Monte Carlo Importance Sampling for the MCNP™ General Source

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ABSTRACT

Research was performed to develop an importance sampling procedure for a radiation source. The procedure was developed for the MCNP radiation transport code, but the approach itself is general and can be adapted to other Monte Carlo codes. The procedure, as adapted to MCNP, relies entirely on existing MCNP capabilities. It has been tested for very complex descriptions of a general source, in the context of the design of spent-reactor-fuel storage casks. Dramatic improvements in calculation efficiency have been observed in some test cases. In addition, the procedure has been found to provide an acceleration to acceptable convergence, as well as the benefit of quickly identifying user-specified variance reduction in the transport that effects unstable convergence.

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I. INTRODUCTION

The Monte Carlo method has evolved a rich set of variance-reduction techniques, many of which are available in MCNP,[1] an XTM radiation transport code that is used world wide. The basic objective of such techniques is to optimize computing resources devoted to important Monte Carlo histories, where the metric for importance is the degree to which a history contributes to the computed results.

Among radiation transport applications well suited for Monte Carlo simulations is the design of storage casks for spent reactor fuel. In designing storage casks, the computed result is the radiation dose, exterior to the cask, that would be measured in the analogous physical experiment.

One variance-reduction technique is importance-sampling the source. Rather than allowing source-particle attributes (*i.e.*, position and velocity), to be sampled as governed by physical laws, the sampling is biased to favor particle attributes that would ultimately lead to significant tally contributions (*i.e.*, the computed result). The particle weight, a statistical attribute assigned to each particle history, is adjusted so as to preserve the fair Monte Carlo game.

Importance sampling is mechanically straightforward; the difficulty is determining which particle attributes are important in a given scenario. The theoretical source importance function is the optimum characterization of the biased source distributions, but it is ordinarily as difficult to compute the importance function as it is to compute the dose. Such a circuitous dilemma is circumvented by a fortuitous circumstance: even

a crude knowledge of the importance function can deliver substantial benefits.

II. SIMULATION SCENARIO

The design of spent-fuel storage casks deals with models comprising complex geometry (thousands of fuel rods) and complex fixed source, distributed in energy, direction, and position (for all the rods). These scenarios are characteristic of deep-penetration radiation shielding, typically among the most difficult calculations to converge.

The specific details of complexity in this scenario, however, are incidental to the description of the present importance-sampling procedure. It suffices to visualize the physical model as a cylindrical container that serves to shield a symmetric arrangement of fuel assemblies (32 in this instance), each assembly comprising 264 rods. The rod axes are parallel to the container axis.

III. THE SOURCE IMPORTANCE-SAMPLING (SIS) PROCEDURE

An obscure MCNP option, which analyzes a tally with respect to a history's source attributes, is precisely the tool needed for the present research objective. This option is the so-called "FTn SCX card," described in the "Special Treatments for Tallies" section of the MCNP manual[1] (page 3-89). When this option is activated for each of the source distributions to be biased, the corresponding computed tallies become approximate source-importance biasing functions. The appropriate normalization is performed by MCNP in its input-processing stage.

Thus, this source importance-sampling (SIS) procedure comprises an analog-source preliminary run to generate an approximate importance function for the subsequent

refined run. The latter utilizes the importance function generated in the former to bias the general source for an efficient convergence of the shielding calculation. To simplify the discussions below, the term *analog-source* may imply source biasing based on information other than that generated by the SIS procedure. But it is important to bear in mind the sometimes counter-intuitive nature of deep penetration scenarios.

The gains in calculational efficiency have been impressive. This novel MCNP procedure (to the author's knowledge, not previously reported) has the advantage of being completely general in its applicability. It also obviates the need for clairvoyance on the part of the user; only a little common-sense judgement is useful to massage the computed estimates of the source importance function. This smoothing can be automated eventually within the code.

IV. BENCHMARK CALCULATIONS

The complex analog-source models were adapted from existing MCNP input models. The latter had been prepared by staff of Holtec International, which sponsored part of this research. In benchmarking the SIS procedure, only source biasing and tally definitions were modified to gauge SIS effectiveness. As discussed below, instances of inadequate variance reduction, aside from source biasing, were unaltered, so as to focus attention on the SIS procedure itself.

A. Improvement of Efficiency

Of the model definitions available to test the SIS approach, one case was very difficult to converge based on analog-source sampling. It involved essentially an isotropic

photon source in the spent fuel rods with an energy probability density ranging over [0.3,3.0] MeV. The modeled input specified tallies (and corresponding transport variance reduction) for both the top (plane surface) and side (curved surface) exterior of the container. For the purpose of benchmarking the SIS procedure, only the tally at the top was analyzed.

The analog-source case was executed on an IBM-590 cluster, using 6 nodes in parallel-virtual-machine (PVM) mode.[2] After 200 million histories (a $\frac{1}{5}$ *giga-history*!) and a total of 216 cpu-hours (*hours*!) for the 6 nodes, it still had not converged, where all references to convergence, herein, imply MCNP's 10 statistical tests as the criteria (refer to the "Forming Statistically Valid Confidence Intervals" section of the MCNP manual,[1] page 2-105). At that point, the computed figure-of-merit (FOM) was 0.051, where the FOM is inversely proportional to the product of variance with compute time ($\sim \frac{1}{\sigma^2 \tau}$).

For the SIS procedure comparison, the tally was analyzed with respect to the following binned source distributions: energy; rod bundle; position along the rod axis; and direction with respect to the rod axis. The tally was not analyzed with respect to individual rod positions, because there were simply too many (8448) to get statistically viable estimates of the corresponding importances.

Using the same cluster in PVM mode, the SIS procedure converged this problem in 43 cpu-minutes, with a computed FOM of 3.2. The ratio of the SIS FOM to the analog-source FOM represents an efficiency-improvement factor of 63. Purists may

wonder how this improvement is affected if the compute time (185 cpu-minutes) for the preliminary, importance-generating run was included in calculating the SIS FOM. In so doing, the SIS FOM reduces to 0.60 and the efficiency-improvement factor becomes 12, still a respectable improvement. If, however, the generated importances are applicable to a suite of related calculations, the effect of the preliminary compute time on the improvement factor diminishes.

Not all these tests showed order-of-magnitude improvement. Part of the reason for the above cited gain was that the analog-source model was deficient in its transport variance reduction (which was unaltered for the SIS calculation). Additionally, the original energy-biasing, based on intuition, overemphasized the high-energy bins, as compared with the biasing prescribed by the SIS importance-generating run.

B. Acceleration to Acceptable Convergence

In another benchmark case that was better behaved (with respect to its variance reduction in the transport), the computed FOM was 33, after a compute time of 152 cpu-minutes. The corresponding SIS run produced an FOM of 53, in a compute time of 32 cpu-minutes. That is only a 61% improvement in efficiency.

But how quickly a particular problem can be computed to *acceptable* convergence (using MCNP's 10 statistical tests as the criteria) is another issue of interest. Since the FOM comprises two factors, one can imagine circumstances where an acceptable, albeit higher, variance (σ^2) would be desirable in return for a shorter compute time (τ).

In the case presently cited, the relatively small improvement in efficiency (*i.e.*, ratio

of FOMs) had a concomitant reduction in compute time by a factor of almost five. That is what may be defined as an "acceleration to acceptable convergence." The latter improvement is very important in computing-intensive design studies.

C. Identifying Unstable Convergence

In the last scenario to be described herein, the SIS procedure displayed chaotic convergence/divergence, after a relatively short run time of 4 cpu-minutes. The corresponding analog-source benchmark appeared to have converged after 2 million histories (in a running time of 50 cpu-minutes). All of the MCNP criteria for forming valid confidence intervals had been satisfied for the analog-source run. Such a situation presented cause for concern.

It appeared that the convergence of the analog-source run, accepted by MCNP criteria, required further examination, if the SIS results were to be believed. Consequently, the analog-source model was continued for longer compute time. It remained converged up to 6 million histories. But at 8 million histories, the computed tallies began diverging, no longer passing all the statistical tests that define MCNP convergence; at 10 million histories, it remained unconverged. Such behavior is pathologically deceptive.

The MCNP statistical tests are designed to detect an unstable convergence, but the caveat that convergence is not *guaranteed* has always been explicitly stated. Recently,[3] an extension, in the form of a rule-of-thumb, has been suggested to improve the detection of such pathological instability; it calls for extension of compute times to double the number of histories required for initial convergence. But in this particular benchmark,

such an extension still would have declared stable convergence for this problem, because the *apparent* stability survived way beyond the compute time specified by the rule-of-thumb.

In this particular case, the culprit may have been the modeler's attempt to compute the dose at the top, bottom, and side of the container, simultaneously. It is obvious that the requisite transport variance reduction for dose at the top and bottom is different, and that the side dose is much more impacted by peripheral rod-bundles than are the end doses. Thus the failure to de-couple the three dose tallies for this model necessitated a transport variance reduction that was self-conflicting and was, at best, a compromise.

This result demonstrates another advantage of the SIS procedure: it detected a convergence instability in a running time that was a factor of 50 shorter than for the analog-source benchmark. Moreover, it did so for a scenario where the current MCNP trouble-shooting mechanisms were fooled.

V. SUMMARY

A procedure has been developed to importance-sample a Monte Carlo general source. This SIS procedure has been demonstrated to function with the production version of MCNP, but it could be adapted to any other Monte Carlo radiation transport code, provided such a code offers a general source, a source biasing, and a tally analysis capability.

The SIS procedure has 3 capabilities that have, thus far, been identified and demonstrated: (1) improvement of computing efficiency; (2) acceleration to acceptable conver-

gence; and (3) early detection of an unstable convergence. The first cited capability has an obvious advantage. The second capability is advantageous in situations where minimal criteria for convergence are acceptable in return for requisite short running jobs. The third capability is complementary to the statistical analysis package in MCNP. The latter has always included the caveat that passage of this suite of tests is not a guarantee of stable convergence. A situation has been demonstrated where a calculation converged so deceptively that it was undetected by the current statistical package, even when recently specified cautionary recommendations were followed. But the SIS procedure detected the inherent instability quickly.

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