PROPOSED SOLUTION TO THE "KEFF OF THE WORLD" PROBLEM

by

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In 1971 Whitesides posed a Monte Carlo (MC) problem which he called "computing the k_{eff} of the world." This problem is still troublesome today. The problem arose in MC studies of a 9 x 9 x 9 configuration of weakly coupled Pu spheres, initially identical, with the whole array surrounded by water. The MC eigenvalue for this array was .93. When the central sphere was replaced by another, just critical in isolation, the MC eigenvalue was still .93. Here we consider a model problem somewhat analogous to Whitesides', and use it (a) to illustrate the difficulties in the simplest traditional MC approach, and (b) to explore an alternative approach.

The model problem is a one-group slab diffusion eigenvalue problem in difference form, with reflecting boundaries:

\[- \left[ D \left( \phi_{i+1}^{g+1} - 2\phi_i^{g+1} + \phi_{i-1}^{g+1} \right) / h^2 \right] + \sum_a \phi_i^{g+1} = S_{fi}^{g} / \lambda^g,\]

\[S_{fi}^{g} = (v \Sigma_p) \phi_{fi}^{g}, \quad \lambda^g = \sum_{i=1}^{N_c} S_{fi}^{g} / N_s \]

\[i = 1, 2, \ldots, N_c, \quad \phi_0^{g} = \phi_{i}^{g}, \quad \phi_{N_c+1}^{g} = \phi_{N_c}^{g}.\]

Here g means "generation", i is the mesh-cell number, N_c is the number of cells and N_s is the number of neutron-starters per generation.

In the simplest MC version of the power method, as applied to Eq. (1), one chooses N_s starting sites by sampling from the pdf

\[p_{ai}^{g} = S_{fi}^{g} / \sum_{j=1}^{N_c} S_{fj}^{g}.\]

Once a starting-cell (i.e. a starting i) is chosen the starter is placed in that cell and given three options. It can jump left with probability p_L:

\[p_L = (D / h^2) / (\Sigma_a + 2D / h^2)\]
or right with probability \( p_R = p_L = p \), or it can be absorbed. If a starter jumps across the left- or right-hand boundary it is reflected. The next-generation fission source in any box, \( i \), is the sum \( S_i^{g+1} \), of the fission contribution, \( (\nu \Sigma_f / \Sigma_s) \), of each particle absorbed in that box.

To understand the performance of this method in the low-coupling case, i.e. for \( p_R + p_L < < 1 \), it's helpful to consider the no-coupling case \( h = \infty, p_L = p_R = 0 \). In this case (1) in every generation there is a finite probability that no starters will be chosen from box \( i \), even if \( S_i^{g+1} > 0 \), and (2) since every starter is absorbed in the cell where it's born, \( S_i \) for that \( i \) will then vanish in all future generations. It follows that, as \( g \to \infty \), the MC will converge to a fission source which occupies only a single mesh box; and that this final mesh box can, with nonzero probability, be any cell \( i \) with \( 0 < (\nu \Sigma_f / \Sigma_s)_i < \infty \). The MC eigenvalue will then be equal to the ratio \( (\nu \Sigma_f / \Sigma_s)_i \) in that cell. Thus both the source shape and the eigenvalue may be grossly incorrect, while the apparent variances are very small.

In all our test cases \( N_s = 41, D = 1/3, \Sigma_s = .2, (\nu \Sigma_f)_i = \Sigma_s \) for \( i \neq 21 \), \( (\nu \Sigma_f)_i = .22 \) for \( i = 21 \). Computations were run for \( h = 10 \) and \( h = 100 \). Typical MC results for \( h = 100 \) are shown in Figure 1. It will be seen that the apparently converged results are close to those expected in the no-coupling limit. We note that all problems were run with \( N_s = 2000 \), skipping the first 1000 generations. It was not our goal to study convergence rates, but only to examine anomalies in apparently converged solutions.

To alleviate this anomalous behavior we replace the random source-sampling with stratified source-sampling. Specifically:

1. As before define the pdf
   \[
   p_i^g = \frac{S_i^g}{\sum_j S_j^g}.
   \]

2. The expected number of starters in box \( i \) is
   \[
   \langle N_s^{gi} \rangle = p_i^g \cdot N_s.
   \]

3. Define a cutoff threshold \( N_{cut} < < 1 \).

4. \( \langle N_s^{gi} \rangle < N_{cut} \):

   - Play roulette. With probability \( p_{\text{start}} = \langle N_s^{gi} \rangle \) start one neutron from cell \( i \) with unit weight. With probability \( 1 - p_{\text{start}} \), start none from cell \( i \).

5. \( \langle N_s^{gi} \rangle \geq N_{cut} \):

   - Define \( \bar{N}_s^{gi} = \text{nint} \left( \langle N_s^{gi} \rangle \right) \)

   - If \( \bar{N}_s^{gi} = 0 \), take 1 starter from box \( i \) with weight = \( \langle N_s^{gi} \rangle \).
C. Otherwise take \( \bar{N}_s^{\text{gi}} \) starters, each with weight = \( \frac{<N_s^{\text{gi}} \geq 1/>N_s^{\text{gi}}}{N_s^{\text{gi}}} \).

6. Where, in the conventional method, one normalizes by \( N_s \), the number of starters, one should still normalize by \( N_s \), which is now the expected weight of all starters.

Using this method we now find (see Fig. 2) perfectly reasonable results for \( N_s = 10 \), where conventional sampling still gives bizarre results for \( N_s = 200 \). Other computations, show similar behavior for \( h = 10 \).

REFERENCE:

Figure 1: CONVENTIONAL SOURCE-SAMPLING, h=100.

Estimated eigenvalue: 1.000000
Standard deviation: 0.000000
True eigenvalue: 1.099634

Estimated eigenvector:
- NPRGEN=10
- NPRGEN=200
True eigenvector: ×

Mesh-box number

Source, normalized to 1.
Figure 2: STRATIFIED SAMPLING, $h=100.$, NPRGEN=10, CUTOFF=0.

Estimated eigenvector: 
True eigenvector: 

Estimated eigenvalue: 1.099654
Standard deviation: 0.2934809e-4
True eigenvalue: 1.099634