Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources

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INTRODUCTION

In Monte Carlo (MC) criticality calculations, the parameters of interest (e.g., fundamental mode eigenvalue and flux) can only be tallied after the fission source distribution is sufficiently converged. To avoid contamination of the results by an inadequately converged fission source distribution, which can lead to undersampled tally estimates, MC practitioners specify a number of inactive cycles, often referred to as “skipped cycles”, to be discarded before beginning the tallies.

Conventionally, the initial source distribution is specified by the user or by default in the MC code. The default in the SCALE/KENO [1] MC codes is to start neutrons uniformly throughout all regions containing fissile material. The closer the initial starting source is to the actual converged source distribution, the fewer the number of skipped cycles required to reach source convergence, thereby improving the efficiency of the MC criticality calculation. Also, an accurate initial starting source can reduce the likelihood of undersampling problems due to inadequate source convergence [2].

The goal of this work was to evaluate an automated approach to defining deterministic-based starting sources for improving the reliability and efficiency of MC criticality calculations. Two approaches were considered: 1) a starting source based on the fission distribution from an eigenvalue deterministic calculation and 2) a starting source based on flux from a fixed-source adjoint deterministic calculation.

A new capability is under development within the SCALE code system for providing an automated capability to specify initial starting sources in MC criticality calculations based on information from relatively fast, approximate deterministic transport calculations. For automating the coupling between deterministic calculations with the Denovo code [4] and MC criticality calculations with the KENO-VI code [5], the capability uses the functionality from the hybrid shielding analysis sequence MAVRIC [6] for creating Denovo input files and processing Denovo output. Two options are currently available in this capability for the starting source of the MC calculations. The first option is based on forward fluxes, \( \phi(\vec{r}, E) \) from a Denovo eigenvalue calculation according to,

\[
 s(\vec{r}, E) = \chi(E) \int_{E=0}^{\infty} v(E') \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') dE',
\]

where \( \chi(E) \) is the fission spectrum, \( v(E) \) is the average neutrons emitted per fission, and \( \Sigma_f(\vec{r}, E) \) is the fission cross-section. The second is based on the spatial distribution of the adjoint fluxes, \( \phi^+(\vec{r}, E) \) of a fixed-source adjoint calculation (Eq. 2) in which the fixed adjoint source is defined as \( v(E) \Sigma_f(\vec{r}, E) \).

\[
 s(\vec{r}, E) = \chi(E) \int_{E=0}^{\infty} \phi^+(\vec{r}, E') dE'.
\]

The calculated starting sources are normalized and restricted to the fissionable materials by KENO.

TEST PROBLEMS

The first test problem represents a “Pin-cell array with irradiated fuel” (Pin-cell) [3]. It consists of a reflected LWR spent fuel pin with more reactive end regions separated by a less reactive region. Two cases were considered in this analysis: the first case (denoted as Case2_1 in Ref. 3) has a symmetric axial composition and the second case (Case2_3) has an asymmetric axial composition. The second test problem (Spheres) represents an unreflected 5×5×1 array of HEU metal spheres in air with the center sphere being larger than the others [3].

Three starting sources were used for the MC calculation of the Pin-cell problem: 1) an axially uniform source, 2) a starting source based on a forward eigenvalue deterministic calculation, and 3) a starting source based on a fixed-source adjoint deterministic calculation. For the second problem, the four starting sources used were: 1) a source uniformly distributed among all spheres, 2) a nonuniform source distribution with more neutrons in one of the corner spheres, 3) a source based on a forward eigenvalue deterministic calculation, and 4) a source based on a fixed-source adjoint deterministic calculation. As indicated in Ref. 3, the goal of using the unrealistic nonuniform starting source distribution was to test the robustness of the criticality codes to converge to the
correct source distribution with a bad starting source guess. For this starting source, the largest number of neutrons was placed in one of the least reactive units.

For all the test problems considered, the deterministic calculations used less than 1,000 spatial mesh cells and the SCALE 27 neutron group ENDF-7 library. The macromaterials approach [7] was used for enhancing the fidelity of the deterministic models. For each problem, the time taken in running the deterministic calculations was small compared to the MC simulation time.

RESULTS

Using a large number of skipped and active cycles, a reference $k_{\text{eff}}$ value was calculated for each problem. For the Pin-cell problem, the reference $k_{\text{eff}} = 1.07793 \pm 6.5E-05$ was calculated for Case2_1 using a uniform starting source with 1,501 total cycles and 501 skipped cycles and the reference $k_{\text{eff}} = 1.07792 \pm 2.3E-05$ was calculated for Case2_3 using a uniform starting source with 10,000 total cycles and 1,000 skipped cycles. For the Spheres problem, the reference $k_{\text{eff}} = 1.11765 \pm 2.1E-05$ was calculated using $1.25 \times 10^6$ neutrons per cycles, 1,500 skipped cycles, and 3,000 total cycles.

The variations of Shannon entropy [8] and $k_{\text{eff}}$ as functions of the cycle number are shown in Fig. 1 for the Pin-cell problem and in Fig. 2 for the Spheres problem.

Calculating the number of skipped cycles was solely based on the Shannon entropy because it converged slower than $k_{\text{eff}}$ for all the cases. With a uniform starting source, the average entropy and its population standard deviation were calculated for the last 940 cycles for Case2_1 and the last 500 cycles for Case2_3 using 1,000 total cycles for the Pin-cell problem and for the last 1,300 cycles using 1,400 total cycles for the Spheres problem. The numbers of skipped cycles, shown as circles in Fig. 1 and Fig. 2, represent the number of cycles at which the entropy falls inside a bandwidth determined by these asymptotic values. The calculations were repeated using these numbers of skipped cycles and a threshold standard deviation of 2.0E-04, which was used to terminate the execution of the KENO-VI runs once achieved.

The parameters used in the Pin-cell problem calculations are shown in Table 1 and the results are shown in Table 2 for the three different starting sources. All the calculations used 100,000 histories per cycle. The speedup factor in Table 2 is the ratio between the time taken by the MC calculation with the uniform starting source to reach the uncertainty threshold in $k_{\text{eff}}$ and the total simulation time (deterministic + MC) with the other starting sources.

**TABLE 1. Calculations parameters for Pin-cell problem**

<table>
<thead>
<tr>
<th>Cycles</th>
<th>Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Skip.</td>
<td>Active</td>
</tr>
<tr>
<td>Case2_1</td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>56</td>
</tr>
<tr>
<td>Forward</td>
<td>1</td>
</tr>
<tr>
<td>Adjoint</td>
<td>20</td>
</tr>
<tr>
<td>Case2_3</td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>490</td>
</tr>
<tr>
<td>Forward</td>
<td>192</td>
</tr>
<tr>
<td>Adjoint</td>
<td>451</td>
</tr>
</tbody>
</table>

The use of deterministic-based starting sources provided a factor of 1.6 to 1.8 enhancement of the overall efficiency of the criticality calculation using a forward eigenvalue deterministic calculation and a factor of 1.1 to 1.3 using a fixed-source adjoint calculation.
The parameters and results for Spheres problem calculations are shown in Table 3 and Table 4 respectively. These calculations used 125,000 neutrons per cycles.

For the Spheres problem, the use of a starting source based on a forward eigenvalue calculation provided a slight increase in the efficiency of the overall simulation. The differences between the calculated $k_{eff}$ values with the uniform and the nonuniform starting sources and the reference $k_{eff}$ are on the order of three standard deviations (3σ) in the calculated $k_{eff}$. This indicates that the fission source, which appears to be converged according to a relatively constant entropy criterion, might not be fully converged or might be converged to the wrong source distribution. Also, the number of active cycles for reaching the uncertainty threshold varies by approximately 50% for some of the different starting sources. Further investigation is being conducted for this problem.

**CONCLUSIONS**

An automated approach that uses an approximate deterministic solution for providing the starting fission source for a MC eigenvalue calculation was evaluated and demonstrated to speed up source convergence and effectively increases the efficiency of the overall simulation. The approach based on the fission source distribution from an eigenvalue deterministic calculation performed best for the test cases evaluated. In addition to speeding up the calculations, this automated approach takes the guess-work out of defining an appropriate, problem-dependent starting source, and hence should significantly reduce the likelihood of users producing wrong answers due to improper source convergence. This latter reliability improvement aspect will be the subject of further evaluation in the future. Finally, this work complements on-going activities to accelerate MC reactor analyses with the FW-CADIS method, which requires a forward deterministic eigenvalue calculation [9]. So, in future work for MC reactor analyses, the deterministic fission distribution will be used as the starting source for the MC calculations.

**REFERENCES**