send_integer_array ((/ value /), target, tag, domain, error)
    end subroutine mpi90_send_integer

348e <Implementation of mpi90 procedures 346a>+≡ (345a) <348d 349a>
    subroutine mpi90_send_double (value, target, tag, domain, error)

```

```

    real(kind=default), intent(in) :: value
    integer, intent(in) :: target, tag
    integer, intent(in), optional :: domain
    integer, intent(out), optional :: error
    call mpi90_send_double_array ((/ value /), target, tag, domain, error)
end subroutine mpi90_send_double

349a  <Implementation of mpi90 procedures 346a>+≡ (345a) <348e 349c>
    subroutine mpi90_send_integer_array (buffer, target, tag, domain, error)
        integer, dimension(:), intent(in) :: buffer
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_send.*_array 349b>
    end subroutine mpi90_send_integer_array

349b  <Body of mpi90_send.*_array 349b>≡ (349)
    integer :: local_domain, local_error
    external mpi_send
    <Set default for domain 347b>
    call mpi_send (buffer, size (buffer), datatype, target, tag, &
        local_domain, local_error)
    <Handle local_error 346c>

349c  <Implementation of mpi90 procedures 346a>+≡ (345a) <349a 349d>
    subroutine mpi90_send_double_array (buffer, target, tag, domain, error)
        real(kind=default), dimension(:), intent(in) :: buffer
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_send_double_array"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        <Body of mpi90_send.*_array 349b>
    end subroutine mpi90_send_double_array

349d  <Implementation of mpi90 procedures 346a>+≡ (345a) <349c 350a>
    subroutine mpi90_send_integer_array2 (value, target, tag, domain, error)
        integer, dimension(:, :), intent(in) :: value
        integer, intent(in) :: target, tag
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(size(value)) :: buffer
        buffer = reshape (value, shape(buffer))
        call mpi90_send_integer_array (buffer, target, tag, domain, error)

```

```

        end subroutine mpi90_send_integer_array2

350a  <Implementation of mpi90 procedures 346a>+≡ (345a) <349d 350c>
        subroutine mpi90_send_double_array2 (value, target, tag, domain, error)
            real(kind=default), dimension(:,,:), intent(in) :: value
            integer, intent(in) :: target, tag
            integer, intent(in), optional :: domain
            integer, intent(out), optional :: error
            real(kind=default), dimension(size(value)) :: buffer
            buffer = reshape (value, shape(buffer))
            call mpi90_send_double_array (buffer, target, tag, domain, error)
        end subroutine mpi90_send_double_array2

350b  <Declaration of mpi90 types 350b>≡ (345a)
        type, public :: mpi90_status
            integer :: count, source, tag, error
        end type mpi90_status

350c  <Implementation of mpi90 procedures 346a>+≡ (345a) <350a 351a>
        subroutine mpi90_receive_integer (value, source, tag, domain, status, error)
            integer, intent(out) :: value
            integer, intent(in), optional :: source, tag, domain
            type(mpi90_status), intent(out), optional :: status
            integer, intent(out), optional :: error
            integer, dimension(1) :: buffer
            call mpi90_receive_integer_array (buffer, source, tag, domain, status, error)
            value = buffer(1)
        end subroutine mpi90_receive_integer

350d  <Interfaces of mpi90 procedures 348c>+≡ (345a) <348c 353a>
        interface mpi90_receive
            module procedure &
                mpi90_receive_integer, mpi90_receive_double, &
                mpi90_receive_integer_array, mpi90_receive_double_array, &
                mpi90_receive_integer_array2, mpi90_receive_double_array2
        end interface

350e  <Set defaults for source, tag and domain 350e>≡ (351c 353c)
        if (present (source)) then
            local_source = source
        else
            local_source = MPI_ANY_SOURCE
        end if
        if (present (tag)) then
            local_tag = tag
        else

```

```

        local_tag = MPI_ANY_TAG
    end if
    <Set default for domain 347b>
351a <Implementation of mpi90 procedures 346a>+≡ (345a) <350c 351b>
    subroutine mpi90_receive_double (value, source, tag, domain, status, error)
        real(kind=default), intent(out) :: value
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        call mpi90_receive_double_array (buffer, source, tag, domain, status, error)
        value = buffer(1)
    end subroutine mpi90_receive_double
351b <Implementation of mpi90 procedures 346a>+≡ (345a) <351a 351e>
    subroutine mpi90_receive_integer_array &
        (buffer, source, tag, domain, status, error)
        integer, dimension(:), intent(out) :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_receive.*_array 351c>
    end subroutine mpi90_receive_integer_array
351c <Body of mpi90_receive.*_array 351c>≡ (351b 352a)
    integer :: local_source, local_tag, local_domain, local_error
    integer, dimension(MPI_STATUS_SIZE) :: local_status
    external mpi_receive, mpi_get_count
    <Set defaults for source, tag and domain 350e>
    call mpi_recv (buffer, size (buffer), datatype, local_source, local_tag, &
        local_domain, local_status, local_error)
    <Handle local_error 346c>
    if (present (status)) then
        call decode_status (status, local_status, datatype)
    end if
351d <Declaration of mpi90 procedures 345b>+≡ (345a) <348b 354d>
    private :: decode_status

```



Can we ignore ierror???

```

351e <Implementation of mpi90 procedures 346a>+≡ (345a) <351b 352a>
    subroutine decode_status (status, mpi_status, datatype)

```



```

type(mpi90_status), intent(out) :: status
integer, dimension(:), intent(in) :: mpi_status
integer, intent(in), optional :: datatype
integer :: ierror
if (present (datatype)) then
    call mpi_get_count (mpi_status, datatype, status%count, ierror)
else
    status%count = 0
end if
status%source = mpi_status(MPI_SOURCE)
status%tag = mpi_status(MPI_TAG)
status%error = mpi_status(MPI_ERROR)
end subroutine decode_status

```

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

```

subroutine mpi90_receive_double_array &
    (buffer, source, tag, domain, status, error)
real(kind=default), dimension(:), intent(out) :: buffer
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_receive_double_array"
integer, parameter :: datatype = MPI_DOUBLE_PRECISION
<Body of mpi90_receive.*_array 351c>
end subroutine mpi90_receive_double_array

```

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

```

subroutine mpi90_receive_integer_array2 &
    (value, source, tag, domain, status, error)
integer, dimension(:,:), intent(out) :: value
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
integer, dimension(size(value)) :: buffer
call mpi90_receive_integer_array &
    (buffer, source, tag, domain, status, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_receive_integer_array2

```

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

```

subroutine mpi90_receive_double_array2 &
    (value, source, tag, domain, status, error)
real(kind=default), dimension(:,:), intent(out) :: value
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status

```

```

integer, intent(out), optional :: error
real(kind=default), dimension(size(value)) :: buffer
call mpi90_receive_double_array &
    (buffer, source, tag, domain, status, error)
value = reshape (buffer, shape(value))
end subroutine mpi90_receive_double_array2
353a <Interfaces of mpi90 procedures 348c>+≡ (345a) <350d 354e>
interface mpi90_receive_pointer
    module procedure &
        mpi90_receive_integer_pointer, mpi90_receive_double_pointer
end interface
353b <Implementation of mpi90 procedures 346a>+≡ (345a) <352c 354c>
subroutine mpi90_receive_integer_pointer &
    (buffer, source, tag, domain, status, error)
integer, dimension(:), pointer :: buffer
integer, intent(in), optional :: source, tag, domain
type(mpi90_status), intent(out), optional :: status
integer, intent(out), optional :: error
character(len=*), parameter :: FN = "mpi90_receive_integer_pointer"
integer, parameter :: datatype = MPI_INTEGER
<Body of mpi90_receive_*.pointer 353c>
end subroutine mpi90_receive_integer_pointer
353c <Body of mpi90_receive_*.pointer 353c>≡ (353b 354c) 353d>
integer :: local_source, local_tag, local_domain, local_error, buffer_size
integer, dimension(MPI_STATUS_SIZE) :: local_status
integer :: ierror
external mpi_receive, mpi_get_count
<Set defaults for source, tag and domain 350e>
353d <Body of mpi90_receive_*.pointer 353c>+≡ (353b 354c) <353c 353e>
call mpi_probe (local_source, local_tag, local_domain, &
    local_status, local_error)
<Handle local_error 346c>

```



Can we ignore ierror???

```

353e <Body of mpi90_receive_*.pointer 353c>+≡ (353b 354c) <353d 354a>
call mpi_get_count (local_status, datatype, buffer_size, ierror)
if (associated (buffer)) then
    if (size (buffer) /= buffer_size) then
        deallocate (buffer)
        allocate (buffer(buffer_size))
    end if

```

```

else
    allocate (buffer(buffer_size))
end if

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

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

354c  <Implementation of mpi90 procedures 346a>+≡ (345a) <353b 355a>
    subroutine mpi90_receive_double_pointer &
        (buffer, source, tag, domain, status, error)
        real(kind=default), dimension(:), pointer :: buffer
        integer, intent(in), optional :: source, tag, domain
        type(mpi90_status), intent(out), optional :: status
        integer, intent(out), optional :: error
        character(len=*), parameter :: FN = "mpi90_receive_double_pointer"
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
    <Body of mpi90_receive_*_pointer 353c>
end subroutine mpi90_receive_double_pointer

```

L.3 Collective Communication

```

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

354e  <Interfaces of mpi90 procedures 348c>+≡ (345a) <353a>
    interface mpi90_broadcast
        module procedure &
            mpi90_broadcast_integer, mpi90_broadcast_integer_array, &
            mpi90_broadcast_integer_array2, mpi90_broadcast_integer_array3, &
            mpi90_broadcast_double, mpi90_broadcast_double_array, &
            mpi90_broadcast_double_array2, mpi90_broadcast_double_array3, &
            mpi90_broadcast_logical, mpi90_broadcast_logical_array, &
            mpi90_broadcast_logical_array2, mpi90_broadcast_logical_array3
    end interface

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

```

```

else
    local_domain = MPI_COMM_WORLD
end if

355a  <Implementation of mpi90 procedures 346a>+≡ (345a) <354c 355b>
    subroutine mpi90_broadcast_integer (value, root, domain, error)
        integer, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_integer_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_integer

355b  <Implementation of mpi90 procedures 346a>+≡ (345a) <355a 355c>
    subroutine mpi90_broadcast_double (value, root, domain, error)
        real(kind=default), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        real(kind=default), dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_double_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_double

355c  <Implementation of mpi90 procedures 346a>+≡ (345a) <355b 355d>
    subroutine mpi90_broadcast_logical (value, root, domain, error)
        logical, intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        logical, dimension(1) :: buffer
        buffer(1) = value
        call mpi90_broadcast_logical_array (buffer, root, domain, error)
        value = buffer(1)
    end subroutine mpi90_broadcast_logical

355d  <Implementation of mpi90 procedures 346a>+≡ (345a) <355c 356b>
    subroutine mpi90_broadcast_integer_array (buffer, root, domain, error)
        integer, dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error

```

```

        character(len=*), parameter :: FN = "mpi90_broadcast_integer_array"
        integer, parameter :: datatype = MPI_INTEGER
        <Body of mpi90_broadcast_*_array 356a>
    end subroutine mpi90_broadcast_integer_array

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

356b <Implementation of mpi90 procedures 346a>+≡ (345a) <355d 356c>
    subroutine mpi90_broadcast_double_array (buffer, root, domain, error)
        real(kind=default), dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, parameter :: datatype = MPI_DOUBLE_PRECISION
        character(len=*), parameter :: FN = "mpi90_broadcast_double_array"
        <Body of mpi90_broadcast_*_array 356a>
    end subroutine mpi90_broadcast_double_array

356c <Implementation of mpi90 procedures 346a>+≡ (345a) <356b 356d>
    subroutine mpi90_broadcast_logical_array (buffer, root, domain, error)
        logical, dimension(:), intent(inout) :: buffer
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, parameter :: datatype = MPI_LOGICAL
        character(len=*), parameter :: FN = "mpi90_broadcast_logical_array"
        <Body of mpi90_broadcast_*_array 356a>
    end subroutine mpi90_broadcast_logical_array

356d <Implementation of mpi90 procedures 346a>+≡ (345a) <356c 357a>
    subroutine mpi90_broadcast_integer_array2 (value, root, domain, error)
        integer, dimension(:,:), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        integer, dimension(size(value)) :: buffer
        buffer = reshape (value, shape(buffer))
        call mpi90_broadcast_integer_array (buffer, root, domain, error)
        value = reshape (buffer, shape(value))
    end subroutine mpi90_broadcast_integer_array2

```

357a *<Implementation of mpi90 procedures 346a>+≡* (345a) <356d 357b>
`subroutine mpi90_broadcast_double_array2 (value, root, domain, error)`
`real(kind=default), dimension(:,,:), intent(inout) :: value`
`integer, intent(in) :: root`
`integer, intent(in), optional :: domain`
`integer, intent(out), optional :: error`
`real(kind=default), dimension(size(value)) :: buffer`
`buffer = reshape (value, shape(buffer))`
`call mpi90_broadcast_double_array (buffer, root, domain, error)`
`value = reshape (buffer, shape(value))`
`end subroutine mpi90_broadcast_double_array2`

357b *<Implementation of mpi90 procedures 346a>+≡* (345a) <357a 357c>
`subroutine mpi90_broadcast_logical_array2 (value, root, domain, error)`
`logical, dimension(:,,:), intent(inout) :: value`
`integer, intent(in) :: root`
`integer, intent(in), optional :: domain`
`integer, intent(out), optional :: error`
`logical, dimension(size(value)) :: buffer`
`buffer = reshape (value, shape(buffer))`
`call mpi90_broadcast_logical_array (buffer, root, domain, error)`
`value = reshape (buffer, shape(value))`
`end subroutine mpi90_broadcast_logical_array2`

357c *<Implementation of mpi90 procedures 346a>+≡* (345a) <357b 357d>
`subroutine mpi90_broadcast_integer_array3 (value, root, domain, error)`
`integer, dimension(:,:,:), intent(inout) :: value`
`integer, intent(in) :: root`
`integer, intent(in), optional :: domain`
`integer, intent(out), optional :: error`
`integer, dimension(size(value)) :: buffer`
`buffer = reshape (value, shape(buffer))`
`call mpi90_broadcast_integer_array (buffer, root, domain, error)`
`value = reshape (buffer, shape(value))`
`end subroutine mpi90_broadcast_integer_array3`

357d *<Implementation of mpi90 procedures 346a>+≡* (345a) <357c 358>
`subroutine mpi90_broadcast_double_array3 (value, root, domain, error)`
`real(kind=default), dimension(:,:,:), intent(inout) :: value`
`integer, intent(in) :: root`
`integer, intent(in), optional :: domain`
`integer, intent(out), optional :: error`
`real(kind=default), dimension(size(value)) :: buffer`
`buffer = reshape (value, shape(buffer))`
`call mpi90_broadcast_double_array (buffer, root, domain, error)`

```

        value = reshape (buffer, shape(value))
    end subroutine mpi90_broadcast_double_array3
358  <Implementation of mpi90 procedures 346a>+≡ (345a) <357d
    subroutine mpi90_broadcast_logical_array3 (value, root, domain, error)
        logical, dimension(:,:,:), intent(inout) :: value
        integer, intent(in) :: root
        integer, intent(in), optional :: domain
        integer, intent(out), optional :: error
        logical, dimension(size(value)) :: buffer
        buffer = reshape (value, shape(buffer))
        call mpi90_broadcast_logical_array (buffer, root, domain, error)
        value = reshape (buffer, shape(value))
    end subroutine mpi90_broadcast_logical_array3

```

—M— IDEAS

M.1 Toolbox for Interactive Optimization

Idea: Provide a OpenGL interface to visualize the grid optimization.

Motivation: Would help multi channel developers.

Implementation: Coding is straightforward, but interface design is hard.

M.2 Partially Non-Factorized Importance Sampling

Idea: Allow non-factorized grid optimization in two- or three-dimensional subspaces.

Motivation: Handle nastiest subspaces. Non-factorized approaches are impossible in higher than three dimensions (and probably only realistic in two dimensions), but there are cases that are best handled by including non-factorized optimization in two dimensions.

Implementation: The problem is that the present `vamp_sample_grid0` can't accomodate this, because other auxiliary information has to be collected, but a generalization is straightforward. Work has to start from an extended `divisions` module.

M.3 Correlated Importance Sampling (?)

Idea: Is it possible to include *some* correlations in a mainly factorized context?

Motivation: Would be nice ...

Implementation: First, I have to think about the maths ...

M.4 Align Coordinate System (i.e. the grid) with Singularities (or the hot region)

Idea: Solve **vegas**' nastiest problem by finding the direction(s) along which singularities are aligned.

Motivation: Automatically choose proper coordinate system in generator generators and separate wild and smooth directions.

Implementation: Diagonalize the covariance matrix $\text{cov}(x_i x_j)$ to find better axes. Caveats:

- damp rotations (rotate only if eigenvalues are spread out sufficiently).
- be careful about blow up of the integration volume, which is $V' = V d^{d/2}$ in the worst case for hypercubes and can be even worse for stretched cubes. (An adaptive grid can help, since we will have more smooth directions!)

Maybe try non-linear transformations as well.

M.5 Automagic Multi Channel

Idea: Find and extract one singularity after the other.

Motivation: Obvious.

Implementation: Either use multiple of **vegas**' $p(x)$ for importance sampling. Or find hot region(s) and split the integration region (à la signal/background).

—N—

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N.1 Identifiers

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