LA-UR-07-1123

Title: | Convergence Testing for MCNP5
Monte Carlo Eigenvalue Calculations

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Intended for: | M&C+SNA-2007,
ANS Mathematics & Computation Topical Meeting
Monterey, CA, 15-19 April 2007

Los Alamos
NATIONAL LABORATORY
——— EST.1943 ———

CONVERGENCE TESTING FOR MCNP5 MONTE CARLO EIGENVALUE CALCULATIONS

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ABSTRACT

Determining convergence of Monte Carlo criticality problems is complicated by the statistical noise inherent in the random walks of the neutrons in each generation. The latest version of MCNP5 incorporates an important new tool for assessing convergence: the Shannon entropy of the fission source distribution, H_{src}. Shannon entropy is a well-known concept from information theory and provides a single number for each iteration to help characterize convergence trends for the fission source distribution. MCNP5 computes H_{src} for each iteration, and these values may be plotted to examine convergence trends. Convergence testing should include both k_{eff} and H_{src}, since the fission distribution will converge more slowly than k_{eff}, especially when the dominance ratio is close to 1.0.

Key Words: Monte Carlo, criticality, Shannon entropy, MCNP

1. INTRODUCTION

Monte Carlo-based criticality calculations make use of the basic numerical method called power iteration [1,2]. 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. Upon convergence, tallies are started and iterations continued until statistical uncertainties become small enough.

Determining convergence of Monte Carlo criticality problems is complicated by the statistical noise inherent in the random walks of the neutrons in each generation. In the early years of Monte Carlo criticality calculations (roughly, from the 1950s through the 1970s), computers

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were slow enough that most calculations sought results just for k_{eff} and did not compute detailed power distributions. As a result, nearly all computational tools for assessing convergence were based on the trends in k_{eff} as a function of the number of iterations. 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. Unfortunately, most Monte Carlo codes still assess convergence only using k_{eff}, without examining convergence of the source distribution. This practice can lead to significant errors in the computed power distributions, since the source distribution will converge more slowly than k_{eff} [1,3,4].

Recent research into the convergence of Monte Carlo criticality calculations [4-7] has established that the Shannon entropy of the fission source distribution, H_{src}, is an effective diagnostic indicator. In 2006, the MCNP5 Monte Carlo code [8] was enhanced to compute and plot H_{src} as a function of iteration to assess the convergence of the fission source distribution [3]. In this paper, we review the theory of H_{src} and convergence, examine the behavior of H_{src} for different iteration schemes, and investigate candidate techniques for automated convergence testing.

2. THEORY FOR CONVERGENCE AND SHANNON ENTROPY

It can be readily shown [1,3,4] that k_{eff} and the fission source distribution will converge during power iteration as

$$\Psi^{(n+1)}(\vec{r}) = \vec{u}_0(\vec{r}) \ + \ \tfrac{a_1}{a_0}\rho^{n+1}\cdot\vec{u}_1(\vec{r}) \ + \ ...$$

$$(1)$$

$$k_{eff}^{(n+1)} = k_0\cdot\left[1 \ - \ \tfrac{a_1}{a_0}\rho^n(1-\rho)g_1 \ + \ ...\right]$$

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. (1) 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}.

Shannon entropy is a well-known concept from information theory and provides a single number for each iteration 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. iteration. The Shannon entropy of the discretized source distribution for an iteration is given by:

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

$$(2)$$

where N is the number of tally bins for the source distribution, and P_J is the fraction of the source distribution occurring in bin J. That is, P_J is found by integrating $\Psi^{(n+1)}$ from Eq. (1) over the volume of tally bin J. H_{src} varies between 0 for a point distribution to $ln_2 N$ for a uniform distribution. Also note that as P_J approaches 0, $P_J ln_2 P_J$ approaches 0.

3. NUMERICAL RESULTS: H_{src} FOR DIFFERENT ITERATION STRATEGIES

For a given iteration, determining H_{src} from Eq. (2) involves choices for the number and configuration of spatial tally bins, and for the number of neutrons followed per iteration. To determine the effects of these choices on assessing convergence using H_{src}, four different criticality test problems were used. These test problems were run with different numbers of neutrons per iteration to determine confidently when k_{eff} and H_{src} had converged, and then were repeated using different numbers and sizes of spatial tally bins for Eq. (2).

Figure (1) provides an example of increasing the number of spatial bins used in computing H_{src}. The test problem was Benchmark 3 from the OECD/NEA benchmarks for source convergence [9], with slabs of 18 cm of fuel on the left, 20 cm of water in the middle, and 20 cm of fuel on the right. Using 100 or 1000 bins in computing H_{src} results in convergence plots which are easy to interpret. Using a very large number of bins, 10000 or more, leads to a loss of detail and makes it more difficult to assess convergence. Other test problems show similar results. It is thus recommended that a few dozen or hundred bins be used, rather than many thousands, in computing H_{src}.

Figure (2) shows the behavior of H_{src} for a 2D vs 3D layout of the spatial tally bins for a standard MCNP test problem (*inp24*, [8]) that represents a 3D , ¼ core PWR. Using a 2D binning arrangement for computing H_{src}, where the z-dependence is integrated out, results in seemingly faster convergence of H_{src}, compared to the 3D binning where the axial variations affect H_{src}. However, since both runs had exactly the same Monte Carlo distribution of source points in each cycle, hence the same actual convergence behavior of the source distribution, it is clear that 3D binning should be used for computing H_{src} for 3D problems. Using a 2D binning for a 3D problem can give an incorrect assessment of convergence.

Figure 1. H_{src} convergence for different numbers of spatial tally bins
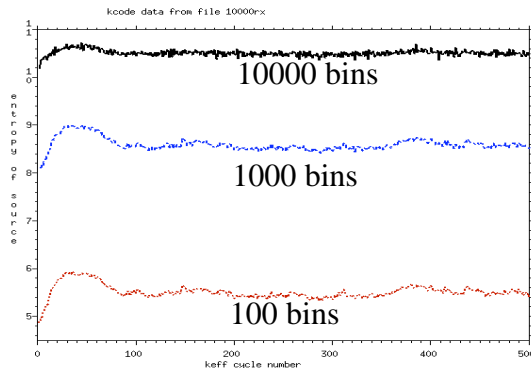

Figure 2. H_{src} convergence for 2D vs 3D spatial tally bins

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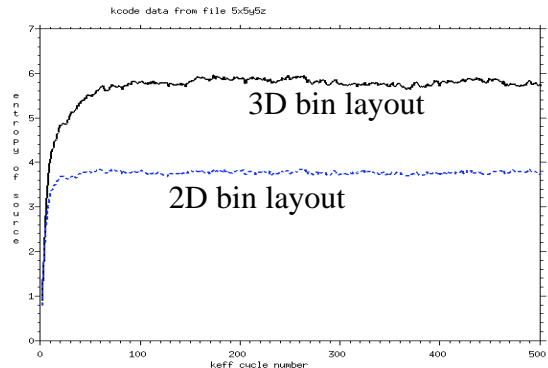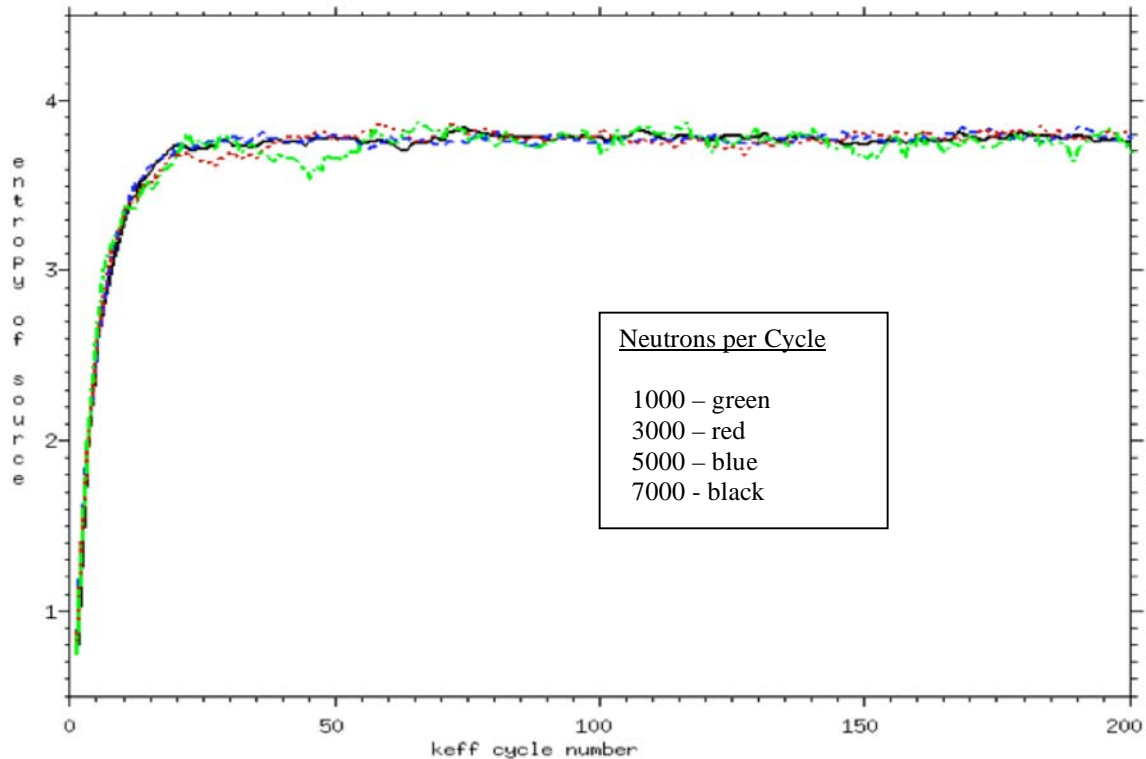
3/7

Figure 3. H_{src} convergence for different numbers of particles per cycle
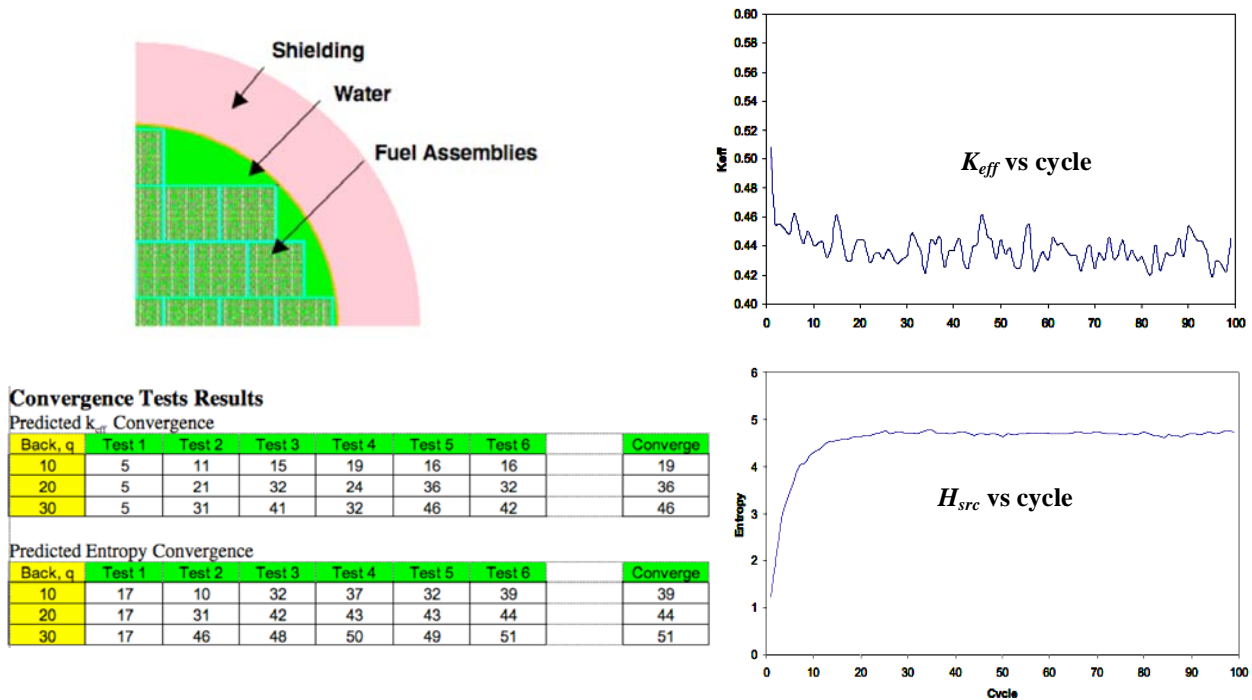

Figure (3) shows the behavior of H_{src} for the 3D MCNP test problem *inp24* when different numbers of neutrons per cycle are used with a fixed grid for the H_{src} computation. Since convergence does not depend on the number of neutrons per cycle, H_{src} converges to the same value, independent of the number of neutrons per cycle. With smaller numbers per cycle, however, more noise is present in the H_{src} plots, making it more difficult to assess convergence.

4. NUMERICAL RESULTS: CONVERGENCE TESTING USING H_{src}

To investigate the feasibility of completely automating the determination of convergence, six different convergence tests were created and applied to both k_{eff} and H_{src} in MCNP5 criticality calculations for five different test problems. The goal was to enable MCNP to determine the iteration at which convergence is reached for both k_{eff} and H_{src}. This series of tests was successful in all but the most difficult cases, i.e. problems with a very high dominance ratio. The six tests were as follows:

- Check if value has not increased/decreased 5 times in a row
- Check if average of previous q values has not increased/decreased 5 times in a row
- Check if slope of previous q values has not changed sign
- Check if slope of previous q values is zero within t-statistic test
- Check rate of change of average of previous q values is < 0.001
- Normality check over previous q values, using the Shapiro-Wilk test [10]

Figure 4. Convergence tests for *inp24* test problem

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	11	15	19	16	16		19
20	5	21	32	24	36	32		36
30	5	31	41	32	46	42		46

Predicted Entropy Convergence

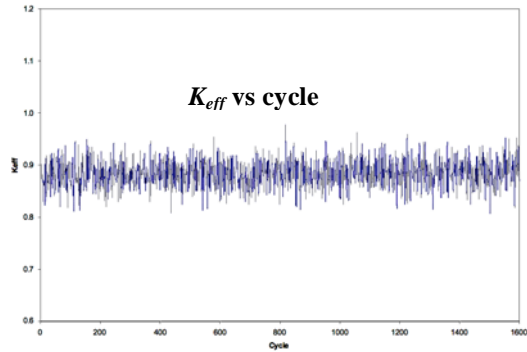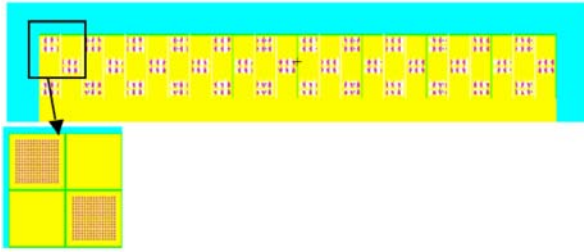| Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	17	10	32	37	32	39		39
20	17	31	42	43	43	44		44
30	17	46	48	50	49	51		51

For these numerical tests, q was varied among 10, 20, and 30 cycles for back-averaging. The six tests were applied separately to k_{eff} and H_{src}, and convergence was declared only if all six tests were satisfied.

Figure (4) shows the geometry and convergence behavior for the *inp24* test problem. Using $q=10$ results in quite reasonable estimates of convergence, as seen in the plots of k_{eff} and H_{src} vs cycle, while $q=20$ or $q=30$ results in overly conservative convergence criteria. Tests for other typical PWR or BWR problems show results similar to those in Figure (4) and suggest that it is not difficult to reliably automate the convergence assessment for "ordinary" reactor problems.

Figure (5) shows the geometry and convergence behavior for Benchmark 1 from the OECD/NEA benchmarks for source convergence [9], similar to a large, loosely-coupled fuel storage vault. The convergence tests work reasonably well for k_{eff}, which converges within 15 or 20 cycles, but fail miserably for H_{src}, where over 1000 cycles are needed for actual source convergence, rather than the 36-78 estimated by the tests. Other criticality-safety types of problems showed similar behavior: For loosely-coupled problems or problems with unusual arrangements of materials, the 6 tests on k_{eff} and H_{src} did not reliably predict convergence.

As a result of these initial numerical experiments in assessing convergence, it was decided to <u>not</u> incorporate the tests into the standard versions of MCNP5. While the tests performed well for routine reactor problems, they sometimes badly misjudged the convergence of more difficult problems. More research and numerical testing are needed before convergence testing can be fully automated.

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5/7

Figure 5. Convergence tests for OECD/NEA Benchmark 1

K_{eff} vs cycle

Convergence Tests Results

Predicted k_{eff} Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	5	10	13	14	13	15		15
20	5	20	20	21	30	25		30
30	5	30	30	33	31	35		35

Predicted Entropy Convergence

Back, q	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6		Converge
10	7	10	35	35	36	36		36
20	7	20	71	51	72	74		74
30	7	48	76	73	77	78		78

H_{src} vs cycle
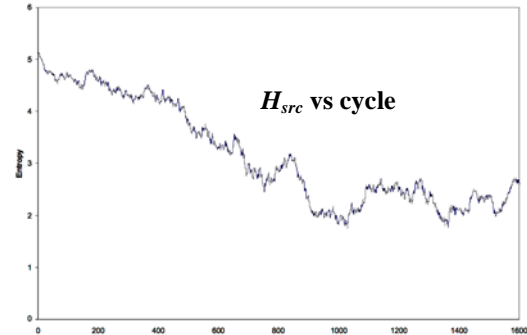
5. CONCLUSIONS

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 (version 1.40) includes capabilities for computing and plotting the Shannon entropy of the fission distribution as an important new tool for assessing problem convergence. The recommended MCNP5 procedures for defining spatial tally bins and computing H_{src} have been shown to be effective for a variety of typical criticality problems. Automation of convergence testing shows promise, but further research in this area is needed to improve robustness. It is highly recommended that both k_{eff} and H_{src} be carefully checked for convergence in all Monte Carlo criticality calculations.

ACKNOWLEDGMENTS

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7/7