On the Use of Shannon Entropy of the Fission Distribution for Assessing Convergence of Monte Carlo Criticality Calculations

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Abstract

Monte Carlo calculations of k-eigenvalue problems are based on a power iteration procedure. To obtain correct results free of contamination from the initial guess for the fission distribution, it is imperative to determine when the iteration procedure has converged, so that a sufficient number of the initial batches are discarded prior to beginning the Monte Carlo tallies. In this paper, we examine the convergence behavior using both theory and numerical testing, demonstrating that k_{eff} may converge before the fission distribution for problems with a high dominance ratio. Thus, it is necessary to assess convergence of both k_{eff} and the fission distribution to obtain correct results. To this end, the Shannon entropy of the fission distribution has been found to be a highly effective means of characterizing convergence of the fission distribution. The latest version of MCNP5 includes new capabilities for computing and plotting the Shannon entropy of the fission distribution as an important new tool for assessing problem convergence. Examples of the application of this new tool are presented for a variety of practical criticality problems.

KEYWORDS: Monte Carlo, k_{eff}, convergence, Shannon entropy, MCNP

1. Introduction

Monte Carlo calculations of k-eigenvalue problems are based on a power iteration procedure [1,2], where single-generation random walks are carried out for a "batch" of neutrons to estimate k_{eff} and the next-generation fission distribution. The iteration process is repeated until the fission distribution has converged, at which point any previous results are discarded, tallies are started, and the iteration process is continued until acceptably small statistical uncertainties are obtained. To obtain correct results, free of contamination from the initial guess for the fission distribution, it is imperative to determine when the iteration procedure has converged, so that a sufficient number of the initial batches are discarded. Batches are thus divided into two types: inactive, where the distribution is not yet converged, and active, where stationarity has been reached and Monte Carlo tallies are accumulated. Determining convergence is complicated by the statistical noise inherent in the random walks of the neutrons in each generation; statistical variations in the single-generation estimates of k_{eff} and the fission distribution may be larger than the incremental changes from the power iteration procedure.

The current method to determine convergence in MCNP5 [3] and other codes is to perform a preliminary calculation and assess convergence by post-processing examination of the resulting trends in single-generation k_{eff} estimators. After setting the number of inactive and active cycles, the calculation is then repeated to obtain results. The principal difficulty with this conventional approach is that convergence testing should include both k_{eff} and the fission source distribution, since the fission distribution will converge more slowly than k_{eff}.

In Section 2, the theory of power iteration convergence is examined, to demonstrate the different convergence behavior of k_{eff} and the fission distribution. In Section 3, the Shannon entropy of the fission distribution is defined and discussed in terms of application to Monte Carlo k-eigenvalue calculations. In Section 4, numerical results are presented for assessing the convergence of both k_{eff} and the fission source distribution for several practical problems. Conclusions and recommendations for assessing convergence of criticality problems are presented in Section 5.

2. Convergence of k_{eff} and the Fission Source Distribution

The k-eigenvalue transport equation in standard form

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

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 [1,4]

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

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 u_J of Eq. (1), $\vec{u}_J=1/k_J\cdot F\vec{u}_J$, with $k_0>k_1>k_2>\ldots$, substituted into Eq. (4), and rearranged with some straightforward algebra, then

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

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-ρ) 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}.

3. Shannon Entropy of the Fission Distribution

Recent research into assessing the convergence of the fission source distribution for MCNP5 has involved computing a quantity called the Shannon entropy of the fission source distribution, H_{src} [5-7]. The Shannon entropy is a well-known concept from information theory and provides a single number for each batch to help characterize convergence of the fission source distribution. It has been found that the Shannon entropy converges to a single steady-state value as the source distribution approaches stationarity. Line-plots of Shannon entropy vs. batch are easier to interpret and assess than are 2D or 3D plots of the source distribution vs. batch.

To compute H_{src}, it is necessary to superimpose a 3D grid on a problem encompassing all of the fissionable regions, and then to tally the number of fission sites in a batch that fall into each of the grid boxes. These tallies may then be used to form a discretized estimate of the source distribution, $\{P_J, J=1,N_s\}$, where N_s is the number of grid boxes in the superimposed mesh, and P_J = (number of source sites in J-th grid box)/(total number of source sites). Then, the Shannon entropy of the discretized source distribution for that batch is given by:

$$H_{src} = -\sum_{J=1}^{N} P_J \cdot \ln_2(P_J) \qquad (6)$$

H_{src} varies between 0 for a point distribution to $ln_2(N_s)$ for a uniform distribution. Also note that as P_J approaches 0, $P_J ln_2(P_J)$ approaches 0.

MCNP5 computes and prints H_{src} for each batch of a criticality calculation. Plots of H_{src} vs. batch can also be obtained during or after a calculation, using the built-in plotting capabilities. The user may specify a particular grid to use in determining H_{src} or can let MCNP5 automatically determine a grid which encloses all of the fission sites for the batch. The number of grid boxes will be determined by dividing the number of histories per cycle by 20, and then finding the nearest integers which give that many equal-sized grid boxes, although not fewer than 4x4x4 will be used.

Upon completion of the problem, MCNP5 will compute the average value of H_{src} for the last half of the active cycles, as well as its (population) standard deviation. MCNP5 will then report the first cycle found (active or inactive) where H_{src} falls with one standard deviation of its average for the last half of cycles, along with a recommendation that at least that many cycles should be discarded (inactive). Plots of H_{src} vs. cycle should be examined to further verify the number of inactive cycles that are required for convergence. When running criticality calculations with MCNP5, it is essential that users examine the convergence of both k_{eff} and the fission source distribution (using Shannon entropy). If either k_{eff} or H_{src} is not converged prior to starting the active cycles, then results from the calculations will not be correct.

4. Numerical Results

The convergence behavior of both k_{eff} and the fission source distribution have been examined for many practical criticality problems using MCNP5. One example is shown in Fig. 1, where k_{eff} and H_{src} are plotted vs. batch for a typical 3D ¼-core PWR model. While it is difficult to determine precisely where k_{eff} has converged due to the statistical noise in the k_{eff} plot, a conservative estimate would be about 40 batches. Examining the H_{src} plot, it can be seen that about 70 cycles are required for the 3D fission source distribution to fully converge.

A second example for a 3D whole-core PWR model is shown in Fig. 2. For this example, k_{eff} appears to have converged after about 10 batches, whereas examining H_{src} indicates that it takes about 50 batches for the fission source to converge.

A third example is Benchmark Problem 1 from the OECD/NEA Source Convergence Benchmarks [8]. This problem represents a very large, loosely-coupled array of fuel assemblies in a fuel storage vault. Examining the plots in Fig. 3, it appears that k_{eff} converges almost immediately, whereas it takes about 1500 batches for the fission distribution to converge. Any power distributions or local reaction rates computed for this problem would show serious bias if fewer than 1500 batches were discarded in the Monte Carlo calculation.

5. Conclusions

Based on both theory and numerical testing, it has been demonstrated that k_{eff} may converge before the fission distribution for Monte Carlo criticality problems, especially for those with a high dominance ratio. Thus, it is necessary to assess convergence of both k_{eff} and the fission distribution to obtain correct results. To this end, the Shannon entropy of the fission distribution has been found to be a highly effective means of characterizing convergence of the fission distribution. The latest version of MCNP5 includes capabilities for computing and plotting the Shannon entropy of the fission distribution as an important new tool for assessing problem convergence.

It is highly recommended that both k_{eff} and H_{src} be carefully checked for convergence in all Monte Carlo criticality calculations. The capability to calculate and plot H_{src} should be added to other Monte Carlo codes that are used for criticality calculations.

Figure 1. Convergence plots of k_{eff} and H_{src} vs. batch for a 3D ¼-core PWR

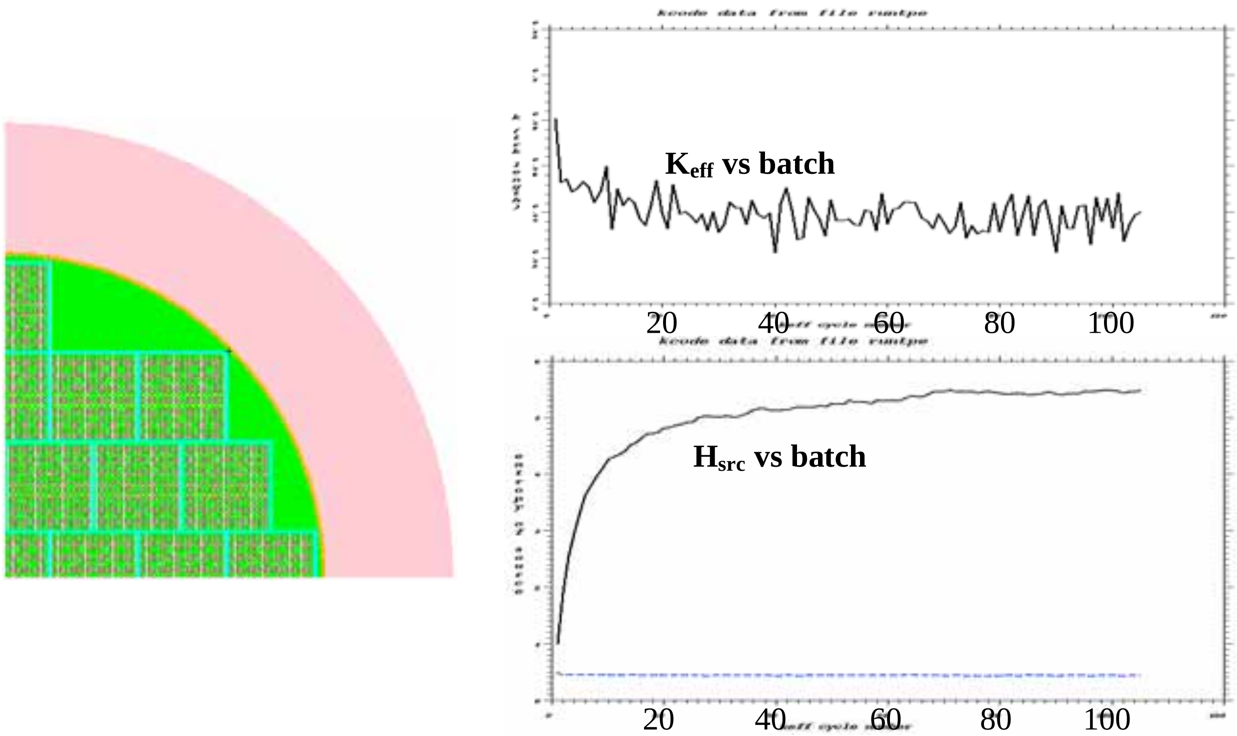


Figure 2. Convergence plots of k_{eff} and H_{src} vs. batch for a 3D whole-core PWR

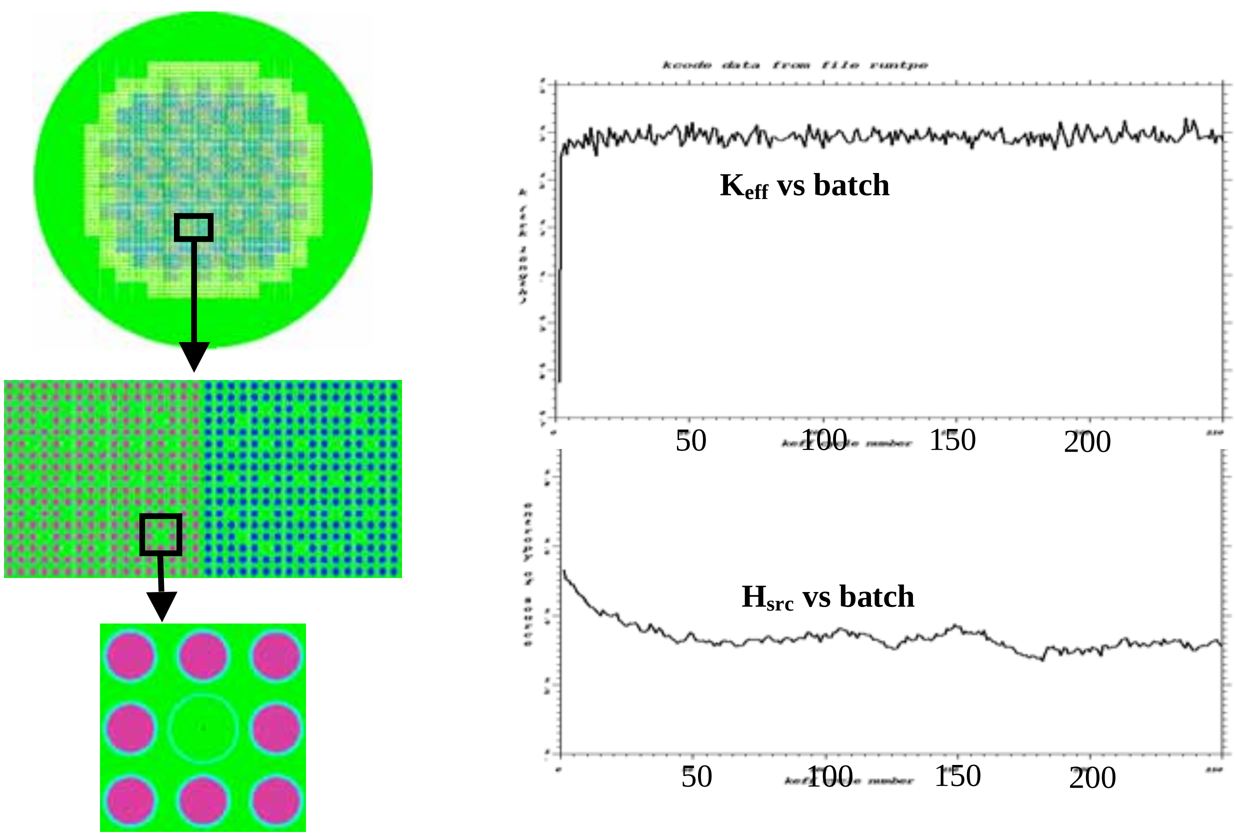
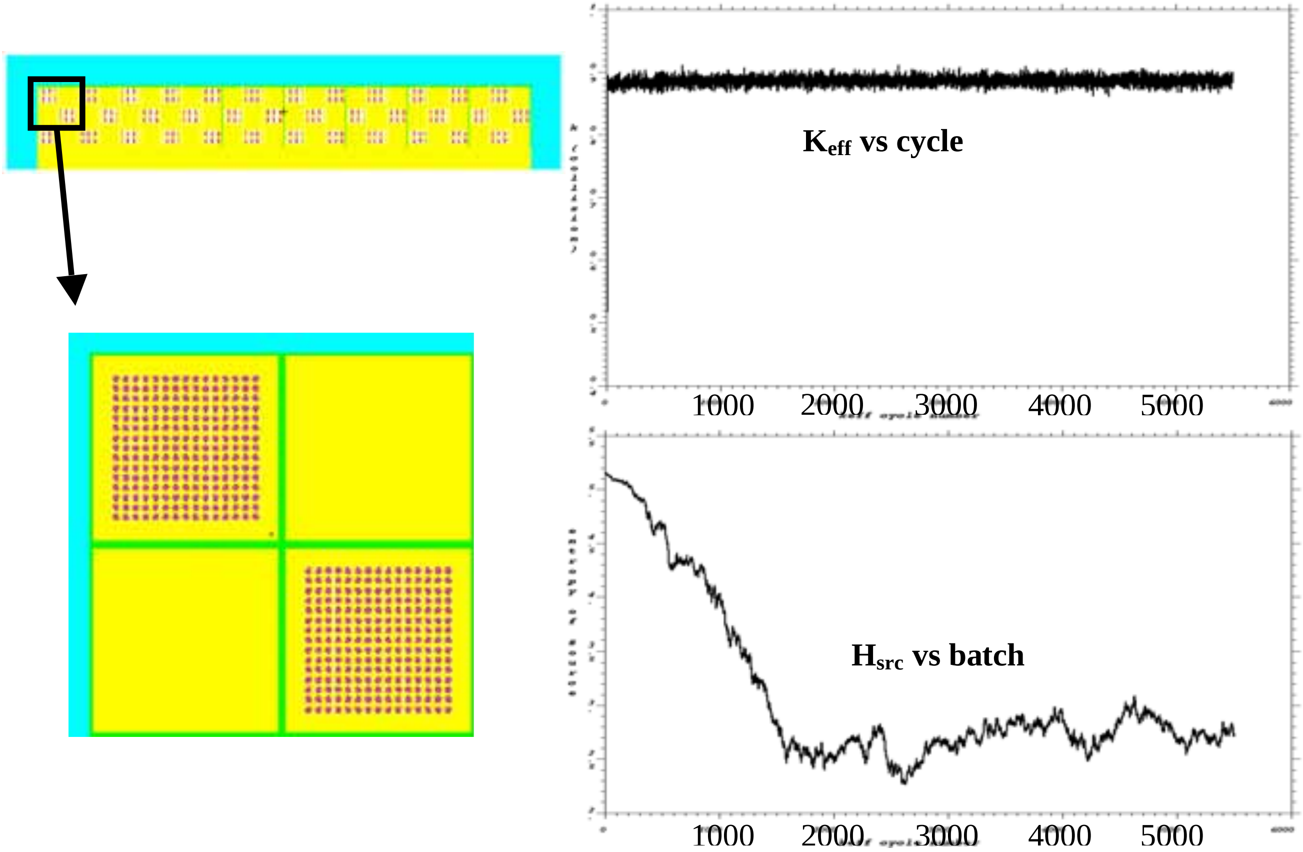


Figure 3. Convergence plots of k_{eff} and H_{src} vs. batch for OECD Benchmark 1



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