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"The keff of the World"

by

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Pitfalls in Criticality Safety Monte Carlo Computations: "The keff of the World"

by

Ely M. Gelbard

In work originally published in 1971,⁽¹⁾ Elliot Whitesides brought to our attention a problem still unsolved today. This was a problem he called "computing the keff of the world", a name which has survived for many years.

The specific example which Whitesides discussed was a 9 x 9 x 9 array of plutonium spheres, surrounded by a water reflector. The computed keff of the array was .93. When the central sphere was replaced by a sphere which, when isolated, was exactly critical, the computed eigenvalue was still .93. It seems important to note that there are at least two potential sources of difficulty in such problems. One is an inadequate number of generations; the other is an inadequate number of starters per generation or, more precisely, inadequate sampling of physical detail within each generation. It is easy to see that these are really different types of difficulties. If sampling within each generation is inadequate increasing the number of generations won't help. And clearly increasing the amount of information gathered per generation won't help if the number of generations is inadequate. In a way the error due to undersampling within a generation is analogous to course-mesh errors in deterministic calculations, while inadequate source convergence acts similarly both in deterministic calculations and Monte Carlo.

It has been shown that the Monte Carlo eigenvalue bias is given by the relations⁽²⁾

$$\Delta = - \frac{N}{2} \left(\sigma^2 - \sigma_{APP}^2 \right) \quad (1)$$

where: Δ is the eigenvalue bias: σ^2 is the variance in the eigenvalue: σ_{APP}^2 is the apparent variance in the eigenvalue computed as if eigenvalues in different generations were independent of each other: N is the number of generations. As the number of generations goes to infinity the variances decrease like $1/N$, so that the bias eventually reaches an asymptote; it does not go to zero. It is pointed out in Ref. 3 that, if $N < 200$ and the relative standard deviations in eigenvalue is less than .25%, then $\Delta \leq \sigma$. But in criticality safety calculations both of these conditions may be violated.

Of course sampling per generation can always be improved simply by increasing the number of starters in each generation, but obviously this approach can be costly. Instead various devices may be used to improve sampling efficiency. In different ways each device uses knowledge of the importance of different regions in space and/or energy. In absorption-weighted tracking the details of the procedure determine which volumes of phase space will be emphasized. But other simple strategies may also be useful. Consider, as an example, the use of source biasing.

In the Whiteside $9 \times 9 \times 9$ array the difficulty seems to be that few fission sites are created in any one of the spheres. Suppose we know the eigenvalue of each sphere in isolation. Probably one ought to know at least that much about any array before it is assembled. Given these eigenvalues, one could divide the whole configuration into zones and require a specified number of starters in each zone. Starting weights would be adjusted accordingly. For example in the $9 \times 9 \times 9$ array one could surround the central sphere by a cube and place, let's say, a quarter of all starters in this cube. In the given case this method might suffice to give a reasonably good eigenvalue for the system. There could, however, still be important regions which remain undersampled. This might be true, for example, of spheres near the central sphere. But mapping of important zones could be considerably more detailed if necessary. It should be noted that in the interior of regular array it isn't necessary to sample the structure of the array in great detail, since neutrons traveling in one sphere are equivalent to neutrons in the other spheres. Only near irregularities is it necessary to sample details of the lattice structure.

Unfortunately this sort of source biasing can't be carried out at the beginning of each generation. Otherwise weight fluctuations would accumulate from one generation to another, increasing the variance in the eigenvalue. Source biasing could be repeated periodically, but infrequently.

In any slowly convergent Monte Carlo eigenvalue calculation there is still another problem. Probably most eigenvalue calculations give us what has been called above the "apparent" variance, computed as if eigenvalues in different generations we're uncorrelated. In fact in weakly coupled systems successive eigenvalues are strongly positively correlated, and variances computed ignoring this correlation can be too small. The underestimation of variance is bothersome because it may give the user a false sense of security. Clearly the true statistical uncertainty is something we would like to know for its own sake. But the true standard deviation is useful also because of its connection with the eigenvalue bias. In fact we see from Equ. (1) that, if we know the true eigenvalue variance we can compute the bias, and vice versa.

The true eigenvalue variance can often be roughly estimated by MacMillan's method,⁽⁴⁾ but it still isn't clear just how reliable this method is. Probably a more reliable estimate can be obtained directly by replicating the eigenvalue calculation several times, using new starting random numbers for each replica. Of course this procedure increases running times but, on new parallel machines, or on parallelized networks, the cost of replicated Monte Carlos is not prohibitive. It probably isn't necessary to carry out such replications very frequently, but studies using replication would be useful, at this stage, to give us a better understanding of eigenvalue biases in difficult criticality safety problems. Such studies could also give us valuable information on the accuracy and reliability of MacMillan's method.

Finally, the replication process itself needs to be better understood. Certainly it gives an unbiased estimate of the eigenvalue variance, but it may still give a misleading estimate. One finds this situation, for example, in fixed source shielding calculations if rare events are crucially important. Suppose, in a criticality safety calculation, events in which fissions

occur in one relatively small portion of phase space are rare but crucially important. Then very infrequently one replica will give a very different eigenvalue from the great majority of others. In other words the estimated variance will be unbiased, but the distribution of estimates will be pathological. It would then be difficult to get a true variance by replication. In short we have a lot to learn about criticality safety Monte Carlo; but we now have the computing capacity and the theory to make a study of this sort of Monte Carlo application very fruitful.

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