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ACCELERATION OF MONTE CARLO CRITICALITY CALCULATIONS USING DETERMINISTIC-BASED STARTING SOURCES*

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ABSTRACT

A new automatic approach that uses approximate deterministic solutions for providing the starting fission source for Monte Carlo eigenvalue calculations was evaluated in this analysis. By accelerating the Monte Carlo source convergence and decreasing the number of cycles that has to be skipped before the tallies' estimation, this approach was found to increase the efficiency of the overall simulation, even with the inclusion of the extra computational time required by the deterministic calculation. This approach was also found to increase the reliability of the Monte Carlo criticality calculations of loosely coupled systems because the use of the better starting source reduces the likelihood of producing an undersampled k_{eff} due to the inadequate source convergence. The efficiency improvement was demonstrated using two of the standard test problems devised by the OECD/NEA Expert Group on Source Convergence in Criticality-Safety Analysis to measure the source convergence in Monte Carlo criticality calculations. For a fixed uncertainty objective, this approach increased the efficiency of the overall simulation by factors between 1.2 and 3 depending on the difficulty of the source convergence in these problems. The reliability improvement was demonstrated in a modified version of the "k_{eff} of the world" problem that was specifically designed to demonstrate the limitations of the current Monte Carlo power iteration techniques. For this problem, the probability of obtaining a clearly undersampled k_{eff} decreased from 5% with a uniform starting source to zero with a deterministic starting source when batch sizes with more than 15,000 neutron/cycle were used.

Key Words: Monte Carlo criticality, Source convergence, Hybrid Monte Carlo/deterministic

1. INTRODUCTION

Monte Carlo (MC) methods, which allow detailed and accurate modeling of the full geometry and energy of nuclear systems, are routinely used in criticality safety analysis. An MC criticality simulation involves computing the fission source distribution iteratively until the source distribution is sufficiently converged, and only then the statistical sampling of certain parameters (e.g., fundamental mode eigenvalue, reaction rates, and fluxes) can take place. The parameters of interest can only be tallied after an acceptable source convergence because the contamination of

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the results by an inadequately converged fission source distribution can lead to under-predicted tally estimates (wrong answers) [1].

Traditionally, the initial source distribution is specified by the user or by default in the MC code. For example, the default in the SCALE/KENO [2] MC codes is to start neutrons uniformly throughout all regions containing fissile material. Since the initial "guessed" distribution does not usually represent the true (fundamental) fission source distribution, MC practitioners specify a number of inactive cycles, often referred to as "skipped cycles," to be discarded before accumulating the tallies. The closer the initial starting source is to the fundamental source distribution, the fewer the number of skipped cycles is required to reach source convergence, thereby improving the efficiency of the MC criticality calculation. In addition to speeding up the calculations, an accurate initial starting source can increase the reliability of the MC calculation by reducing the likelihood of producing inaccurate tally estimates because of the undersampling problems caused by the insufficient sampling of some portion of the systems [3, 4, 5].

The goal of this work is to evaluate an automated approach to defining deterministic-based starting sources for MC criticality calculations. A quick deterministic eigenvalue calculation is used for calculating the fission distribution on a coarse mesh. The deterministically calculated fission distribution is then used as the starting source for the MC eigenvalue calculation.

Two widely used test problems developed by the Organisation for Economic Co-operaton and Development/Nuclear Energy Agency (OECD/NEA) Expert Group on Source Convergence in Criticality-Safety Analysis [1] and a modified version [4] of the "k_{eff} of the world" problem [5] were used for this evaluation. The results show that, even with the inclusion of the computational efforts of the deterministic calculation, using a deterministic-based starting source increases the efficiency of the overall eigenvalue simulation due to the significant decrease in the number of skipped cycles needed in the MC calculation. The results also show that using deterministic starting sources increases the reliability of the k_{eff} calculation for difficult criticality safety problems where the coupling between the multiplying media is very small.

2. METHODOLOGY

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 [6] and MC criticality calculations with the KENO-VI code [7], this new capability uses some of the functionality of the SCALE hybrid shielding analysis sequence, Monaco with Automated Variance Reduction using Importance Calculations (MAVRIC) [8] for creating Denovo input files and processing Denovo output. The starting source, $s(\vec{r},E)$, is calculated from a Denovo eigenvalue calculation according to,

$$s(\vec{r},E) = \chi(E)\int_{E'=0}^{\infty} \nu(E')\Sigma_f(\vec{r},E')\phi(\vec{r},E')dE' \quad , \tag{1}$$

where $\chi(E)$ is the fission spectrum, $\upsilon(E)$ is the average neutrons emitted per fission, $\Sigma_f(\vec{r},E)$ is the fission cross section, and $\phi(\vec{r},E)$ is the energy- and space-dependent flux.

In this analysis, the MC calculations used either continuous-energy or fine multigroup (238 neutron groups) ENDF/B-VII libraries, while the deterministic calculations used a 27 neutron group ENDF/B-VII library. The macromaterials approach [9], which uses a volume-weighted average of the MC materials present in each cell of the mesh used in the deterministic calculation, was used to enhance the fidelity of the deterministic models that used relatively coarse meshes.

2.1. Efficiency of k_{eff} Calculations

Prior to the efficiency comparison calculations, both the k_{eff} and the Shannon entropy [10] plots were examined for the two standard OECD/NEA test problems, but the Shannon entropy plots solely determined the number of skipped cycles because the Shannon entropy converged more slowly than k_{eff} for all the tested problems. The number of skipped cycles was determined from the number of cycles at which the entropy falls inside a bandwidth determined by the average and the population standard deviation of the asymptotic values of the entropy plots with a uniform starting source. Since it is possible to calculate relatively constant entropy without the complete convergence of the fission source distribution in MC criticality calculations [4, 11], the source distribution was analyzed for the OECD/NEA test problems using deterministic and uniform starting sources. Additionally, the fission rate in one of the least reactive regions of the OECD/NEA test problems was tallied as a function of different numbers of skipped cycles to analyze the effects of using deterministic starting sources on the MC source convergence in low reactive regions.

For comparing the efficiency of the k_{eff} calculations, an uncertainty threshold ($1\sigma = 0.0002$) was specified to terminate the KENO-VI calculations. The efficiency improvements caused by using deterministic starting sources were measured by comparing the time needed by the MC calculation to achieve the uncertainty threshold using a uniform starting source to the total time (deterministic + MC) needed to reach the same uncertainty threshold using deterministic starting sources.

2.2. Reliability of k_{eff} Calculations

For assessing the reliability of the MC k_{eff} calculations, multiple independent MC trials were run using different random number seeds for the modified version of the k_{eff} of the world problem. The reliability of the MC calculations was defined as the probability of not obtaining a clearly undersampled k_{eff} in these independent replicas.

3. TEST PROBLEMS

Two of the four idealized test problems in Ref. [1] were used in this analysis. The problems, which represent cases previously encountered in criticality safety analyses, were defined by the OECD/NEA Expert Group on Source Convergence in Criticality Safety Analysis with the intention of being used as a basis for measuring the performance of source convergence in MC criticality calculations [1].

The first problem, "spheres," represents an unreflected 5 × 5 × 1 array of highly enriched uranium metal spheres in air with the center sphere being larger than the others. A layout of the geometry for the spheres problem's configuration is shown in Fig. 1.

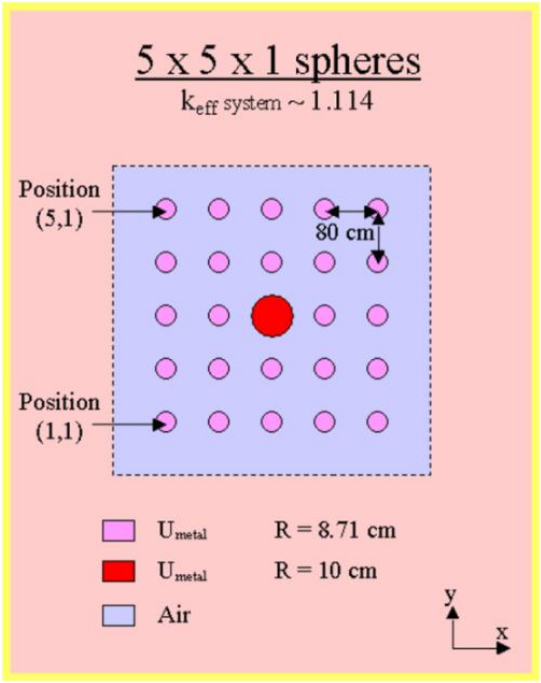

Figure 1. Geometry of spheres problem (Source: Ref. 1).

The second problem, "pin-cell array with irradiated fuel" (pin-cell), represents a reflected light water reactor spent fuel pin with more-reactive (low-burnup) end regions separated by a less-reactive (high-burnup) central region. The model has reflective boundaries in the horizontal directions and vacuum boundaries at the top and the bottom. Figure 2 shows the geometry of the pin-cell problem.

Two pin-cell cases were considered in this analysis: the first case (denoted as Case2_1 in Ref. [1]) has a symmetric axial composition; the second case (Case2_3) has an asymmetric axial composition. For Case2_3, the lower regions of the fuel element have higher burnup (less-reactive) than the upper regions.

The third problem is a modified version of the k_{eff} of the world problem. The original k_{eff} of the world problem was introduced in 1971 by G. E. Whitesides to caution the MC users of the possibility of obtaining incorrect k_{eff} due to the inadequate sampling of the significant regions of criticality problems [5]. The problem represents a 9 × 9 × 9 array of subcritical plutonium spheres spaced on 60 cm centers. The center unit of the array is replaced by a sphere of plutonium, which is exactly critical as a bare unit. The array is surrounded on all sides by a thick water reflector.

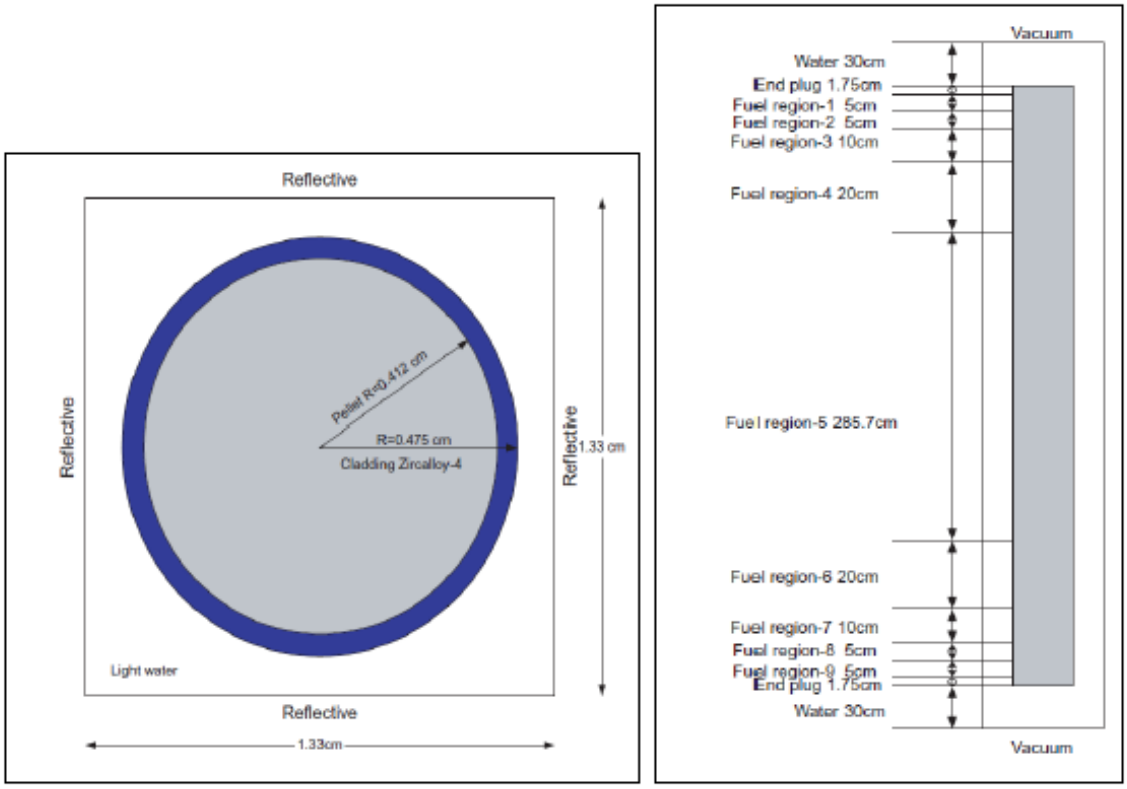

Figure 2. Horizontal and axial views of the pin-cell problem (Source: Ref. 1).

When this problem was tried in 1971, the k_{eff} was always underestimated due to the failure of the MC calculations to converge to the fundamental source mode. With more powerful computing hardware and using the recommended "Best Practices" [3] for MC criticality calculations, the problem was revisited in 2010. By discarding enough initial cycles (150 or more) and using enough neutrons per cycle (10^4 or more), it was shown that the k_{eff} of the world problem "is actually not a difficult problem to solve" using today's tools [11]. A modified, more challenging in terms of source conversion, version of the k_{eff} of the world problem was introduced by B. Kiedrowski specifically to evaluate the limitations of the current MC power iteration techniques. To decrease the coupling among the spheres, the regions between the spheres were flooded with water, and, to create an asymmetry in the coupling between the most reactive region and the other regions, a 0.5 cm layer of natural cadmium was placed around the center sphere. While fast neutrons from the central sphere are easily transported out of the cadmium layer, slowed down neutrons from other spheres cannot easily overcome the cadmium layer around the central sphere. The radii of the subcritical spheres were reduced from 3.90 cm to 3.75 cm, and the radius of the critical sphere was reduced from 4.93 cm to 4.33 cm. It was shown that even with reasonable batch sizes (5×10^3 to 10^4 neutron/cycle) and a reasonable number of skipped cycles (250), numerous independent MC calculations yielded incorrect results for k_{eff} with nontrivial probability [4].

Fig. 3 shows the original and the modified versions of the k_{eff} of the world problem.

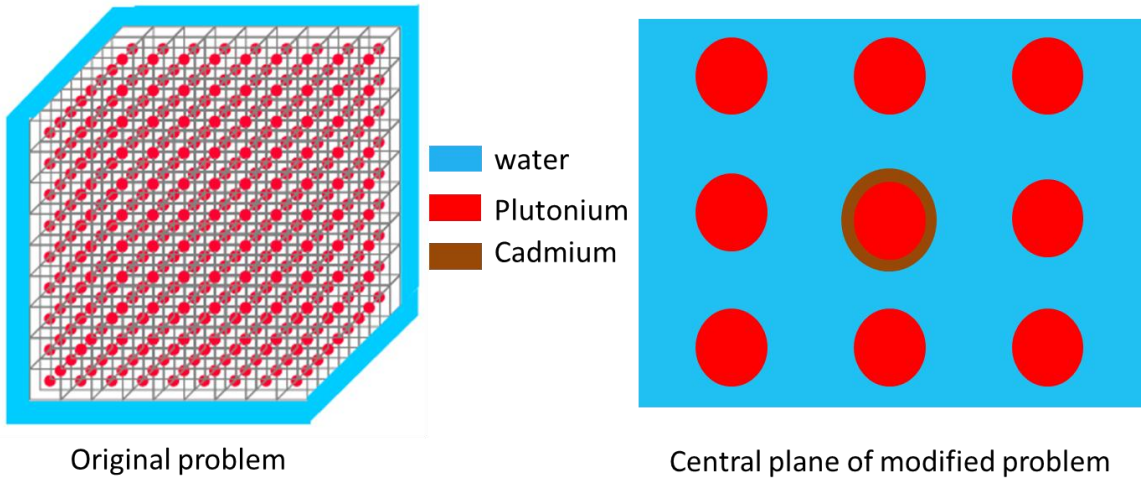

Figure 3. Original and modified k_{eff} of the world problem (Source: Ref. 4).

4. RESULTS

For the results presented in this paper, all the MC calculations of the OECD/NEA standard test problems used the fine multigroup (238 neutron groups) ENDF/B-VII library and the MC calculations of the modified k_{eff} of the world problem used continuous ENDF/B-VII library.

4.1. Efficiency of k_{eff} Calculation

4.1.1. Determination of reference k_{eff} values

Reference k_{eff} values were calculated for the spheres problem and the pin-cell problem using a uniform starting source and a very large number of skipped cycles, as compared to the numbers of skipped cycles that were enough not to cause undersampling in k_{eff} results in Ref. [1]. For the spheres problem, the reference k_{eff} (1.117668 ± 0.000026) was calculated using 4,000 skipped cycles and 14,000 total cycles. For the pin-cell problem, the reference k_{eff} (1.077896 ± 0.000022 for Case2_1 and the reference k_{eff} = 1.077919 ± 0.000023 for Case2_3) were calculated using 1,000 skipped cycles and 10,000 total cycles. The number of neutrons per cycle used in the reference k_{eff} calculations was 125,000 for the spheres problem and 100,000 for the pin-cell problem.

4.1.2. Determination of a sufficient number of skipped cycles

The variations of Shannon entropy and k_{eff} as functions of the cycle number, along with the reference k_{eff} values, are shown in Fig. 4 for the spheres problem and in Fig. 5 for the pin-cell problem for cases using uniform and deterministic starting sources. The numbers of neutrons per cycle are the same numbers used in the reference k_{eff} calculations.

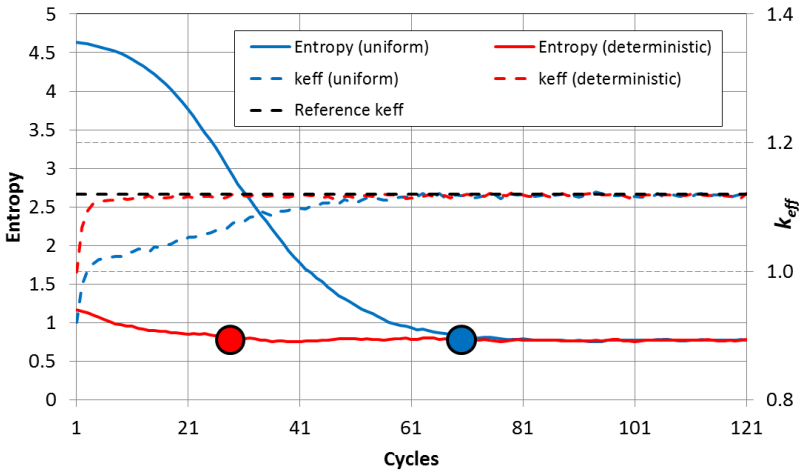

Figure 4. Entropy and k_{eff} variations for spheres problem.

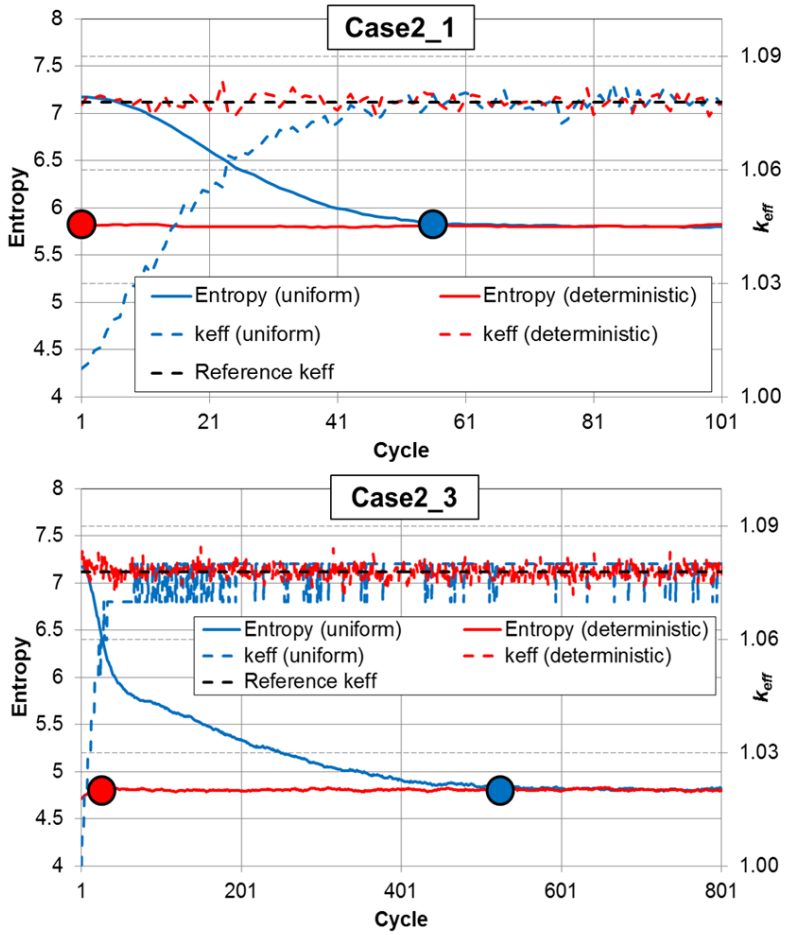

Figure 5. Entropy and k_{eff} variations for pin-cell problem.

The circles in Figs. 4 and 5 indicate the numbers of cycles at which the entropy falls inside a bandwidth determined by the average and the population standard deviation of the asymptotic values of the Shannon entropy. These asymptotic values were calculated using a uniform starting source for the last 1,300 cycles using 1,400 total cycles for the spheres problem, the last 940 cycles using 1,000 total cycle for Case2_1 of the pin-cell problem, and the last 500 cycles using 1,000 total cycles for Case2_3 of the pin-cell problem.

4.1.3. Fission source distribution

Because of the strong coupling between the reactive regions in the spheres problem, the convergence of the fission source distribution was relatively fast. An insufficient number of histories per cycle (125) was intentionally chosen to amplify the effects of undersampling in the spheres problem in Ref. [1]; however, none of the different codes contributing to the benchmark exhibited a single situation in which the central, most reactive sphere remained undersampled during 1,000 cycles [1]. With larger numbers of histories per cycle, the fission source distribution in KENO-VI simulations only required a few minutes. Figure 6 shows the calculated fission source distribution for the spheres problem using a 1-min Denovo calculation and a 5.5-min KENO-VI calculation that used a uniform starting source, 12,500 neutron/cycle, 400 skipped cycles, and 1,000 active cycles. The fission source distribution did not change when the number of active and skipped cycles was increased; it was similar in shape to the distribution calculated deterministically.

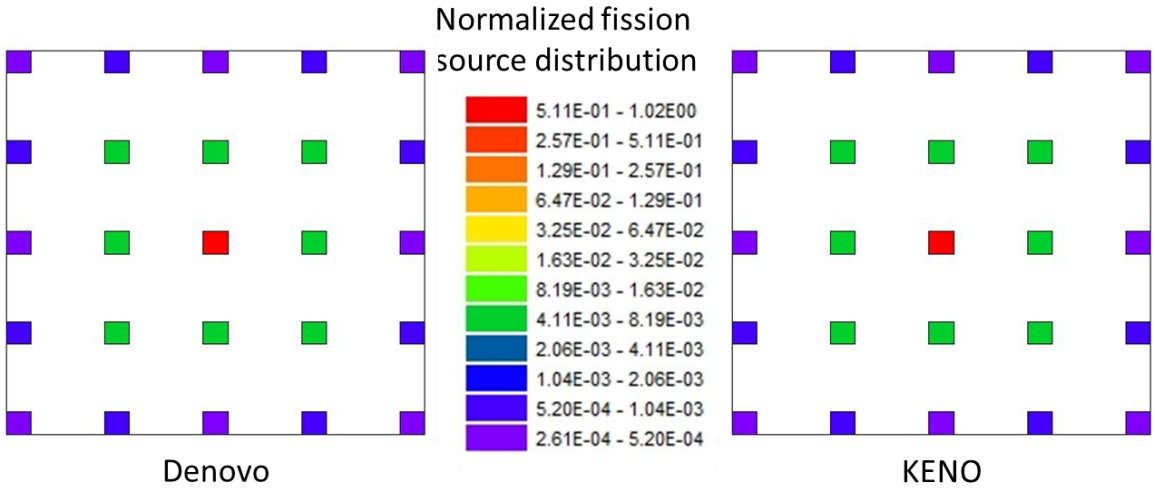

Figure 6. Fission source distribution on the central plane of the spheres problem.

For the pin-cell problem, the convergence of the fission source distribution was relatively easy for Case2_1 but was difficult for Case2_3. Figure 7 shows the axial fission source distribution for the two pin-cell problem cases. The fission source distribution calculated from the approximate Denovo calculation was used to calculate the starting source for the KENO-VI calculation with the deterministic starting source. All the KENO-VI calculations used 500 active

cycles, 500 skipped cycles, and 10^5 neutron/cycle except for the reference calculation, which used the parameters mentioned in Sect. 4.1.1.

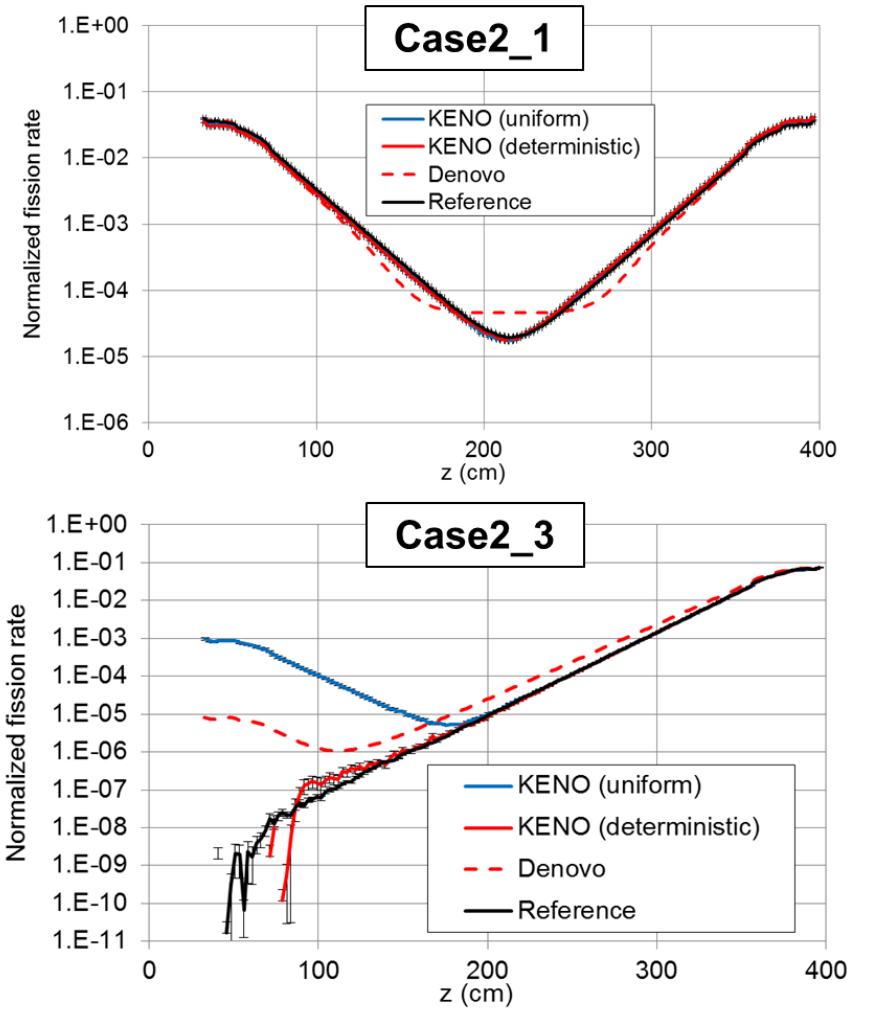

Figure 7. Fission source distribution in the pin-cell problem.

Both KENO-VI calculations with uniform and deterministic starting sources converged to a similar distribution as the reference calculation for Case2_1. For the axial fission source distribution of Case2_3, the KENO-VI calculation with a deterministic starting source had a better agreement with the reference calculation than the KENO-VI calculation with a uniform starting source. Note that the Denovo results were purposely based on a fast-running, fairly coarse representation and no effort was spent trying to further resolve those results. With a uniform starting source, the differences in the fission rates, as compared to the reference results, were less than 3σ between 124 cm and 213 cm from the bottom of the least-reactive region, which is denoted as "region-5" in Fig. 2. Above that, the differences in the fission rates between the KENO-VI calculation with a uniform starting source and the reference calculation did not exceed 2.5%, but they were increasingly higher than the statistical uncertainties in the fission

rates of the KENO-VI calculation with a uniform starting source and reached 14 σ at the upper end of the fuel element. This discrepancy may be caused by an underestimation in the uncertainties of fission rates of the MC calculation with a uniform starting source. In contrast, the differences in the fission rates between the KENO-VI calculation with a deterministic starting source and the reference KENO-VI calculation did not exceed a few standard deviations after the first 15 cm of the bottom of region-5. Below that, at the lower end of region-5 and in lower regions, the differences between the fission rates of the KENO-VI calculation with a deterministic starting source and the reference KENO-VI calculation were higher than the statistical uncertainties in the KENO-VI calculation with a deterministic starting source and both the KENO-VI calculations did not have fission scores in large portions in these regions. The fission rates did not converge in these lower regions even with higher numbers of neutrons per cycle (10^6–10^7) and hundreds of skipped cycles in other simulations. The fission rates of the KENO-VI calculation with a uniform starting source were at least four orders of magnitude higher than the fission rates of the other two KENO-VI calculations in these regions.

To determine the effects of the use of deterministic starting sources on the fission source distribution in low reactive regions, the fission rate in the first 20 cm of region-5 in Case2_3 was investigated further. Figure 8 shows the fission rate in the lowest 20 cm portion of region-5 as a function of the number of skipped cycles for KENO-VI calculations with a deterministic starting source and with a uniform starting source. A constant number of neutrons per cycle (10^5) was used for all the KENO-VI calculations. The number of active cycles was also kept to be constant at 1,000, except for the reference calculation, which used 10^4 active cycles, 10^4 skipped cycles, and a uniform starting source. This reference case used more skipped cycles than the reference case described in Sect 4.1.1 because it is more difficult for the fission source to converge in the low reactive regions.

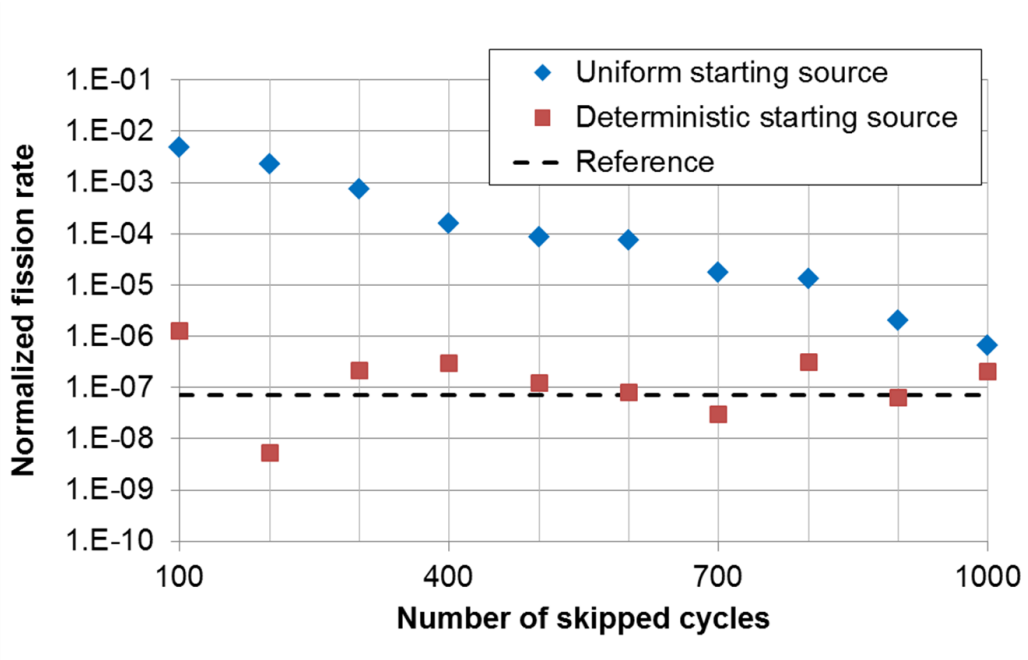

Figure 8. Fission rate in lowest 20 cm portion of region-5 of Case2_3 of pin-cell problem (all uncertainties <25%).

Because of the high number of neutrons initially sampled in low reactive regions with a uniform starting source, the fission rate at the lowest 20 cm of region-5 was much higher than the reference value, which used 10^4 skipped cycles and the same uniform starting source. The fission rate with a uniform starting source decreased with increasing numbers of skipped cycles, but even with 900 skipped cycles, the fission rate was still more than one order of magnitude higher than the reference value. With a deterministic starting source, the fission rate in the lowest 20 cm region crossed the reference value with 200 skipped cycles and started oscillating around that value when more skipped cycles were used. Even though a reliable estimate for the fission rate in the low reactive region could not be achieved with a deterministic starting source and a reasonable number of skipped cycles, it is apparent that the MC calculation with a deterministic starting source performed much better than the MC calculation with a uniform starting source in calculating the reaction rates in low reactive regions.

4.1.4. k_{eff} Calculation efficiency comparisons

After the number of skipped cycles was determined, the k_{eff} calculations were repeated using the uncertainty threshold ($1\sigma = 0.0002$) to terminate the KENO-VI execution. The k_{eff} calculations used the same numbers of neutrons per cycle as the reference calculations. The parameters used in the spheres problem calculations and the pin-cell problem calculations are shown in Table I and Table II, respectively.

Table I. Calculation parameters for spheres problem

Starting source	Cycles		Time (min)	
	Skipped	Active	Denovo	Keno
Uniform	69	139	0.00	9.43
Deterministic	26	133	0.91	7.67

Table II. Calculation parameters for pin-cell problems

Starting source	Cycles		Time (min)	
	Skipped	Active	Denovo	Keno
Case2_1				
Uniform	56	79	0.00	60.20
Deterministic	1	74	3.69	33.75
Case2_3				
Uniform	490	138	0.00	278.25
Deterministic	10	140	25.28	68.28

The results of the calculations for the spheres and the pin-cell problems are shown in Table III and Table IV for the different starting sources. All the calculated k_{eff} agreed with the reference k_{eff} within 3σ.

Table III. Spheres problem results

Starting source	k_{eff}	Speedup
Uniform	1.11707 ± 0.00019	1.0
Deterministic	1.11758 ± 0.00019	1.2

Table IV. Pin-cell problem results

Starting source	k_{eff}	Speedup
Case2_1		
Uniform	1.07783 ± 0.00019	1.0
Deterministic	1.07807 ± 0.00019	1.6
Case2_3		
Uniform	1.07806 ± 0.00018	1.0
Deterministic	1.07809 ± 0.00017	3.0

The speedup provided by the use of the deterministic starting source increased with the difficulty of the convergence of the fission source distribution. A slight increase in the efficiency of the overall simulation was noticed for the spheres problem and for Case2_1 of the pin-cell problem. As shown in Figs. 6 and 7, the fission source distribution varies by only three orders of magnitude throughout the geometry in these cases. A greater increase in the efficiency of the k_{eff} calculation was noticed for Case2_3 of the pin-cell problem, where the variation of the fission source distribution is more than six orders of magnitude.

4.2. Reliability of k_{eff} calculation

The decoupling features added to the modified version of the k_{eff} of the world problem increase the difficulty of calculating a reliable k_{eff} even with today's tools [4]. The calculated k_{eff} for a uniform array of subcritical spheres with similar radii was 0.94957 ± 0.00043. For a system with the same dimensions but with no spheres other than the central coated larger sphere, k_{eff} was calculated to be 1.00015 ± 0.00014. The composite system should be supercritical but because the mass of the fissile material in the whole system is much larger than mass of the fissile material in the critical unit, it is difficult for the sampling techniques to distinguish between the units. For that reason, both KENO-VI and MCNP [12] can produce incorrect k_{eff} results for this problem, even with seemingly reasonable calculational parameters [4].

Figure 9 shows the probability distribution function of the calculated k_{eff} using a uniform starting source with different random number seeds and different numbers of neutrons per cycle. Nine different numbers of neutrons per cycle varying between 1,000 and 25,000 were used to calculate k_{eff} in this analysis. For each number of neutrons per cycle, the k_{eff} calculation was repeated one hundred times with different random number seeds. The 900 cases used 250 skipped cycles and variable numbers of active cycles. The number of active neutrons was set to be constant (10^6) for all the runs with the different numbers of neutrons per cycle and the different random number seeds. The KENO-VI run times varied between 25 and 160 min for all cases.

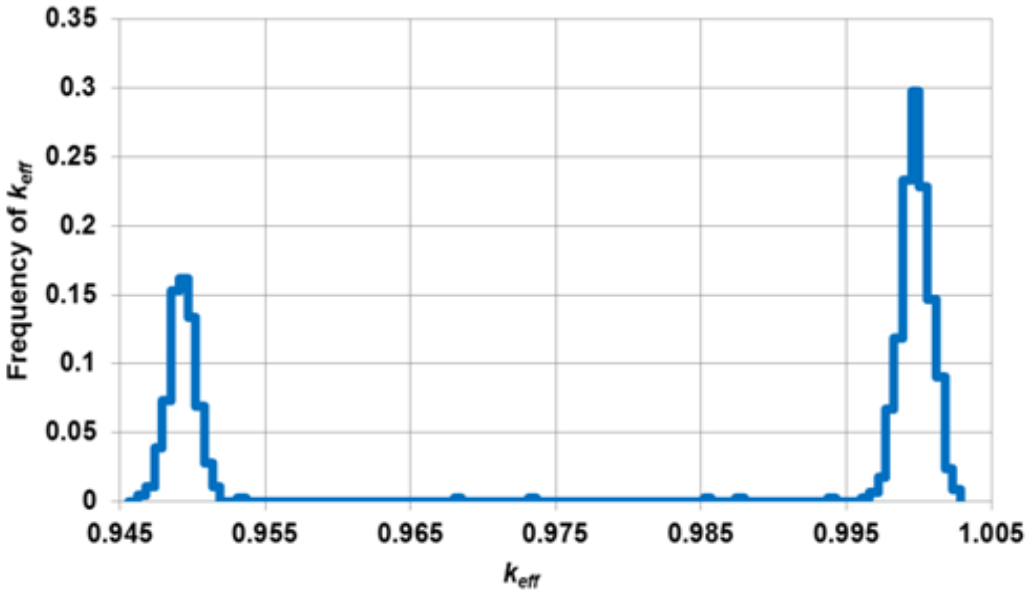

Figure 9. Probability density function of the calculated k_{eff} for the modified "k_{eff} of the world" problem.

The calculations were repeated with a deterministic starting source from a 55-min Denovo calculation. Figure 10 shows the probability of obtaining a clearly undersampled k_{eff} (k_{eff}~0.95) as a function of the number of neutrons per cycle using uniform and deterministic-based starting sources.

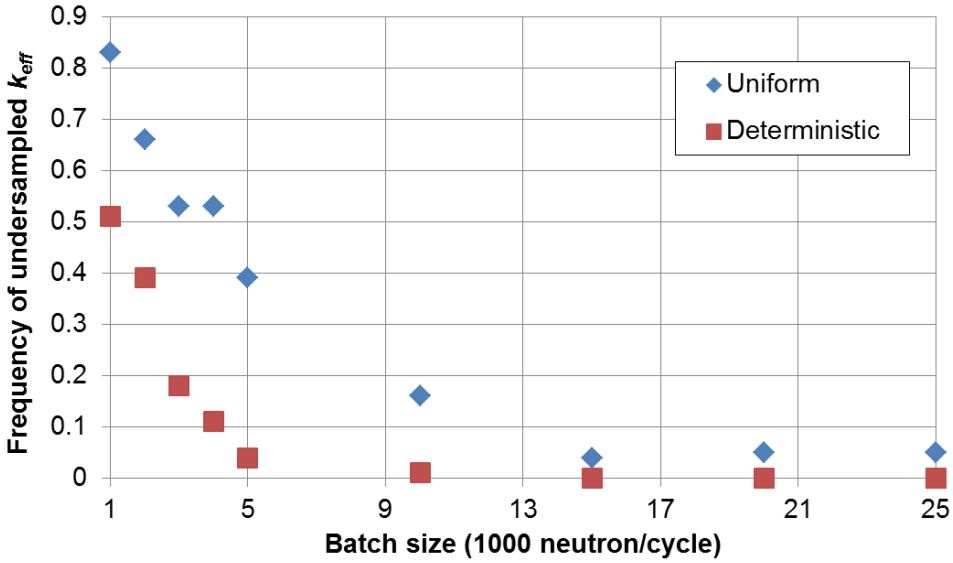

Figure 10. Frequency of undersampling of k_{eff} for the modified k_{eff} of the world problem.

The effectiveness of using a deterministic starting source to improve the reliability of the k_{eff} MC calculations is shown in Fig. 10. Due to enhancing the fission source distribution throughout the multiplicative regions and increasing the probability of the adequate sampling of the highest reactive regions, the probability of calculating a clearly undersampled k_{eff} for this problem was always less with a deterministic starting source. The probability of calculating the incorrect k_{eff} reached zero with a deterministic starting source at 15,000 neutrons/cycle, but a nontrivial probability that reached 5% with 25,000 neutron/cycle remained with a uniform starting source.

5. CONCLUSIONS

For improving the efficiency and reliability of source convergence in MC criticality calculations, a new approach that automates the coupling between deterministic and MC eigenvalue calculations is under development within the SCALE code system. The approach, which uses information from a relatively fast, approximate deterministic transport calculation to provide the starting fission source for an MC eigenvalue calculation, takes the guesswork out of defining an appropriate, problem-dependent starting source.

Due to a significant decrease in the number of skipped cycles necessary before the MC tally accumulation can begin, the new approach was found to increase the efficiency of the overall criticality simulation, even with the inclusion of the time necessary to run the deterministic calculation. In addition to speeding up the calculations, the approach was found to increase the reliability of the MC calculation of k_{eff} in problems for which the coupling between the multiplying media is very small. As compared to typical user-provided or code-defaulted starting sources, the more accurate starting source provided by the deterministic calculation decreases the probability of producing inaccurate tally estimates associated with undersampling problems caused by inadequate source convergence. The efficiency improvement of this approach was demonstrated using standard test problems defined by the OECD/NEA Expert Group on Source Convergence in Criticality-Safety Analysis and the reliability improvement was demonstrated using a modified version of the k_{eff} of the world problem.

This work complements ongoing activities to accelerate MC reactor analyses with the FW-CADIS method [13], which requires a forward deterministic eigenvalue calculation [14]. Therefore, in future work for MC reactor analyses, the deterministic fission distribution will be used as the starting source for the MC calculations to improve tally efficiency and reliability. The efficiency of MC eigenvalue calculations with starting sources from fixed-source adjoint deterministic calculations were evaluated and found to be less effective as compared to starting sources from forward eigenvalue deterministic calculations [15]. Starting sources from adjoint eigenvalue deterministic calculations were also evaluated and their effectiveness was found to be comparable to starting sources from forward eigenvalue deterministic calculations. This work concentrated on starting sources based on forward eigenvalue deterministic calculations because the fluxes from a forward eigenvalue deterministic calculation will be available during the implementation of the FW-CADIS method.

6. ACKNOWLEDGMENTS

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