Evaluating Source Convergence by Shannon Entropy in Monte Carlo Inactive Cycles with pCMFD or pFMFD Acceleration

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1. Introduction

Evaluating the number of inactive cycles needed to obtain a sufficiently converged fission source distribution during Monte Carlo neutronics analysis, and avoiding unnecessary inactive cycles, can reduce the computing cost of such analyses.

Prior literature suggests that the Shannon entropy of the source distribution is a more robust indicator of source convergence than other commonly used indicators, such as the neutron multiplication factor [1]. Thus, an algorithm that can automatically detect sufficient convergence in the Shannon entropy is needed.

Prior literature also suggests that large sets of convergence criteria are necessary for this to avoid early false positives. Recently, however, a relatively simple rebound condition was tested with promising results on Monte Carlo using pCMFD convergence acceleration [2].

This study seeks to follow up on this recent work with a more thorough investigation of the robustness of rebound-based convergence criteria.

2. Methodology

The pCMFD and pFMFD source convergence acceleration schemes were implemented on the iMC Monte Carlo neutronics analysis code [3].

2.1 Convergence Acceleration with pCMFD or pFMFD

The partial-current coarse mesh finite difference, or pCMFD, method accelerates the convergence of the neutron source distribution by adjusting the Monte Carlo simulation with a lower-order deterministic solution [4].

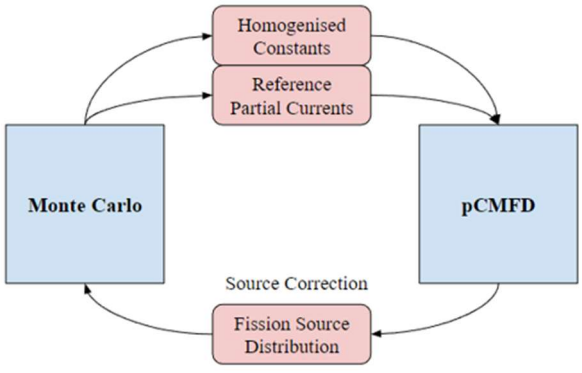


Fig. 1. Convergence acceleration with pCMFD

The pCMFD method begins with discretising the problem geometry into nodes and the construction of neutron balance equations, as shown in Eq. 1.

$$\sum_j \frac{A_{ij}}{V_i}\left(J_{ij+} - J_{ij-}\right) + \Sigma_{a,i}\phi_i = \frac{1}{k_{eff}}\nu_i\Sigma_{f,i}\phi_i \qquad (1)$$

The notations are conventional.

The partial current J_{ij+} is expressed with an adjusted diffusion-like scheme, as below.

$$J_{ij+} = \widetilde{D}_{ij}\left(\phi_i - \phi_j\right) + \widehat{D}_{ij}\phi_i \qquad (2)$$

The first term on the right-hand side represents the finite difference method partial current using the diffusion approximation. The second term is an adjustment that is included to ensure that the pCMFD partial current J_{ij+} matches the Monte Carlo partial current J_{ij}^{ref} tallied in the preceding cycle. The correction factor $\widehat{D}_{ij}$ is thus calculated as below.

$$\widehat{D}_{ij} = \frac{J_{ij+}^{ref} - \widetilde{D}_{ij}\left(\phi_i - \phi_j\right)}{\phi_i} \qquad (3)$$

Substituting these values into Eq. 1 for every node in the reactor problem produces a system of linear equations that is an eigenvalue problem where the dominant eigenvalue is $\frac{1}{k_{eff}}$ and the eigenvector is the vector of all node-average fluxes ϕ_i. This can then be solved with the usual iterative methods.

Once the pCMFD solution is obtained, the Monte Carlo source weights can be adjusted to match the pCMFD fission source distribution, as shown in Eq. 4.

$$\frac{w_{MC,new}}{w_{MC,old}} = \frac{w_{pCMFD}}{\sum w_{pCMFD}} \frac{\sum w_{MC,old}}{\sum_i w_{MC,old}} \qquad (4)$$

The following cycle of the Monte Carlo simulation may then proceed with these revised source weights.

Conventional pCMFD uses a coarse mesh where each mesh node is radially coextensive with one fuel assembly. A variant, using the same formulation on a fine mesh where each mesh cell corresponds to one fuel pin, is called the partial-current fine-mesh finite difference, or pFMFD, method.

2.2 Source Distribution Shannon Entropy

The Shannon entropy measures the semantic information entropy of a probability distribution. It can be calculated for the fission source distribution in a neutronics analysis problem.

$$H = -\sum_i \{p_i log(p_i)\} \quad (5)$$

Because the initial neutron source distribution used in the current study is flat, in neutronics analysis the Shannon entropy of the source distribution always begins at its maximum value and converges downwards towards an equilibrium value. Increases in the Shannon entropy would thus indicate that the converging trend is weaker than the stochastic cycle-wise variation, which suggests sufficient convergence.

The relative difference condition is shown in Eq. 6. If the shown inequalities are satisfied, sufficient convergence is assumed at cycle c.

$$\frac{|H_c - H_{c-1}|}{|H_1 - H_2|} < \varepsilon \,, \frac{|H_{c-1} - H_{c-2}|}{|H_1 - H_2|} < \varepsilon \quad (6)$$

In this study, $\varepsilon = 10^{-3}$ was used. Preliminary calculations suggested that this is suitable.

Two different variants of the rebound convergence criterion were tested. In the qualified rebound convergence criterion variant, the Shannon entropy is judged to have converged if the Shannon entropy rises from one cycle to the next after a certain minimum number of inactive cycles. Preliminary calculations suggested that aggressive convergence acceleration schemes tended to produce early overshoots in the Shannon entropy, so rebounds in the first four inactive cycles are ignored. If Eq. 7 is satisfied, sufficient convergence is assumed at cycle $c + 2$.

$$H_c > H_{c-1} \,, c > 4 \quad (7)$$

The stride-2 rebound convergence criterion variant requires that the Shannon entropy increase across two inactive cycles. If the inequality below is satisfied, sufficient convergence is assumed at cycle $c + 2$.

$$H_c > H_{c-2} \,, c > 4 \quad (8)$$

3. Procedure

These criteria were applied to two model problems.

3.1 Problem Descriptions

The APR1400 model problem is based on the conventional pressurised water reactor of the same name [5]. The pin pitch is 1.30cm, the assembly pitch 20.88cm, and the active core height 381cm. Structural elements above and below the active core are simplified.

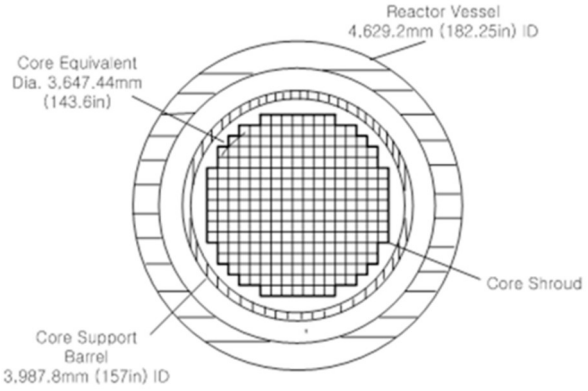


Fig. 2. Radial layout of the APR1400 problem

The MOX1000 model problem is based on a sodium-cooled fast reactor benchmark problem created by the Nuclear Energy Agency [6]. The pin pitch is 0.913cm, the assembly pitch 16.25cm, and the active core height 114.94cm. Structural elements above and below the active core are simplified, leaving only the lower axial reflector and the upper gas plenum.

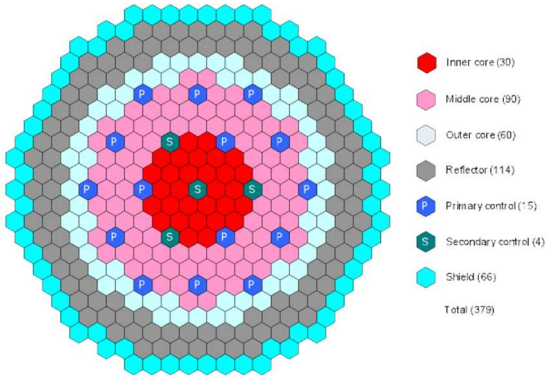


Fig. 3. Radial layout of the MOX-1000 core

3.2 Testing Procedure

For this study, it is assumed that convergence criteria are reliable if the Shannon entropy at the cycle in which sufficient convergence is evaluated to be reached does not fall outside the normal range of post-convergence fluctuation more often than would be expected.

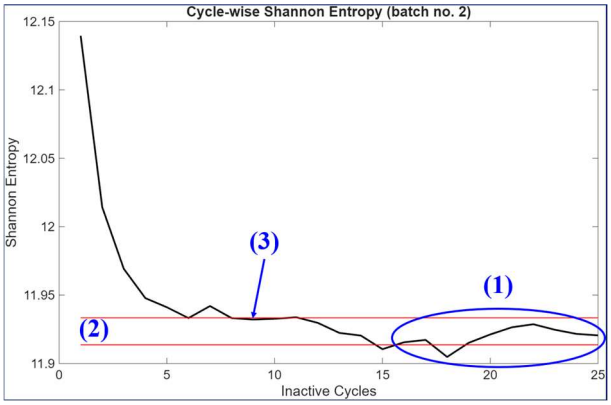


Fig. 4. Judging sufficient convergence

First, as shown in (1), the Shannon entropies calculated in the final 10 cycles of all batches are sampled, for a total sample size ten times as large as the number of batches. Then, as in (2), 1.0-, 1.5-, and 2.0-sigma ranges for this sample are constructed. Finally, as in (3), it is observed whether the Shannon entropy at the point where sufficient convergence is judged to have been reached falls within these ranges.

4. Results

Neutronics analysis was performed with pCMFD using 500,000 and 2 million histories per cycle, and with pFMFD using the necessary number of histories per cycle. 60 batches were performed for each case, except for APR1400 with pFMFD for which 25 were performed.

Axially, for the pCMFD calculations, each fuel assembly in the APR1400 model was divided into 19 axial nodes, each 20.05cm in height, and each driver assembly or equivalent in the MOX1000 model was divided into 5 axial nodes, each 22.99cm in height. For the pFMFD calculations, each fuel pin or equivalent was divided into four times as many cells, one-fourth as high.

Two sets of convergence criteria were tested: Set A, the relative difference criterion and the qualified rebound criterion, and Set B, the relative difference criterion and the stride-2 rebound criterion. Each criteria set judges the Shannon convergence as having converged if any criterion in it is satisfied.

4.1 Verifying Assumptions

The normality of the sample of Shannon entropies from the final 10 cycles of each run was checked using the D'Agostino D normality test.

Table I: Normality evaluation for Shannon entropy samples

Model	**D-value**	**Crit. Range**
APR1400 (500k)	0.28081	(0.2794, 0.2842)
APR1400 (2M)	0.28054	
MOX1000 (500k)	0.28194	
MOX1000 (2M)	0.28041	
MOX1000 (FM-2M)	0.27953	

All calculated D-values fall within the critical range, so there is no reason to reject the assumption of normality.

Sensitivity tests were performed to verify that 25 inactive cycles are sufficient to observe the full convergence behaviour and that samples of the final 10 cycles of each batch produce a sufficiently representative and converged sample.

Table II: Means and standard deviations of sampled entropies

Problem	Final 10 of 25 cycles	Final 5 of 25 cycles	Final 50 of 150 cycles
APR1400, CM (2M)	11.9273 (0.0034)	11.9269 (0.0034)	11.9258 (0.0031)
MOX1000, CM (2M)	9.7581 (0.0003)	9.7581 (0.0003)	9.7581 (0.0003)

The sample means and standard deviations do not change significantly with a smaller sample size or with a larger number of inactive cycles, demonstrating that 25 inactive cycles are sufficient to observe the full convergence behaviour and that the final 10 cycles are a sufficiently large sample.

4.2 APR1400

The number of outliers in which the final Shannon entropy did not fall within the stochastic ranges as described in subsection 3.2 is as below.

Table III: Frequency of outliers

Conditions	>1.0-sigma		>1.5-sigma		>2.0-sigma	
	A	B	A	B	A	B
CM, 500k	11	12	6	2	1	1
CM, 2M	12	16	5	5	3	2
FM, 16M	8	1	2	1	1	0

With 60 batches, the ideal numbers of outliers given a normal distribution are 19.1, 8.0, and 2.8. With 25 batches, they are 8.0, 3.4, and 1.2. The actual number of outliers is never significantly higher in any case.

The minimum, median, and maximum number of cycles required before the criteria sets judged sufficient convergence to have been reached are summarised below.

Table IV: Number of cycles before sufficient convergence

Conditions	Criteria A			Criteria B		
	Min	Mid	Max	Min	Mid	Max
CM, 500k	8	10	15	9	11	15
CM, 2M	9	11	16	10	13	17
FM, 16M	7	8	8	7	7	7

The mean Shannon entropy across all batches in each cycle under each calculation condition is shown in Fig. 5. As the pFMFD mesh is finer than the pCMFD mesh, the nominal Shannon entropy values are higher with pFMFD than with pCMFD. For comparability, the values are normalised such that the initial value is one and the mean value across the final 10 cycles is zero.

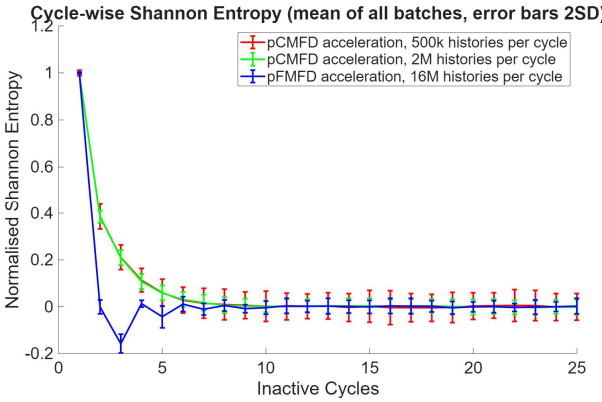


Fig. 5. Normalised entropy for the APR1400 problem

The APR1400 is a thermal reactor problem, so it may take multiple cycles for local perturbations to propagate through the reactor geometry. In such a problem, an aggressive acceleration method like pFMFD may produce overcorrections in the neutron source, leading to overshoots in the Shannon entropy. Rebound convergence criteria have a tendency to catch on the Shannon entropy recovering from such overshoots, leading to the narrow ranges, shown in Table IV, in the number of cycles judged necessary by the convergence criteria. However, fast convergence under pFMFD allows the Shannon entropy to sufficiently converge by cycle 7, so this does not cause outliers to be more common than expected.

4.3 MOX1000

The number of outliers as defined in subsection 3.2 are shown in Table V.

Table V: Frequency of outliers

Conditions	>1.0-sigma		>1.5-sigma		>2.0-sigma	
	A	B	A	B	A	B
CM, 500k	12	11	7	4	3	2
CM, 2M	18	9	8	7	3	5
FM, 2M	14	16	10	9	5	4

The ideal numbers of outliers with 60 batches are 19.1, 8.0, and 2.8. The actual number of outliers is only rarely significantly higher.

The minimum, median, and maximum number of cycles required before the criteria sets judged sufficient convergence to have been reached are summarised below.

Table VI: Number of cycles before sufficient convergence

Conditions	Criteria A			Criteria B		
	Min	Mid	Max	Min	Mid	Max
CM, 500k	8	11	15	10	12	16
CM, 2M	10	12	18	11	14	18
FM, 2M	7	8	12	7	9	13

The mean Shannon entropy across all batches in each cycle under each calculation conditions is shown below. As before, the Shannon entropy values are normalised.

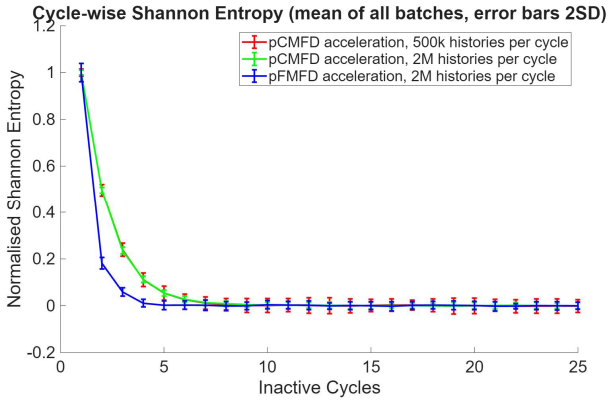


Fig. 6. Normalised entropy for the MOX1000 problem

Because the MOX1000 model is a fast reactor, the problem geometry is more tightly coupled than in the APR1400 problem. Thus, even with pFMFD acceleration, no overshoot is observed and the Shannon entropy converges smoothly.

5. Conclusions

This study investigated the suitability of convergence criteria based on rebounds in the Shannon entropy for generating on-the-fly estimates of the number of inactive cycles it takes for the Shannon entropy to sufficiently converge. Both the qualified rebound criterion and the stride-2 criterion were found to be reasonably robust for all tested cases. The Shannon entropy at the point where convergence was judged to have been reached did not deviate from the post-convergence mean more than would be expected from stochastic variation.

Prior literature notes that Shannon entropy is more reliable than other indicators of source convergence, but verification that the entropy alone can reflect sufficient convergence in the source distribution is still necessary.

With more aggressive convergence acceleration schemes, there may be overshoots in the Shannon entropy during convergence. The results demonstrate the importance of criteria that are robust in such overshoots.

Developing similarly simple convergence criteria that are robust against very difficult neutronics problems, such as a spent fuel storage pool, which converge very slowly even with an efficient acceleration scheme, may also be a useful future complement to this study.

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