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A REVIEW OF BEST PRACTICES FOR MONTE CARLO CRITICALITY CALCULATIONS

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Monte Carlo methods have been used to compute k_{eff} and the fundamental mode eigenfunction of critical systems since the 1950s. While such calculations have become routine using standard codes such as MCNP and SCALE/KENO, there still remain 3 concerns that must be addressed to perform calculations correctly: convergence of k_{eff} and the fission distribution, bias in k_{eff} and tally results, and bias in statistics on tally results. This paper provides a review of the fundamental problems inherent in Monte Carlo criticality calculations. To provide guidance to practitioners, suggested best practices for avoiding these problems are discussed and illustrated by examples.

I. INTRODUCTION

Monte Carlo methods have been used to compute k_{eff} and the fundamental mode eigenfunction of critical systems since the 1950s [Refs. 1-4]. While such calculations have become routine using standard codes (e.g., MCNP [Ref. 5], SCALE/KENO [Ref. 6]), there remain 3 principal concerns 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 statistics on k_{eff} and reaction rate tallies must be recognized and dealt with.

Unfortunately, the user manuals and tutorials provided with standard Monte Carlo codes provide little or no discussion of these 3 concerns. Theoretical papers from the 1960s - 1980s do not provide practical examples showing the magnitude of the difficulties, and provide little or no practical guidance to code users. This paper provides a brief review of the 3 concerns, illustrating each with realistic practical examples. Guidance for users is offered as recommended “best practices.”

I.A Criticality Calculations and the Power Method

The k-eigenvalue transport equation in standard form

$$\begin{aligned} [\Omega \cdot \nabla + \Sigma_t(\vec{r}, E)] \Psi(\vec{r}, E, \Omega) = & \iint \Psi(\vec{r}, E', \Omega') \Sigma_s(\vec{r}, E' \rightarrow E, \Omega \cdot \Omega') d\Omega' dE' \\ & + \frac{1}{k_{eff}} \frac{\chi(E)}{4\pi} \iint v \Sigma_f(\vec{r}, E') \Psi(\vec{r}, E', \Omega') d\Omega' dE' \end{aligned} \quad (1)$$

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

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

Equation (3) may be solved numerically using the standard power iteration method^{5,6}

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

Most Monte Carlo codes use the standard power method for solving k-eigenvalue problems^{7,8}, 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.

I.B. Example Problem Descriptions

To illustrate the computational concerns and to provide guidance to practitioners, 2 realistic, practical problems are used: a detailed 2D quarter-core PWR model (Fig. 1) and a 3D array of steel cans filled with plutonium nitrate solution (Fig. 2). All of the calculations discussed below were performed with MCNP5 (version 1.51) using the new ENDF/B-VII continuous-energy data libraries on a Mac Pro (dual quad-core Xeons, 8 cpus total).

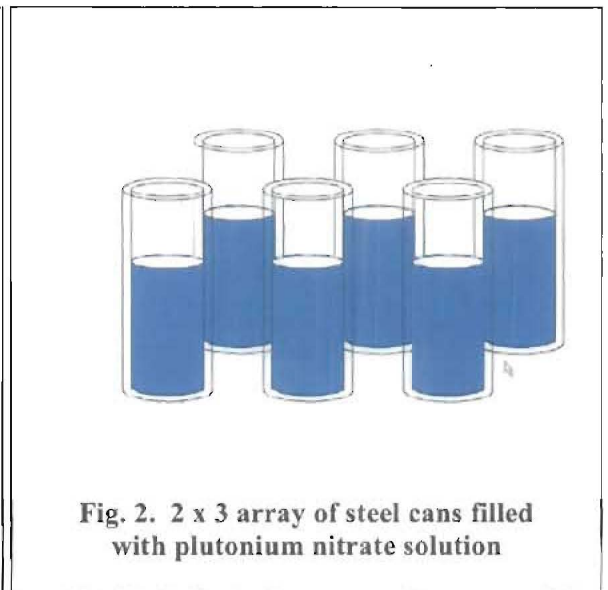
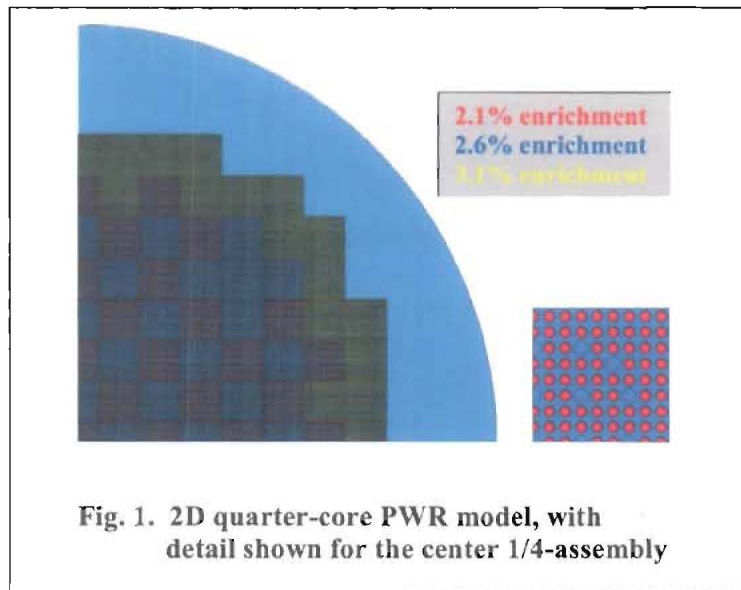
The PWR model has explicit representation of every fuel pin and water tube. This example is based on the specifications given by Nakagawa and Mori⁹ for a 3D whole-core model. In the current 2D quarter-core example, there are 48 1/4 fuel assemblies (each with a 17x17 lattice arrangement), 12,738 fuel pins with cladding, and 1206 1/4 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 $\rho=.96$.

The 2x3 array of steel cans containing plutonium nitrate solution is a simplified version of the problem described in Chapter 5 of the MCNP Criticality Primer¹⁰. There are six stainless steel cylinders arranged in a 2x3 array with a 10 cm separation between cylinders. For simplicity, no external walls or features are included.

II. CONVERGENCE OF THE POWER METHOD

II.A Background

Concerning the relative convergence of k_{eff} and the fission source distribution during the power iteration process, if the initial guess for $\Psi^{(0)}$ is expanded in terms of the eigenvectors $\vec{u}_j$ of Eq. (3), substituted into Eq. (4),



and rearranged with some straightforward algebra, then

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

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 convergence of both the fission source distribution and k_{eff} , not just that of k_{eff} .

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 method¹¹. 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.

The Shannon entropy of the fission source distribution, H_{src} [Refs. 12-14], 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.

II.B Numerical Examples

As discussed in Section II.A, the number of cycles required for convergence of k_{eff} and the fission source distribution depends on the dominance ratio for the problem and on 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 quarter-core PWR example problem, Figure 3 shows the convergence behavior of both k_{eff} and H_{src} for several initial source guesses: a single point at the center of the center quarter-assembly, points at the centers of each quarter assembly along the problem diagonal, and a uniform source throughout the core region. For the 2x3 array of cans, Figure 4 shows the convergence behavior of both k_{eff} and H_{src} for several initial source guesses: a single point at the center of the solution in the front left can, points at the centers of the solution in each of the cans, and a uniform distribution of source points in the solution in each of the cans.

It can be seen in Figures 3 and 4 that plots of k_{eff} vs cycle are not always useful in assessing convergence for these 2 problems; k_{eff} converges in only a few cycles. For H_{src} , source guesses with single points are the poorest choice, requiring 50 to 100 cycles to converge; source guesses at a number of single points are better, but still not representative of the converged source; source guesses distributed uniformly in fissionable regions are reasonably close to the converged sources, and require about 40 cycles for the PWR problem to converge and only 5-10 cycles for the array of cans to converge. Note that this behavior - k_{eff} converging sooner than H_{src} - is consistent with Eqs. (5) and the discussion in Section II.A. 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.

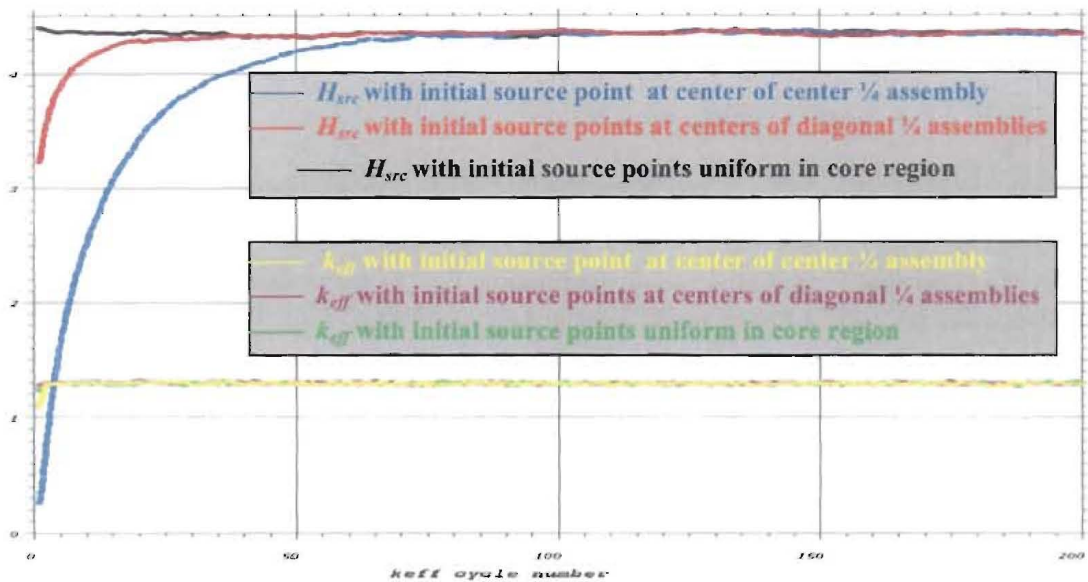
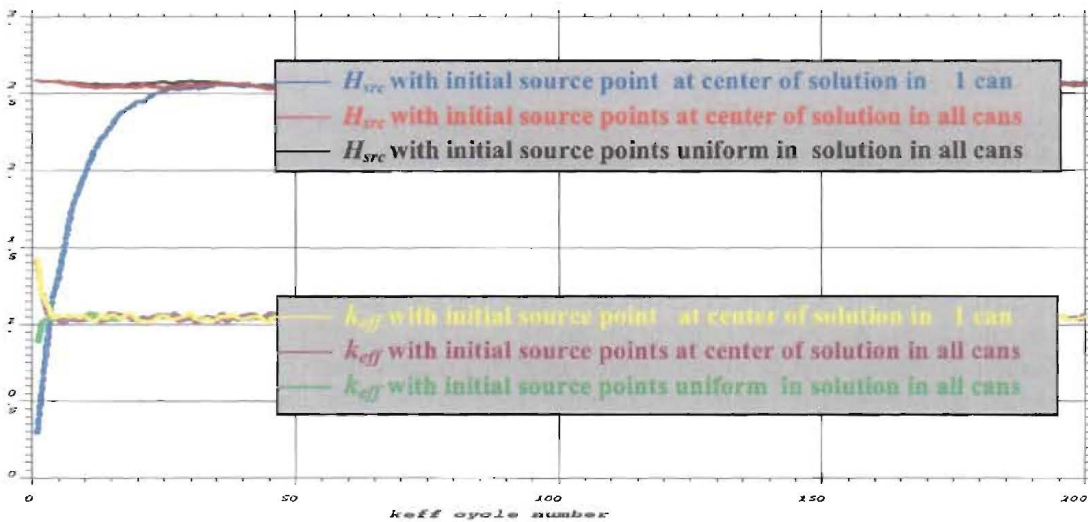


Figure 3. Convergence plots of H_{src} and k_{eff} for quarter-core PWR problem



II.C. Best Practices

For the initial source guess in a criticality calculation, choose a uniform distribution in all fissionable regions of the problem. If only a one or a few source points are used, more cycles will be needed to assure convergence.

For applications where only k_{eff} is sought, examine plots of k_{eff} vs. cycle to determine the proper number of cycles to discard before beginning the k_{eff} tally. For applications where local tallies are required (e.g., local reaction rates, foil measurements, dose fields, fission distributions, etc.) in addition to k_{eff} , examine plots of both k_{eff} vs. cycle and H_{src} vs. cycle to determine the proper number of cycles to discard before beginning the tallies. Be sure that final production runs are made using at least that many discarded cycles; using fewer discarded cycles can bias the results.

III. BIAS IN RESULTS FOR K_{EFF} AND REACTION RATE DISTRIBUTIONS

III.A. Background

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 $E[M_1] = k_{eff} \cdot M_0$. 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^{15,16}. The bias in k_{eff} has been shown to be

$$\Delta k = -\frac{\sigma_k^2}{k_{eff}} \cdot \sum_{j=1}^{\infty} r_j \propto \frac{1}{M_0}, \quad (7)$$

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.

III.B. Numerical Examples

As discussed in Section III.A, 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 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 quarter-core PWR example, Figure 5 shows the computed values for k_{eff} using 500, 1000, 5000, 10000, 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} .

Figure 6 shows the computed values for k_{eff} for the array of cans using 100, 200, 500, 1000, 5000, 10000, and 20000 neutrons per cycle. For this problem it can be seen that using 100 or 200 neutrons per cycle results in a bias of about 200 pcm, and that using 1000 or more neutrons per cycle effectively eliminates the bias in k_{eff} . Also shown in Figure 6 is the k_{eff} result (the green point) for the array of cans using 1000 neutrons per cycle, but using an incorrect number of discarded cycles. In that run, only 3 cycles were discarded before beginning the k_{eff} tallies, rather than 25 cycles for the other runs. The bias introduced by beginning the tallies before convergence is significant.

Table 1 shows the percent errors in the fission distribution tallies for each of the quarter-assemblies in the PWR 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. 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 7 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.

III.C. Best Practices

It is recommended that 1000s of neutrons/cycle be used for all calculations. For large reactor or storage vault problems, 10,000 or more neutrons/cycle is preferred. Problems should never be run using 10s or 100s of neutrons/cycle; that would introduce significant bias in both k_{eff} and any local tallies.

IV. BIAS IN UNCERTAINTIES FOR K_{EFF} AND REACTION RATE DISTRIBUTIONS

IV.A. Background

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 cycles¹⁷. While such correlation

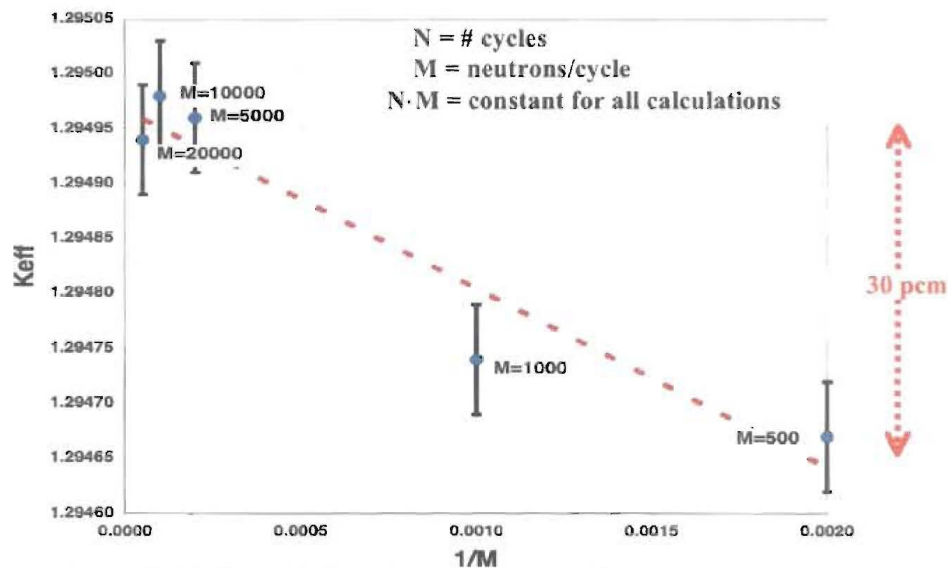


Figure 5. K_{eff} vs $1/M$ for PWR example, M =neutrons/cycle

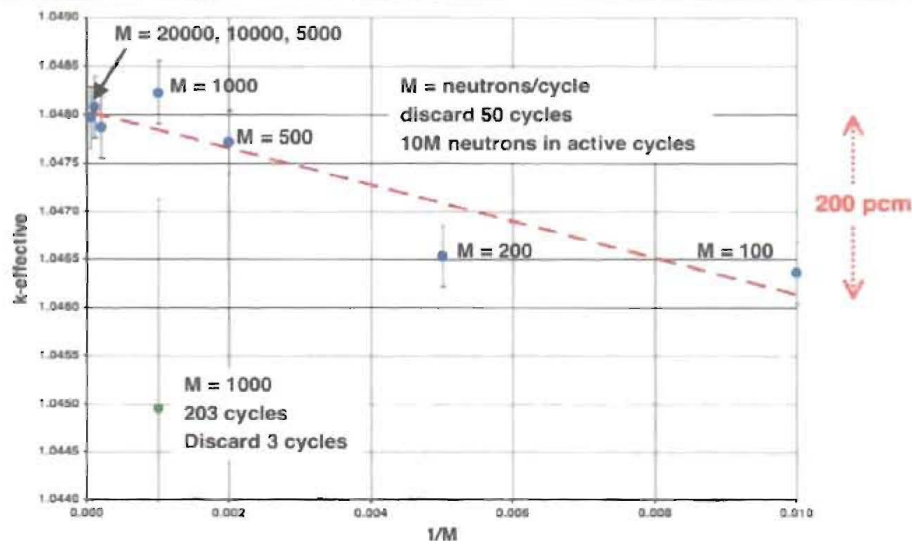


Figure 6. K_{eff} vs $1/M$ for array of cans example, M =neutrons/cycle

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%

does not affect the average results for k_{eff} and local tallies, it can produce significant errors in the computed uncertainties^{15,16,18}. 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:

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

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

$$\sigma_{\bar{X}}^{true} = \sigma_{\bar{X}} \cdot \sqrt{1 + 2 \cdot \sum_{j=1}^{(\infty)} r_j} \quad (9)$$

where $r_J = \text{lag-}J$ 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: $\sigma_{\bar{X}} < \sigma_{\bar{X}}^{\text{true}}$. 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.

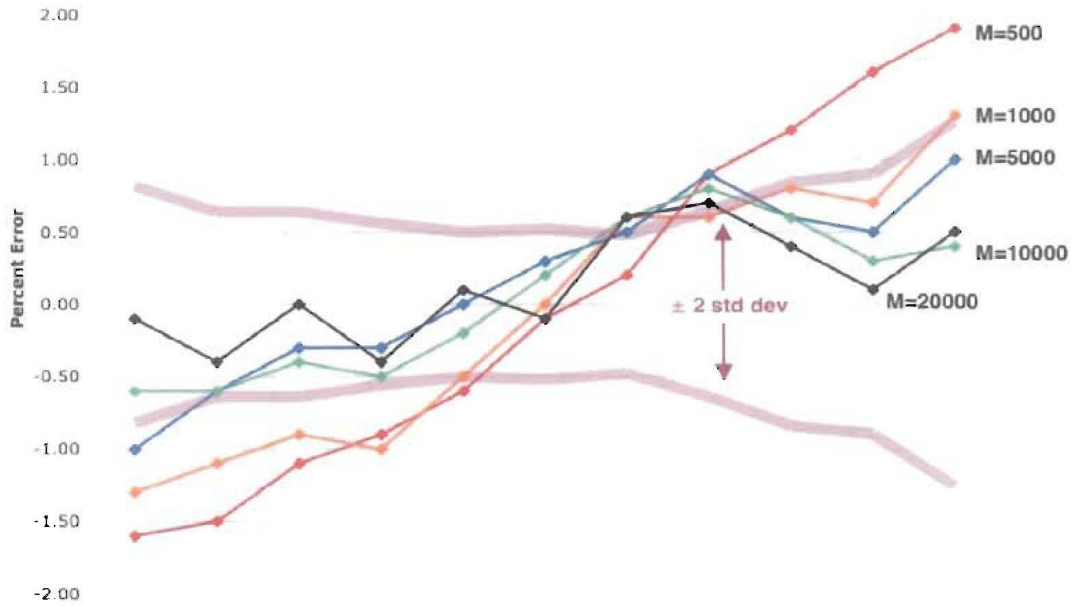


Figure 7. Percent error in fission rates along diagonal, for quarter-core PWR problem (M = neutrons/cycle)

IV.B. Numerical Results

As discussed in Section IV.A, 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 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 this problem, the true uncertainties were calculated by running 25 independent MCNP5 calculations, and then computing the statistics directly from the ensemble of results¹⁸.

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.

IV.C. Best Practices

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 [Ref. 16] and Wielandt's method under development for MCNP5 [Ref. 19,20] 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.

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

While no significant bias in the statistics of keff has been observed, Monte Carlo code users must be aware that localized tallies (e.g., measurement foil absorption, dose rates, heating rates, fission distributions, etc.) may show significant underprediction of the statistics; the true statistics may be factors of 2-5 or more times larger than what the codes report.

V. CONCLUSIONS

Sections I-IV reviewed the theory and limitations of Monte Carlo criticality calculations; provided realistic examples 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; and recommended best practices for Monte Carlo practitioners. These best practices are summarized below:

- 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.

- To improve convergence and reduce the bias in uncertainties, always take advantage of symmetry in the problem geometry. If symmetry permits, using a $1/8^{\text{th}}$ -core or $1/4$ -core geometry model with reflecting or periodic planar boundaries rather than a full-core model will reduce the problem dominance ratio (due to the elimination of several higher radial modes).
- 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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