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Monte Carlo Stratified Source-Sampling*

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DISCLAIMER

Monte Carlo Stratified Source-Sampling

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Abstract

In 1995, at a conference on criticality safety, a special session was devoted to the Monte Carlo "eigenvalue of the world" problem. Argonne presented a paper, at that session, in which the anomalies originally observed in that problem were reproduced in a much simplified model-problem configuration, and removed by a version of stratified source-sampling. The original test-problem was treated by a special code designed specifically for that purpose. Recently ANL started work on a method for dealing with more realistic eigenvalue of the world configurations, and has been incorporating this method into VIM. The original method has been modified to take into account real-world statistical noise sources not included in the model problem. This paper constitutes a status report on work still in progress.

BACKGROUND

The "Eigenvalue of the World" problem was first noted, and named, by Elliot Whitesides in 1971 [1]. The problem was encountered in a Monte Carlo eigenvalue analysis of a highly-decoupled $9 \times 9 \times 9$ array configuration of 4 *cm* identical Plutonium metal spheres. The eigenvalue of the system was computed to be 0.93. When the central sphere was replaced by another which was critical in isolation and the calculation was repeated, the resulting eigenvalue was again 0.93.

In 1995, at a conference on criticality safety, a special session was devoted to the Whitesides' eigenvalue problem. Argonne presented a paper[1], at that session, in which the original anomalies which Whitesides observed were reproduced in a much simplified model-problem configuration; this was a configuration consisting of a set of 41 slabs. The whole slab-array

[1] This was only a presentation given at the Embedded Topical Meeting on Misapplications and Limitations of Monte Carlo Methods Directed Towards Criticality Safety Analysis, USDOE Nuclear Criticality Technology Safety Project Annual Meeting, which was held in San Diego, CA, May 17, 1995. An account of the contents of the presentation can be found in Ref. [3].

was reflected at its left- and right-hand boundaries. All the slabs were identical except for the central slab, whose k-infinity was somewhat higher than that of the others.

Real neutron transport was not treated in the model problem. Instead the differenced diffusion equation was solved by Monte Carlo, with one mesh point at the center of each mesh box. There is a very simple standard Monte Carlo random walk [2] which may be used to solve the differenced diffusion equation. It was essentially this method that was used to treat the model problem, with modifications that avoided the need for detailed Monte Carlo simulation of collisions [3]. These modifications were designed to take advantage of analytic solutions of the difference equations, but without altering, in any way, statistical properties of fission and eigenvalue estimates. It should be noted that, when the simulation of collisions is avoided, collision sites can no longer be used as potential fission sites and, instead, absorption sites served as potential fission sites. Results obtained for the model problem indicated that, for proper convergence to the correct eigenvalue and its corresponding eigenvector, the use of stratified source-sampling techniques dramatically reduces the number of neutron case-histories needed to be run, per generation, over that required if conventional source-sampling methods are used. Consequently, a large reduction in computational cost, and increased reliability, were gained.

The goal of this work is to improve the reliability of Monte Carlo source convergence, subject to a constraint, i.e., that computing time not be substantially increased. We take "reliability" to mean that the chance that a Monte Carlo calculation will converge the fission source to the wrong solution is small. "Small" is to be determined by the user for the purposes of his particular analysis.

There are several important sources of variance in Whitesides' problem which are absent in the original model problem. For example, in the model problem, neutronic decoupling between adjacent slabs was achieved by taking the limit as the thickness of the slabs goes to infinity. At this limit, any neutron that is born in any given slab will, ultimately, be absorbed in that same slab. Consequently, after running one generation of neutron case-histories, the fission-source weight registered in each slab – which is then used to determine its share of source-neutrons for the next generation – becomes directly proportional to the reactivity of the slab. In real transport calculations however, this is no longer the case since potential fission sites are generated at each collision a neutron undergoes along its history. Thus, the number (or weight) of fission sites, at the end of each generation fluctuates among the different fissile objects in the simulation depending on the number of collisions each object's source neutrons produce before their lives are terminated either by absorption or by leakage.

This work has advanced beyond the stage it had reached at the time of the 1997 Nuclear Criticality Technology Safety Project Workshop which was held in Gaithersburg, MD, May 5-9, 1997, but is still far from complete so that this paper is, in effect, a status report on work in progress.

NEW VIM ALGORITHMS

I. Source Stratification

Below we describe the procedures implemented in VIM [4] to deal with the Eigenvalue of the World problem. It will be seen that steps 1 and 2 are precisely the same as in the original algorithm reported at the earlier criticality safety meeting. This algorithm was used, at that time, to treat the very simple model problem sketched above.

Step 1: Stratify the initial fission source guess

For an initial source neutron size of N starters, we divide the sampling domain into K different subdomains; each subdomain k, $k = 1, 2, \ldots, K$, represents a region for which a fraction N^k of the N given starters is assigned. In addition, we associate an initial weight W, typically $W = 1$, with each starting neutron. The initial number (or total weight) of the starting neutrons assigned to each subdomain k, is then $N^k = \frac{N}{K} S_f^k$, where S_f^k is the user's guess of the k^{th} zone's expected fraction of fission source neutrons.

In conventional VIM, the starting neutrons are sampled according to a specified spatial distribution, usually flat, inside a predetermined geometrical shape that envelopes the domain of the problem.

Step 2: Stratify the fission source iteration

In order to stratify the fission source for each subsequent generation, let us first define N_g^k and W_g^k to be the total number of starting neutrons and the weight of a single neutron starter in region k for generation g, respectively. We further define S_g^k to be the total weight of fission sites generated in object k at the end of generation g, then

1. At the end of generation $g-1$, we compute the regionwise probability density function p_g^k,

$$p_g^k = \frac{S_{g-1}^k}{\sum_{k=1}^{K} S_{g-1}^k},$$

2. We calculate the expected normalized total weight of neutron starters in region k for generation g, $\langle W_{tot,g}^k \rangle$

$$\langle W_{tot,g}^k \rangle = p_g^k N,$$

3. We then calculate the number of starters N_g^k and the weight W_g^k of each for generation g. To do so, we define a low weight cutoff threshold, $W_{cut} \ll 1$, so that
   - If $\langle W_{tot,g}^k \rangle < W_{cut}$, a game of Russian roulette is played. With probability $p = \langle W_{tot,g}^k \rangle$, we start one neutron from cell k carrying a unit weight, and with probability $1 - p$ we start none.
   - If $\langle W_{tot,g}^k \rangle \geq W_{cut}$, we define $\tilde{N}$ to be the nearest integer to $\langle W_{tot,g}^k \rangle$, then
     - If $\tilde{N} = 0$, we take one starter from region k with weight $\langle W_{tot,g}^k \rangle$.
     - Otherwise, we take $N_g^k = \tilde{N}$ starters form region k each with weight $W_g^k = \langle W_{tot.g}^k \rangle / \tilde{N}$.
4. The locations of the N_g^k starters in each object k for generation g are then sampled from the fission sites registered at the end of generation $g-1$ in k.

In conventional VIM, as mentioned earlier, fission sites are created through a collision-based algorithm which registers a site weight $S = \frac{\nu\Sigma_f}{C\Sigma_t}$ at each collision, where C is a constant scaling factor. An integer number of S is saved as potential fission sites and a game of Russian roulette is played to select or reject the remaining fragment. A check is then made to see if the fission site bank is full. If it is full, the site is rouletted and banked randomly upon surviving the roulette game, discarding the site that is already there. After the generation's histories are complete, the next generation's starters are obtained by sampling the resulting fission sites bank.

II. Forced Interactions and Absorption-Based Fission Sites

It will be recalled that the basic difficulty in the model problem, and apparently in the original Whitesides Monte Carlo runs, was that the most reactive body was often "lost" in the course of the Monte Carlo computation. If the objects in the computational configuration are loosely coupled then, once an object is left, at the end of a generation, without potential fission-source sites, then it is unlikely that fissions will occur in that object in any later generation. In other words, once the object is lost there is a good chance that it will play no significant role in the remainder of the calculation, so that the random walk will proceed almost as if the object were totally absent. If it is an important object the "converged eigenvalue" may be substantially incorrect.

In the original model problem, in the case of decoupled slabs, there was only one way a slab could be lost; it could be missed completely, in any generation, in the course of the source selection process. The original source-stratification process was designed to eliminate this possibility.

On the other hand in more realistic transport calculations, and in particular in the Eigenvalue of the World problem, there may be another way to lose an object, i.e., all fission neutrons may escape from it uncollided. The two methods below are both designed to eliminate this possibility. In both methods it is guaranteed that at least one potential fission source site will be left in each object at the end of each generation, for each fission neutron born in that object at the beginning of that generation. We have not yet determined the circumstances under which these methods will be useful – that is an important part of the remaining work.

In both of the algorithms below a fragment of each starter is forced to make at least one collision within its birth-object. The algorithms differ only in the methods used to generate potential source-sites from essentially identical random walks. In the first variant these sites are generated at each collision, as is usual in neutronics Monte Carlo codes. In the second, potential source-sites are generated only on absorption, so that each neutron fragment (i.e. the fragment forced to collide internally and the fragment forced to escape uncollided) will leave at most three potential fission source sites.

Implementation of the second option was motivated by some results of early tests of the stratified-source-sampling method. It was noted, in these tests, that anomalously large numbers of scattering collisions could leave correspondingly a large fission-source weight in an unimportant object, which would subsequently attract a large number of starting neutrons. Once this happens there is a substantial probability that this object will be the one that ultimately survives with all the fission weight drawn into it. More generally, variation in the number of scattering collisions per history may add variance to the weight of source-sites in the various objects. But, further, if we create fission sites only on absorption then, to guarantee that every starter leaves a fission-site wherever it was born, it is necessary to force at least one absorption within the source-object.

The first method forces a collision so that the neutron with initial weight W is split into two fragments on its first flight. One fragment, carrying a weight $W_c = W(1 - e^{-\Sigma_t \ell})$, is forced to collide before it leaves its originating region with the result of creating a potential fission site upon collision. Here $(1 - e^{-\Sigma_t \ell})$ is the probability that the neutron will collide before leaving the region, ℓ being the distance between its origin and the surface of the region in its flight direction, The weight of such site would be $S = W_c \frac{\nu\Sigma_f}{\Sigma_t}$. The second fragment is forced to escape, carrying a weight $W_e = We^{-\Sigma_t \ell}$. Each of these two fragments will continue its history in a conventional manner producing additional fission sites upon collision. The weight of each site will then be the weight of the respective fragment (W_c or W_e) times $\frac{\nu\Sigma_f}{\Sigma_t}$.

The second method forces a collision, as above, but the colliding fragment is survival biased, and its absorbed fragment produces a fission site of weight S, as above. The weight of the fragment surviving the forced collision is $W_{cs} = W_c \frac{\Sigma_s}{\Sigma_t}$. In this case, however, each of the two continuing neutron fragments can produce an additional potential fission site only if its life is terminated by absorption in a fissile region (its originating region or any other one). The weight of that fission site will then be the weight of the particle (W_{cs} or W_e) times $\frac{\nu\Sigma_f}{\Sigma_a}$.

When the stratified source-sampling method is successful, the sample population will contain increasing numbers of very low weight particles from fissions in low-importance objects. The method is aimed at preserving all important objects in the sample population, but we will finally wish to "lose" objects that we are sure have low importance. This can be accomplished using a weight cutoff, in which particles with weights smaller than, e.g., 0.1, are rouletted, with the survivors' weights increased appropriately.

Clearly none of these mechanisms will prevent all anomalous results in the Eigenvalue of the World problem. Thus, for example, even if there is a non-zero starting source-weight in an object, if that weight is very small the object may be severely handicapped in the subsequent competition for source neutrons. Furthermore, like the variance reduction techniques commonly used, they incur penalties in computational effort which will have to be noted while comparing the reliability improvements. The performance of alternative methods will have to be tested extensively in Eigenvalue of the World calculations.

PRELIMINARY NUMERICAL RESULTS

The Algorithms described in the preceding section were "hardwired" in VIM. Several debugging test problems were run to ensure their correct implementation and coding. Here we present a sample of such tests. As depicted in Fig. (1), the fission source shape inside a 4 *cm* sphere at the end of the first generation – given an initial flat source guess – evaluated using the stratified sampling with first-flight forced absorptions algorithm (dashed lines) is compared to that evaluated by conventional VIM algorithms (solid lines). These results were obtained by averaging over 10 runs of statistically independent replicas for each of the two different algorithms. Each replica was run with an initial source size of 100,000 neutrons utilizing artificial one-group cross sections that are summarized in the first row of Table (1).

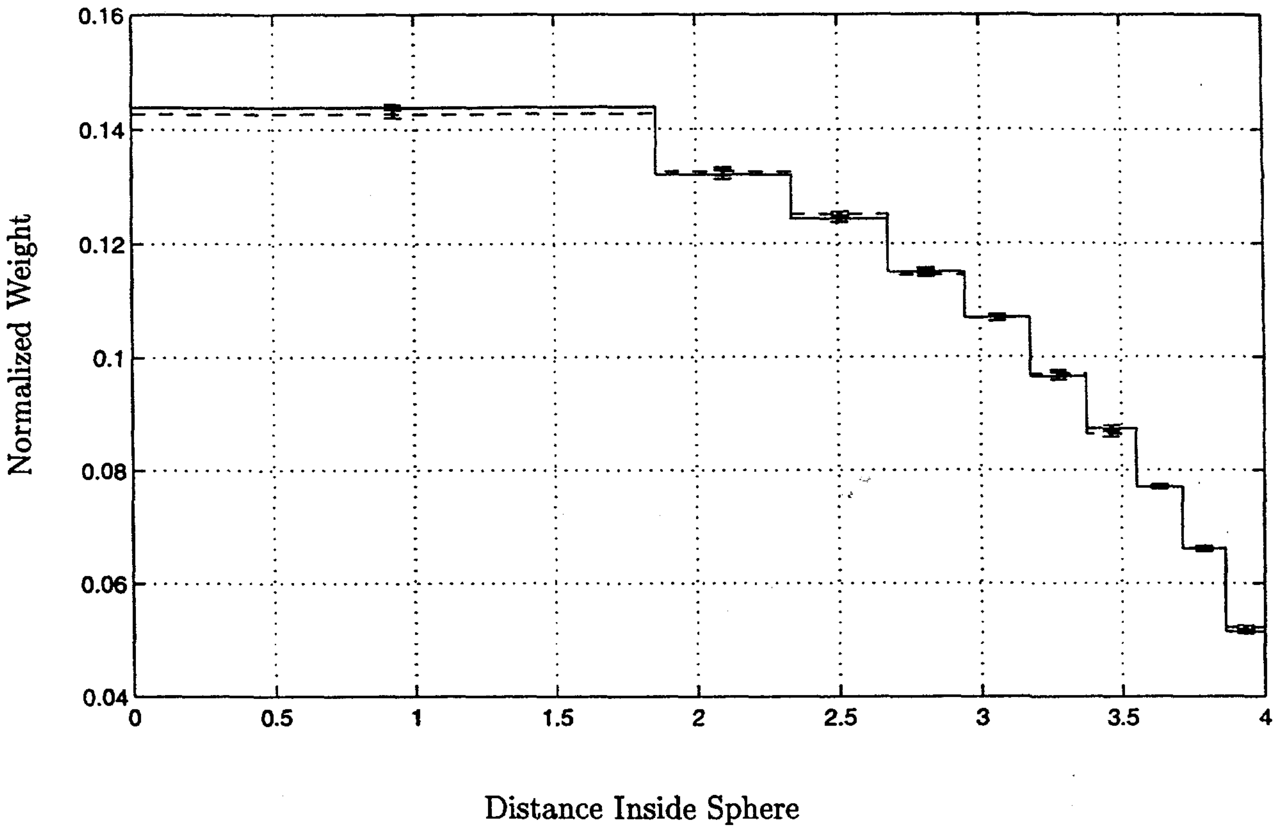

Figure 1: Comparison of Fission Source Shape Inside a Sphere, First Generation.

As can be seen, the two evaluations agree to within statistical bounds (indicated by the error bars). This confirms that the code modifications were made correctly and preserve the evolution of the fission source within an object.

For initial testing to be accomplished in reasonable running times, we used a simple problem that, nonetheless, exercises the tracking complexity in VIM. This is a one-dimensional array of 41 spheres (5 *cm* in radius spaced at a 60 *cm* pitch) configuration, for which 40 spheres were identical ($k_{eff} \sim 0.67$) while the central one had a slightly higher reactivity ($k_{eff} \sim 0.74$). Complete neutronic decoupling was achieved by placing an artificial pure absorbing material in the regions between the different spheres. The various one-group cross sections used in this problem are shown in Table (1).

Table 1: One-Group Cross Sections

	$\nu\Sigma_f$	Σ_a	Σ_s
All Identical Spheres	0.20	0.20	0.80
Untypical Sphere	0.22	0.20	0.80
Region Between Spheres	0.00	5.00	0.00

Table 2: Preliminary Numerical Results

	Reliability %	Starters/Sphere	CPU Time (sec)
Production VIM	95	24	97
Production VIM	40	7	31
Stratified Sampling w/o Forced Absorptions	95	7	39
Stratified Sampling & Forced Absorptions	95	7	55

To evaluate the performance of the various algorithms described above, runs were submitted to search for the minimum number of neutron-starters per sphere to achieve a 95% reliability, i.e. to converge 19 or more out of 20 statistically independent replicas to the correct, non-anomalous result. Table (2) above shows this minimum number of starters and the corresponding CPU time at the end of 200 generations (run times are quoted for a 170 MHz dual processor Sun Sparc 20 machine) for conventional VIM vs. stratified sampling with forced absorptions. The weight cutoff for the later algorithm was set to $W_{cut} = 0.1$.

Furthermore, running VIM with 7 starters/spheres (those needed for a 95% reliability with the stratified sampling and forced absorptions algorithm) produced a reliability of 40% (i.e. only 8 out of 20 replicas converged to the correct solution). In addition, using the same 7 starters/spheres with the stratified sampling algorithm without forced absorptions, the 95% reliability was still preserved. However, the required CPU time for each of these replicas was reduced to 39 seconds.

DISCUSSION

At this point it is necessary to settle on criteria for evaluating performance of the various alternative methods tested above. First and foremost, these methods are designed to diminish the probability that an unwary Monte Carlo user will run into the Eigenvalue of the World anomaly. That the Monte Carlo method, our benchmark standard, can "converge" to an incorrect (but apparently accurate) result is very disturbing; one would like to minimize the probability of such a serious failure although, unfortunately, we see no way to eliminate the possibility completely.

On the other hand it does no good to achieve improved reliability, in the Eigenvalue of the World problem, at a great cost in computing time. Obviously, at some point, computing time becomes prohibitively expensive. But, further, one can always avoid anomalies in standard Monte Carlo just by running a "large enough" number of histories per generation. If the user knows this number, then for him standard Monte Carlo is an option. It is undesirable to increase Monte Carlo running time far beyond the time required by this well-informed user for a standard Monte Carlo run. It is reasonable, then, to compare all running times with that required by this hypothetical well-informed user.

To evaluate computing methods fairly we will need to compare running times at comparable reliabilities, i.e. we will need to define a quantitative measure of reliability. We took this measure to be the running time necessary to give correct ("non-anomalous") results in 95% of replicas.

No test problems comparable to Whitesides' original problems have yet been run. The problems discussed above were preliminary runs, involving much smaller configurations than

Whitesides'. The results presented above show that, for the smaller test problem, the non-analog algorithms have been implemented correctly, and that source stratification does improve reliability. A final evaluation of our various methods will have to wait till results of full scale Eigenvalue of the World calculations become available later.

ACKNOWLEDGMENTS

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