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A REVIEW OF MONTE CARLO CRITICALITY CALCULATIONS – CONVERGENCE, BIAS, STATISTICS

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ABSTRACT

Monte Carlo criticality calculations have been performed for over 50 years for reactor physics and criticality safety applications. With today's faster computers, these calculations are being carried out to greater precision (smaller uncertainties) in k_{eff}, and detailed distributions of power and reaction rates are being computed routinely. This paper provides a review of the fundamental theory of Monte Carlo criticality calculations, with guidance on practical methods for: (1) assuring convergence of both k_{eff} and the source distribution, (2) minimizing the bias in k_{eff} and reaction rate distributions, and (3) dealing with the underprediction bias in uncertainties for k_{eff} and reaction rate distributions.

Key Words: eigenvalue calculations, k-effective, power iteration

1. INTRODUCTION

Monte Carlo methods have been used to compute k_{eff} and the fundamental mode eigenfunction of critical systems since the 1950s [1-4]. With the faster computers of the 1980s through the present, it has become routine to compute detailed power distributions in 2D or 3D Monte Carlo criticality calculations and to compute k_{eff} with uncertainties of a few pcm (rather than 10s or 100s of pcm as in earlier days). Most Monte Carlo codes use the standard power method for solving k-eigenvalue problems [5,6], where each (outer) iteration cycle corresponds to a single fission generation in the simulation. Given a fission neutron source distribution and an estimate of k_{eff}, single-generation random walks are carried out for a "batch" of neutrons to estimate a new k_{eff} and source distribution. Iterations continue until both k_{eff} and the source distribution have converged. After convergence of the power iterations, tallies of k_{eff} and spatial reaction rates are accumulated. While such calculations have become routine using standard codes (e.g., MCNP [7], SCALE/KENO [8]), there remain 3 principal limitations that must be addressed to perform calculations correctly:

1. Sufficient initial cycles must be discarded prior to beginning the tallies, so that contamination of the results by the initial source guess becomes negligible.
2. Sufficient numbers of neutrons must be followed in each cycle so that bias in k_{eff} and reaction rate tallies becomes negligible.
3. Bias in the uncertainties on k_{eff} and reaction rate tallies must be recognized and dealt with.

This paper provides a review of the 3 fundamental problems inherent in Monte Carlo criticality calculations. A realistic 2D quarter-core PWR model is used to illustrate the effects of each and to provide guidance to practitioners.

2. THEORY FOR MONTE CARLO EIGENVALUE CALCULATIONS

The k-eigenvalue transport equation in standard form

$$\left[\Omega\cdot\nabla+\Sigma_T(\vec{r},E)\right]\Psi(\vec{r},E,\Omega)=\iint\Psi(\vec{r},E',\Omega')\Sigma_S(\vec{r},E'\rightarrow E,\Omega\cdot\Omega')d\Omega'dE' + \frac{1}{k_{eff}}\frac{\chi(E)}{4\pi}\iint\nu\Sigma_F(\vec{r},E')\Psi(\vec{r},E',\Omega')d\Omega'dE' \quad (1)$$

can be written as

$$(\mathbf{L}+\mathbf{T})\Psi=\mathbf{S}\Psi+\frac{1}{k_{eff}}\mathbf{M}\Psi \quad (2)$$

and then rearranged to

$$\Psi=\frac{1}{k_{eff}}(\mathbf{L}+\mathbf{T}-\mathbf{S})^{-1}\mathbf{M}\Psi=\frac{1}{k_{eff}}\mathbf{F}\Psi \quad (3)$$

Equation (3) may be solved numerically using the standard power iteration method [5,6]

$$\Psi^{(n+1)}=\frac{1}{k_{eff}^{(n)}}\mathbf{F}\Psi^{(n)},\qquad n=0,1,\ldots,\qquad \text{given } k_{eff}^{(0)} \text{ and } \Psi^{(0)} \quad (4)$$

2.1. Convergence of the Power Method

When calculating k_{eff} and the power distribution for a reactor system, the dominance ratio is the key parameter for determining the convergence rate of the standard power method [9]. For systems with a high dominance ratio, 100s or 1000s of iterations may be required before the method achieves convergence, while systems with a low dominance ratio may require only 10s or 100s of iterations.

Concerning the relative convergence of k_{eff} and the fission source distribution during the power iteration process, if $\Psi^{(0)}$ is expanded in terms of the eigenvectors $\vec{u}_J$ of Eq. (3), substituted into Eq. (4), and rearranged with some straightforward algebra, then

$$\Psi^{(n+1)}(\vec{r})=\vec{u}_0(\vec{r})+\frac{a_1}{a_0}\rho^{n+1}\cdot\vec{u}_1(\vec{r})+\ldots$$
$$k_{eff}^{(n+1)}=k_0\cdot\left[1-\frac{a_1}{a_0}\rho^n(1-\rho)g_1+\ldots\right] \quad (5)$$

where ρ is the dominance ratio (k_1/k_0), k_0 and $\vec{u}_0$ are the fundamental mode eigenvalue (exact k_{eff}) and eigenfunction, k_1 and $\vec{u}_1$ are the first higher mode eigenvalue and eigenfunction, and a_0, a_1, and g_1 are constants determined by the expansion of the initial fission distribution. Eq. (5) shows that higher-mode noise in the fission distribution dies off as ρ^{n+1}, while higher-mode noise in k_{eff} dies off as $\rho^n(1-\rho)$. When the dominance ratio is close to 1, k_{eff} will converge sooner than the fission distribution due to the extra damping factor $(1-\rho)$ which is close to 0. Thus, it is essential to monitor the convergence of both the fission source distribution and k_{eff}, not just that of k_{eff}.

The Shannon entropy of the fission source distribution, H_{src} [10-12], has been shown to be an effective diagnostic measure for characterizing convergence of the fission source distribution. H_{src} is computed by tallying the fractions of fission sites in a cycle on a coarse mesh (P_J) and then evaluating

$$H_{src} = -\sum_J P_J \cdot \ln_2(P_J) \tag{6}$$

Convergence of the power iteration process can be determined by examining plots of both k_{eff} and the fission source distribution (using Shannon entropy) vs. cycle. Both should be converged before tallies of k_{eff} and reaction rates are begun.

2.2. Bias in Results for k_{eff} and Reaction Rate Distributions

In the power iteration process for Monte Carlo, if a fixed number of neutrons M_0 start a cycle and are followed through a single fission generation, then the expected number of neutrons produced, M_1, is $E[M_1] = k_{eff} M_0$. Before beginning the next cycle, the number of neutrons (or alternatively the total neutron weight) must be adjusted by the factor (M_0/M_1) to provide the correct normalization. However, renormalizing each cycle by dividing by a stochastic quantity (M_1) has been shown to introduce a bias in both k_{eff} and any local tallies or distributions [13,14]. The bias in k_{eff} has been shown to be

$$\Delta k = -\frac{\sigma_k^2}{k_{eff}} \cdot \sum_{J=1}^{\infty} r_J \propto \frac{1}{M_0}, \tag{7}$$

where σ_k^2 = population variance in k (computed assuming uncorrelated values of k for each cycle), and r_J = lag-J correlation coefficient between cycle values of k. (The r_J are assumed to approach 0 for large J.) The biases in a tallied reaction rate or a component of a reaction rate distribution are more complicated, and may be positive or negative.

The biases in k_{eff} and local tally results are independent of the number of cycles, N, but are proportional to $1/M_0$ (due to the dependence on σ^2). Thus, bias in k_{eff} and local tallies can be reduced and effectively eliminated by running a sufficient number of neutrons in each individual cycle of the calculation. Section 3 provides a realistic example of the influence of the number of neutrons per cycle on the bias in k_{eff} and local tallies.

2.3. Bias in Uncertainties for k_{eff} and Reaction Rate Distributions

The power iteration process used to solve Monte Carlo eigenvalue calculations is based on a generation model, where next-generation fission neutron sites produced in the current cycle are used as the starting locations for the next cycle. It is clear on physical grounds that there is always some spatial correlation between the fission neutron starting sites in successive cycles (or generations), and that this correlation will be positive. For problems with a small dominance ratio, the correlation effects may be significant for only a few cycles; for problems with a large dominance ratio, correlation effects may persist for dozens or hundreds of cycles [15]. While such correlation does not affect the average results for k_{eff} and local tallies, it can produce significant errors in the computed uncertainties [13,14,16]. Monte Carlo codes such as MCNP

and SCALE/KENO ignore inter-cycle correlation when computing statistics. That is, the codes assume that the individual cycles are independent and ignore correlation. As a result, the codes calculate uncertainties that are too small. For N active cycles, the codes will compute for tally X (where X may be k_{eff}, a tallied reaction rate, or a component of a reaction rate distribution) a mean result and standard deviation given by:

$$\bar{X} = \frac{1}{N} \cdot \sum_{n=1}^{N} X_n, \qquad \sigma_{\bar{X}} = \frac{1}{N} \cdot \sqrt{\frac{1}{N} \cdot \sum_{n=1}^{N} X_n^2 - \bar{X}^2} \tag{8}$$

The true standard deviation, accounting for inter-cycle correlation, is then given for large N by:

$$\sigma_{\bar{X}}^{true} = \sigma_{\bar{X}} \cdot \sqrt{1 + 2 \cdot \sum_{J=1}^{\infty} r_J} \tag{9}$$

where r_J = lag-J correlation coefficient between cycle values, X_J. (The r_J are assumed to approach 0 for large J.) Due to the positive inter-cycle correlation, the significant values of r_J are positive, and the bias in the computed value of $\sigma_{\bar{X}}$ is negative: $\sigma_{\bar{X}} < \sigma_{\bar{X}}^{true}$. It will be demonstrated in Section 3 that the computed uncertainties can be too small by factors of 2-5 for local tallies in fission rates in realistic problems. It must be emphasized that the underprediction errors in uncertainties are present regardless of the number of neutrons per cycle (M_0) or the number of active cycles run (N); the errors in uncertainties are not reduced by running more cycles or more neutrons per cycle.

3. NUMERICAL RESULTS

To provide numerical evidence supporting the theory described in Section 2, calculations were run for a realistic and practical example: a 2D quarter-core PWR model with explicit representation of every fuel pin and water tube. This example is based on the specifications given by Nakagawa and Mori [17] for a 3D whole-core model. In the current 2D quarter-core example, there are 48 ¼ fuel assemblies (each with a 17x17 lattice arrangement), 12,738 fuel pins with cladding, and 1206 ¼ water tubes for control rods or detectors. The assemblies have enrichments of 2.1%, 2.6%, and 3.1%. The dominance ratio for this problem was determined to be ρ=.96. The geometry for the MCNP5 Monte Carlo calculations is shown in Figure 1.

All of the calculations discussed below were performed with MCNP5 (version 1.50) using the new ENDF/B-VII continuous-energy data libraries on a Mac Pro (dual quad-core Xeons, 8 cpus total). Each calculation used an initial source guess that was uniform over the core region; discarded the first 50 cycles; and included 125 M neutrons in the active cycles used for tallies. The MCNP5 mesh tallies were used to calculate the fission rates in each quarter-assembly. (Individual pin-wise fission rates could have been easily calculated, but that would have led to too many results to display reasonably in tables for this paper.)

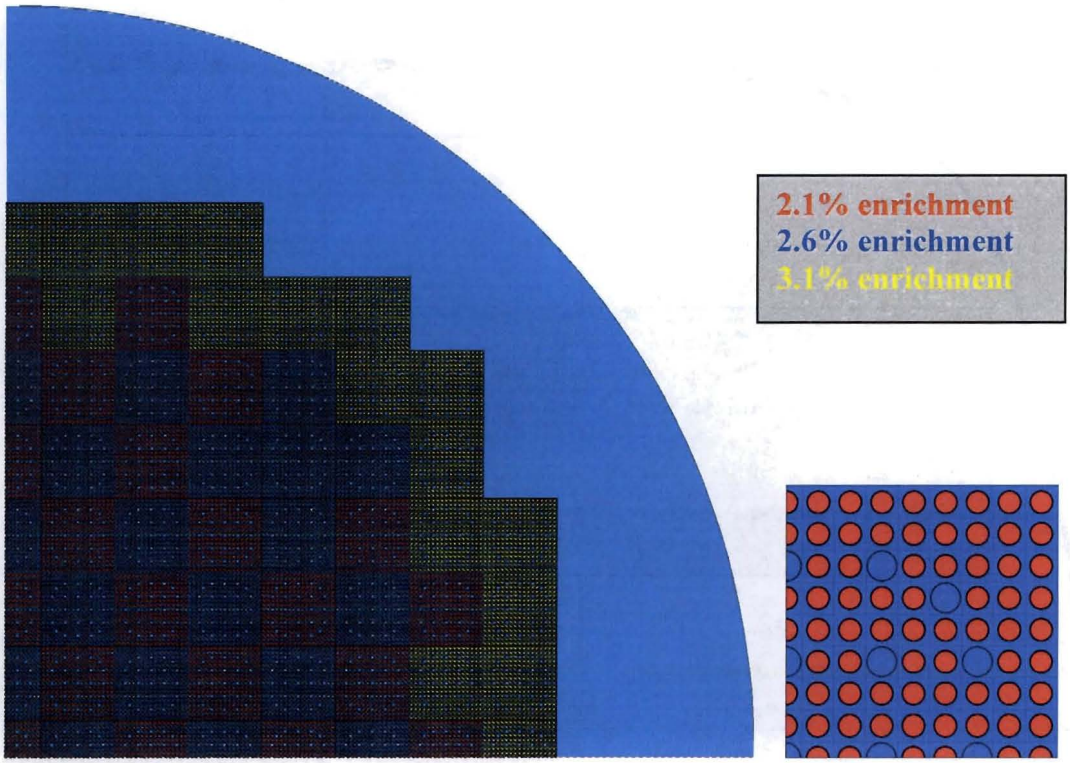

Figure 1. Geometry for MCNP5 calculations of 2D quarter-core PWR model, with detail for the center quarter-assembly

3.1. Convergence

As shown in Section 2.1, the number of cycles required for convergence of k_{eff} and the fission source distribution depends on the dominance ratio for the problem and the selection of the initial guess for the fission source distribution. Problems with dominance ratios close to 1 require more cycles to converge. For a given problem, choosing the initial fission source distribution closer to the actual fundamental mode distribution reduces the number of cycles required for convergence. For the 2D quarter-core PWR example problem, Figure 2 shows the convergence behavior of both k_{eff} and H_{src} for several initial source guesses: (A) a single point at the center of the center quarter-assembly, (B) points at the center of each quarter assembly along the problem diagonal, and (C) a uniform source throughout the core region. These problems were run with 20,000 neutrons/cycle, and a 5 x 5 mesh covering the core region was used for computing H_{src}. It can be seen in Figure 2 that plots of k_{eff} vs cycle are not useful in assessing convergence for this problem; k_{eff} converges in only a few cycles. For H_{src}, source guess (A) is the poorest choice and requires about 100 cycles to converge; source guess (B) is better, but still not representative of the converged source, and requires about 50 cycles to converge; source guess (C) is reasonably

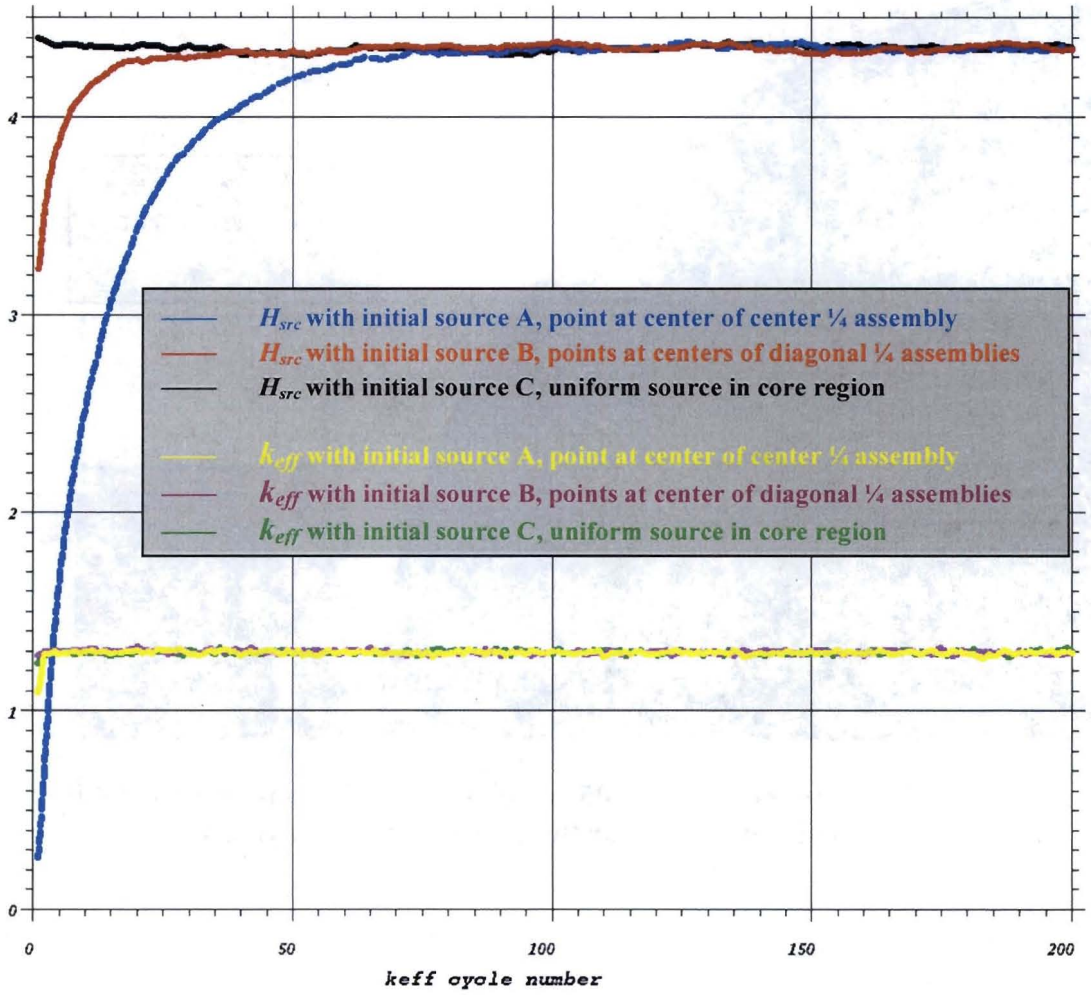

Figure 2. Convergence plots of H_{src} and k_{eff} for 2D quarter-core PWR problem

close to the converged source and requires about 40 cycles to converge. Note that this behavior - k_{eff} converging sooner than H_{src}, is consistent with Eqs. (5) and the discussion in Section 2.1. It should also be noted that the convergence behavior of k_{eff} and H_{src} does not depend on the number of cycles run (N) or on the number of neutrons per cycle (M_0). That is, running a problem with more neutrons per cycle does not cause a problem to converge faster.

For all subsequent calculations for this example problem, the initial source guess is taken to be uniform throughout the core region (source C), and the initial 50 cycles are discarded before beginning tallies.

3.2. Bias in Results for k_{eff} and Reaction Rate Distributions

As discussed in Section 2.2, results for k_{eff} and reaction rate tally distributions exhibit a bias if the number of neutrons per cycle is chosen too small. The "rule-of-thumb" for experienced Monte

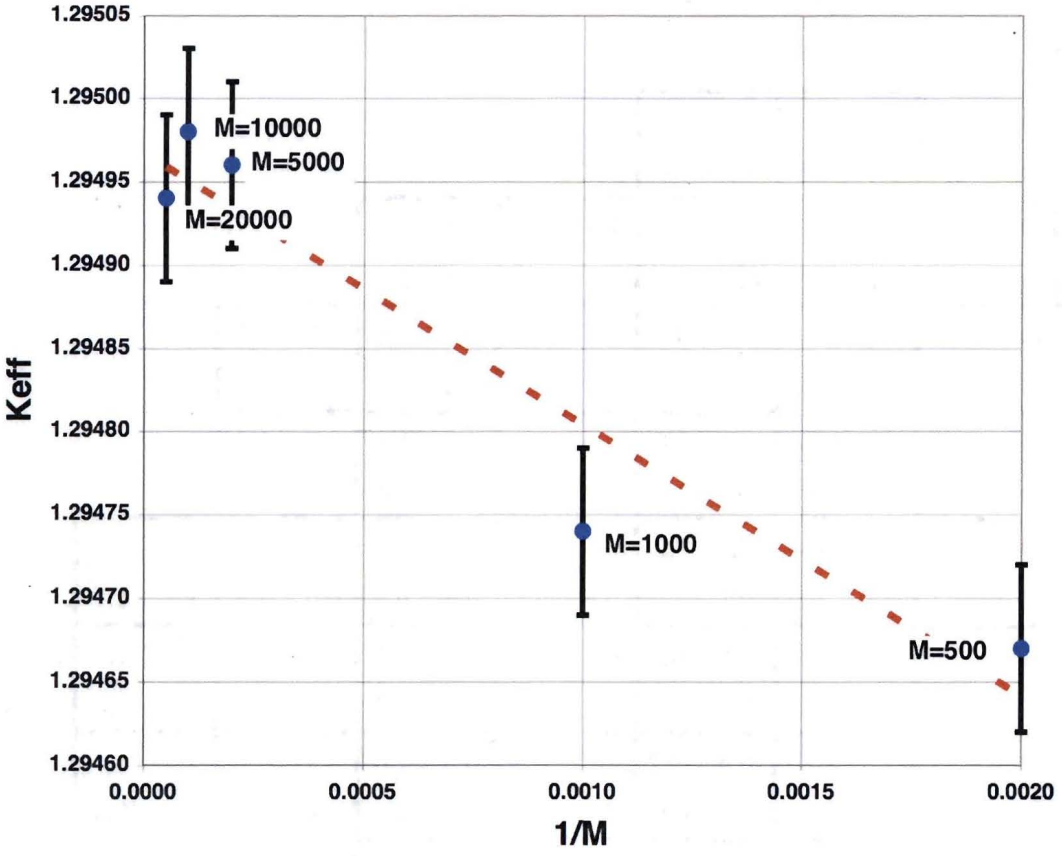

Figure 3. Keff vs M for 2D quarter-core PWR problem (M = neutrons/cycle)

Carlo practitioners has been that 10s or 100s of neutrons per cycle would result in noticeable bias, while several 1000s of neutrons per cycle would be adequate. For the 2D quarter-core PWR example, Figure 3 shows the computed values for k_{eff} using 500, 1000, 5000, 1000, and 20000 neutrons per cycle. For this problem it can be seen that using 500 neutrons per cycle results in a bias of about 30 pcm, and that using 5000 or more neutrons per cycle effectively eliminates the bias in k_{eff}.

Table 1 shows the percent errors in the fission distribution tallies for each of the quarter-assemblies in the problem for the MCNP5 calculation with 500 neutrons per cycle. The bias in the distribution shows a significant tilt, with the inner quarter-assembly fission rates low by up to 1.6% and the outer quarter-assembly fission rates high by up to 3.2%. (The reference for determining the errors in the quarter-assembly fission rates was the ensemble-average of the mesh tallies for 25 independent MCNP5 calculations using 25 M active neutrons each and 20,000 neutrons per cycle.) The bias is significantly larger than the uncertainties on the quarter-assembly fission rates.

Table 1. Percent errors in quarter-assembly fission rates for MCNP calculation for PWR-2D problem using 500 neutrons/cycle

0.0	-0.5	-0.6	-0.2	-0.3	0.5	0.8								
-0.2	-0.7	-0.8	0.1	0.3	0.7	0.6								
-0.5	-0.7	-0.7	0.0	0.3	0.7	1.0	1.3	1.2	1.6	2.0				
-0.1	-0.7	-0.8	0.2	0.3	0.8	1.1	1.2	1.2	1.3	2.4				
-0.4	-0.6	-0.5	0.0	-0.1	0.2	0.7	0.6	1.4	2.0	1.9	2.7	3.2		
-0.7	-0.9	-0.8	-0.4	0.2	0.5	0.4	1.0	1.2	1.6	2.0	1.6	2.6		
-0.6	-0.3	-0.7	-0.6	-0.6	0.3	0.8	1.1	1.2	1.5	1.1	1.7	1.8		
-0.5	-0.8	-1.0	-0.8	-0.5	0.2	0.8	0.9	1.2	1.2	1.4	1.3	1.9		
-0.5	-0.9	-0.8	-1.0	-0.6	0.2	0.2	0.6	0.9	1.1	0.8	0.7	1.1	0.9	1.5
-0.9	-0.9	-1.1	-1.0	-0.9	-0.1	0.2	0.6	0.8	0.6	0.6	0.6	1.3	1.2	1.1
-1.2	-1.3	-1.2	-1.0	-0.6	-0.5	-0.3	0.2	0.9	0.7	1.1	0.9	1.3	1.2	1.1
-1.3	-1.5	-1.0	-0.9	-0.7	-0.5	-0.6	0.3	0.4	0.5	1.3	1.4	2.1	1.9	1.6
-1.7	-1.5	-1.1	-1.1	-0.6	-0.5	-0.2	-0.1	0.3	0.6	1.0	1.7	2.0	2.1	1.9
-1.5	-1.5	-1.4	-1.0	-1.1	-0.8	0.0	0.1	0.3	0.4	1.0	1.0	1.5	3.1	2.3
-1.6	-1.6	-1.2	-1.2	-0.6	-0.7	-0.4	-0.2	0.1	0.2	0.5	1.6	2.1	2.4	2.3

RMS error = 1.1 %
MCNP std deviations: .1% - .3%
True std deviations: .3% - .8%

The biases in the fission distribution are smaller when 1000 neutrons per cycle are used, and smaller still with 5,000 or 10,000 neutrons per cycle. Figure 4 is a plot of the fission tallies in the quarter-assemblies along the diagonal of the problem, showing how the biases in the fission tallies are reduced as the number of neutrons per cycle is increased.

3.3. Bias in Uncertainties for k_{eff} and Reaction Rate Distributions

As discussed in Section 2.3, the uncertainties computed for k_{eff} and reaction rate tally distributions exhibit a bias due to inter-cycle correlation effects that are neglected when performing the Monte Carlo code tallies. The computed uncertainties are always smaller than the true uncertainties for a tally, regardless of the number of cycles run or the number of neutrons per cycle. For the 2D quarter-core PWR problem, Table 2 gives the ratios of the true uncertainty to the MCNP5-calculated uncertainty for each of the quarter-assembly fission rate tallies. For

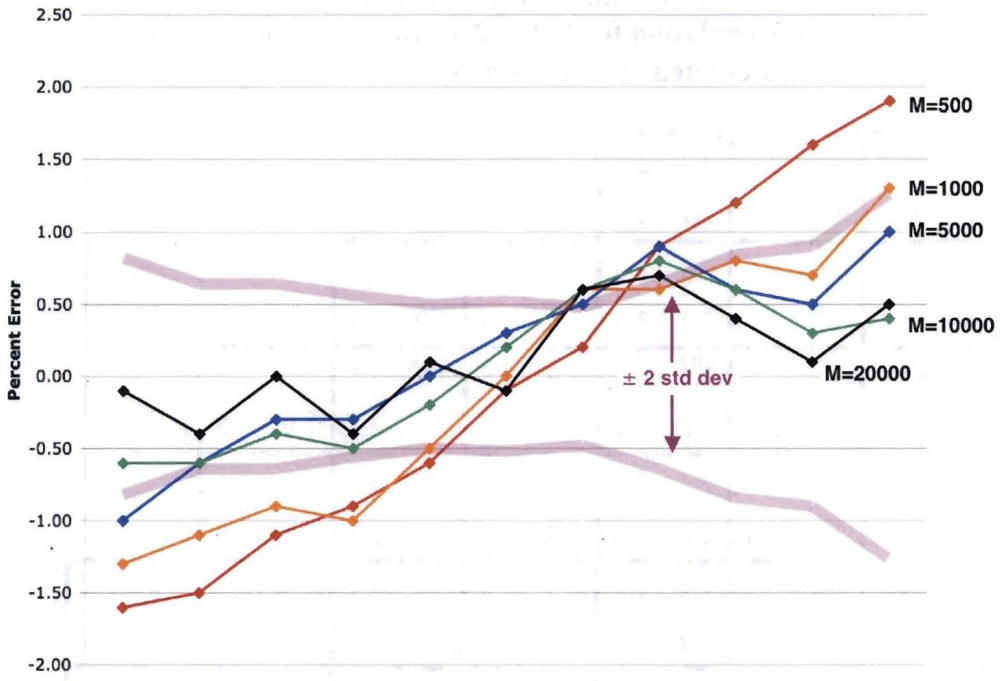

Figure 4. Percent error in fission rates along diagonal, for 2D quarter-core PWR problem (M = neutrons/cycle)

this problem, the true uncertainties were calculated by running 25 independent MCNP5 calculations, and then computing the statistics directly from the ensemble of results [16].

It can be seen from Table 2 that the MCNP5-calculated uncertainties are 1.7 to 4.7 times smaller than the true uncertainties, and 3.1 times smaller than the true uncertainties on average. This is a very significant underprediction bias – in order to reduce the true uncertainties to a specified value, about 10 times as many neutrons must be run as indicated by the MCNP5-computed uncertainties. For problems with dominance ratios even closer to 1, the underprediction bias in uncertainties may be much larger; for problems with smaller dominance ratios, the bias should be smaller.

At present, there is no easy means of overcoming the underprediction bias in the computed uncertainties from Monte Carlo criticality calculations. While there is evidence that modifications to the iteration procedure, such as the superhistory method in MONK [14] and Wielandt's method under development for MCNP5 [18,19] can reduce or eliminate the underprediction bias in uncertainties, these methods are not available yet to general MCNP5 or SCALE/KENO users. A brute-force method for assessing the true uncertainties can be carried out: Make 25 or so independent Monte Carlo criticality calculations, discarding the uncertainties from the individual calculations, and compute the true uncertainties from the ensemble of results from the 25 runs.

Table 2. True relative errors in quarter-assembly fission rates for MCNP calculation for PWR-2D problem, as multiples of MCNP-calculated relative errors, $\sigma_{TRUE} / \sigma_{MCNP}$

3.4	3.1	2.7	2.7	2.6	2.3	2.7								
3.3	3.7	3.6	3.7	3.7	2.7	2.9								
3.8	3.8	3.9	4.0	3.6	3.3	3.0	2.9	2.5	2.5	2.2				
3.8	3.9	4.2	3.3	3.5	3.4	3.2	3.6	3.0	3.0	2.8				
3.9	3.6	3.5	3.3	3.4	3.4	4.0	3.9	3.5	3.2	3.1	2.5	1.7		
4.1	3.8	3.5	3.2	2.9	2.6	2.9	3.2	3.1	2.8	2.7	1.9	1.7		
3.4	3.4	3.2	3.5	2.6	2.4	2.6	3.0	2.9	2.9	2.8	2.3	2.1		
4.2	3.5	3.4	3.1	2.7	2.3	2.0	2.4	2.5	2.5	2.1	2.3	2.3		
3.9	3.6	3.1	2.9	2.3	1.9	1.9	2.3	2.4	2.9	2.7	2.7	2.2	2.8	2.3
3.7	3.3	3.6	2.4	2.2	2.2	2.5	1.8	2.2	2.6	2.7	2.9	2.5	2.4	2.5
3.0	3.1	3.0	2.2	2.2	2.1	2.4	2.5	2.4	2.6	2.7	2.6	2.7	3.0	2.6
2.9	3.7	3.3	2.6	2.5	2.8	3.0	2.9	3.5	3.2	3.3	3.1	3.1	3.2	3.3
3.2	3.1	2.9	3.1	3.2	3.3	3.5	3.5	3.6	3.9	3.7	3.9	3.5	3.4	2.9
3.4	3.0	3.1	3.6	3.4	3.5	3.9	3.7	4.0	4.3	4.0	4.3	3.8	4.2	3.5
3.5	3.2	2.8	3.5	3.8	3.9	3.9	3.9	4.1	4.1	4.6	4.4	4.7	4.5	3.8

Average factor = 3.1

4. CONCLUSIONS

Section 2 reviewed the theory and limitations of Monte Carlo criticality calculations. Section 3 provided a realistic example of the effects of convergence, bias in keff and reaction rate distributions due to the number of neutrons per cycle, and underprediction of uncertainties due to the neglect of correlation effects. From the theory in Section 2 and the numerical evidence in Section 3, the following recommendations may be made to practitioners:

- Before performing long-running Monte Carlo criticality calculations, always review the code input thoroughly and view the problem geometry in a plotter to be sure it is correct.

- To determine the number of cycles needed for convergence of the power iteration method, always make a trial run using ~100 cycles and a moderate number of neutrons per cycle (e.g., 1000). Examine plots of both k_{eff} and H_{src} vs cycle to determine the number of cycles to be discarded before beginning tallies.

- To prevent bias in k_{eff} and reaction rate tallies, at least 5000 or more neutrons per cycle should be used for long production runs. It is preferable to use 10,000, 20,000, 50,000, or more neutrons per cycle, as long as a few hundred active cycles are computed.

- In assessing the uncertainties on computed results, be aware that the true uncertainties may be higher by factors of 5 or more, especially if the dominance ratio is close to 1. It may be helpful to make independent Monte Carlo runs and compare the results and uncertainties from each. It can also be useful to compare the results and uncertainties for different tallies in symmetric locations of a problem, as an indication of how good the computed uncertainties are.

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