Real Variance Reduction in Continuous-Energy Monte Carlo Whole-Core Calculation via p-CMFD Feedback

YuGwon Jo and Nam Zin Cho*

Korea Advanced Institute of Science and Technology (KAIST) 291 Daehak-ro, Yuseong-gu, Daejeon, Korea 34141 *nzcho@kaist.ac.kr

1. Introduction

One of the challenges for the whole-core transport calculation is its slow source convergence. In the previous study of deterministic method of characteristics (MOC) calculation, the coarse-mesh finite difference (CMFD) method [1] was applied to accelerate source convergence of the high-order transport solution by using the low-order CMFD solution. However, the CMFD acceleration method diverges for optically thick coarse-mesh as shown in Fourier convergence analysis, while the partial current-based coarse-mesh finite difference (p-CMFD) method [2-4] is unconditionally stable. In the continuous-energy Monte Carlo (MC) simulation, the p-CMFD acceleration method was applied to reduce the number of inactive iterations (i.e., cycles) for the source convergence [5]. The p-CMFD acceleration method was also combined with the fission and surface source (FSS) iteration method, which is a domain decomposition method, and tested in continuousenergy two-dimensional (2-D) and three-dimensional (3-D) problems [6-8]. It was also used in a threedimensional (3-D) continuous-energy whole-core problem in the context of the transient MC simulations [9,10].

In the previous study [11] of the multigroup MC simulation, it was shown in 1-D and 2-D whole-core problems that the feedback of the CMFD solution not only accelerated MC fission source distributions (FSDs) during inactive iterations, but also led to smaller real standard deviations in MC tallies during active iterations, compared to the conventional power iteration. Recently, the CMFD feedback for the continuous-energy MC simulation [12] leads to around 1.5 times smaller real standard deviations of MC tallies, while the results are restricted to a one-dimensional homogeneous problem. More recently, in Ref. [13], the CMFD method for the continuous-energy MC simulation has been applied to only inactive iterations on a 3-D whole-core problem.

In this paper, the p-CMFD feedback in the continuousenergy MC simulation is investigated for the real variance reduction of local tallies; radial pin powers and assembly powers in a 3-D whole-core problem. We have also refined the tally algorithm to reduce stochastic errors in scattering reaction rates for the p-CMFD parameters (homogenized cross sections and leakage correction factors). The numerical results show that the p-CMFD feedback leads to 1.4 times and 1.9 times smaller averages of real standard deviations in radial pin powers and assembly powers, respectively, at the optimized accumulation condition for the p-CMFD parameters [14], compared to the conventional power iteration.

2. Methodology

2.1. MC simulation with p-CMFD Feedback

Figure 1 shows a schematic flow chart for the MC simulation with the p-CMFD feedback (MC/p-CMFD). To stabilize the fluctuations of FSDs of the MC/p-CMFD, the accumulation scheme 2 in Ref. [14] is applied. We skip the accumulation of the coarse-mesh MC tallies (flux, reaction rates, and partial currents) for the p-CMFD parameters (homogenized cross sections and leakage correction factors) during the initial L_{skip} inactive iterations for the fast convergence of FSDs. Then, for the remaining entire iterations; both inactive and active iterations, the coarse-mesh MC tallies are enqueued in the first-in-first-out (FIFO) queue storage. The FIFO queue length L means that the FIFO queue storage contains the MC tallies of the previous L-1 iterations. When the FIFO queue storage is full, the oldest MC tallies are dequeued and the newest MC tallies are enqueued. The detailed description of the MC/p-CMFD is given in Refs. [5,7].



Fig. 1. Schematic flow chart for the MC/p-CMFD; $S_{MC,i}^{(l)}$ is the number of sampled MC fission sources in the coarse-mesh cell *i*, *M* is the nominal source size, $L_{inactive}$ is the number of inactive iterations, and L_{active} is the number of active iterations.

2.2. Tally of Scattering Reaction Rate

The implicit capture and the Russian roulette are routinely used in the continuous-energy MC code (e.g., MCNP5 [15]) to increase the efficiency of the MC simulation.

In the previous studies of the MC/p-CMFD [5-10], the scattering reaction rates were tallied after the Russian roulette, as line #14 in Fig. 2. In this case, we lose the exact weight of the scattered particle, which may result in the significant increase of stochastic errors in the scattering reaction rates. Therefore, we move line #14 to line #4 in Fig. 2, so that the scattering reaction rate is tallied with the weight before the Russian roulette.

1	A particle collision occurs.
2	Colliding nuclide <i>i</i> is randomly sampled.
3	$W = W(1 - \frac{\sigma_{absoption,i}}{\sigma_{total,i}}).$
4	
5	If $(W < W_{threshold})$ then
6	Do Russian roulette.
7	if (neutron survives) then
8	$W = W_{survive}$
9	else
10	Track the next particle.
11	end if
12	end if
13	Determine outgoing energy and scattered angle for scattered particle.
14	$F_{scatter} = F_{scatter} + W.$
15	Fly until the next collision occurs.

Fig. 2. Collision subroutine in the MC simulation using the implicit capture and the Russian roulette; $F_{scatter}$ is a variable to tally scattering reaction rate.

3. Numerical Results

Figure 3 shows the configurations of a 3-D continuous-energy whole-core test problem, where the material densities and compositions are taken from BEAVRS [16]. The MC simulations in this paper are performed by the in-house 3-D continuous-energy MC code, McBOX [17], using the ENDF/B-VII.0 library.



Fig. 3. Configurations of 3-D continuous-energy whole-core test problem.

The calculational conditions of a single batch run for the MC simulation are 1,000,000 histories per iteration and 400 active iterations; The number of inactive iterations is set as 60 for the MC/p-CMFD, while it is set as 400 for the conventional power iteration. Note that the number of inactive iterations used is not the optimized value but set to be large enough to ensure the fission source convergence.

For the p-CMFD calculation, the coarse-mesh cell is set as a single assembly in x-y plane with 20 divisions in z-axis. It is noted that when the coarse-mesh flux is 10¹⁰ times smaller than the maximum coarse-mesh flux (e.g., peripheral regions of the large whole-core problem, or rodded regions), the MC tallies for this coarse-mesh cell are not reliable due to the too large stochastic errors. Therefore, we treat this type of the coarse-mesh cell as a vacuum region in the p-CMFD calculation and the weights of MC FSDs in this coarse-mesh cell are not corrected. We skip the accumulation of coarse-mesh MC tallies for the p-CMFD parameters during the initial 40 iterations.

To investigate the effect of the FIFO queue length (*L*) in the MC/p-CMFD on the real variance, 50 independent batch runs are performed for several test cases with varying *L* as 0, 1, 3, 5, 10, 20, 40, 160, and 420; The case "*L* = 0" means the conventional power iteration. For each test case, the real standard deviation (σ_{real}), the apparent standard deviation (σ_{app}), and the standard deviation estimated by the history-based batch (HB) method (σ_{HB}) [18] are obtained for radial pin powers and assembly powers.

Figure 4 shows the source convergence of the MC/p-CMFD with several queue lengths by Shannon entropy [19], where the Shannon entropy for each test case is obtained from averaged values of 50 independent batch runs. Note that the reference Shannon entropy is obtained from the conventional power iteration using 20,000,000 histories per iteration. Compared to the conventional power iteration, the MC/p-CMFD shows the faster convergence of the FSDs. It is also shown that the converged Shannon entropy of the MC/p-CMFD is closer to the converged reference Shannon entropy, compared to that of the conventional power iteration. This means that the converged FSDs of the MC/p-CMFD are more accurate than those of the conventional power iteration for the same number of histories (1,000,000) per iteration.



Fig. 4. Comparisons of averaged Shannon entropies of test cases (L = 0, 1, 5, 40, and 420) and reference Shannon entropy.

Figures 5 and 6 show, respectively, radial pin-power and assembly-power distributions and their three standard deviations (σ_{real} , σ_{app} , and σ_{HB}) distributions for test cases. For L = 1 and 5, the σ_{real} distributions of the MC/p-CMFD are smaller than the those of the conventional power iteration. However, when L = 420, the σ_{real} distributions become larger than those of the conventional power iteration.



Fig. 5. Radial pin powers and their three standard deviations (σ_{real} , σ_{app} , and σ_{HB}) for test cases (L = 0, 1, 5, and 420).



Fig. 6. Radial assembly powers and their three standard deviations (σ_{real} , σ_{app} , and σ_{HB}) for test cases (L = 0, 1, 5, and 420).

To investigate the effects of the FIFO queue length on the real variance more clearly, the average of the real standard deviations of local tallies ($\bar{\sigma}_{real}$) is obtained for each test case. Similarly to $\bar{\sigma}_{real}$, the average of apparent standard deviations ($\bar{\sigma}_{app}$) and the average of standard deviations estimated by the HB method ($\bar{\sigma}_{HB}$) are also obtained.

Figure 7 shows the ratios of $\overline{\sigma}_{real}$ in the MC/p-CMFD to $\overline{\sigma}_{real}$ in the conventional power iteration for the various queue lengths. As the queue length increases from 1 to 5, the ratio decreases, while from 10 to 420, the ratio increases. Thus, there appears to be an optimum

queue length L = 5 (for this problem). Figures 8 and 9 compare the three averages of standard deviations ($\bar{\sigma}_{real}$, $\bar{\sigma}_{app}$, $\bar{\sigma}_{HB}$) of radial pin powers and assembly powers, respectively, for the various queue lengths. It is shown that the HB method quite accurately estimate the real variance for the conventional power iteration, while the HB method fails to estimate the real variance when the p-CMFD feedback is used. This is due to the fact that the p-CMFD feedback introduces correlation among the history-based batches.



Fig. 7. The ratios of $\bar{\sigma}_{real}$ in MC/p-CMFD to $\bar{\sigma}_{real}$ in the conventional power iteration for various FIFO queue lengths; 0, 1, 3, 5, 10, 20, 40, 160, and 420.



Fig. 8. Comparisons of three averages of standard deviations $(\bar{\sigma}_{real}, \bar{\sigma}_{app}, \text{and } \bar{\sigma}_{HB})$ of radial pin powers.



Fig. 9. Comparisons of three averages of standard deviations $(\bar{\sigma}_{real}, \bar{\sigma}_{app}, \text{and } \bar{\sigma}_{HB})$ of radial assembly powers.

4. Summary and Conclusions

In this paper, the continuous-energy MC simulation embedding the p-CMFD feedback was investigated for the real variance reduction in local tallies in the 3-D whole-core problem. In contrast to the previous implementation, we also refined the tally algorithm of the scattering reaction rates for the p-CMFD parameters. The numerical results show that the p-CMFD feedback leads to more accurate FSDs and smaller real standard deviations (with optimum queue length L = 5 for the test problem), compared to the conventional power iteration.

Note that the real variance consists of the variance term from a single iteration and the inter-iteration covariance terms. In the MC/p-CMFD, between two successive MC iterations we perform a sufficient number of power iterations in the low-order p-CMFD calculation and the resulting FSDs are used in the next MC iteration. Thus, the real variance of the MC tally is reduced due to the smaller covariance among iterations.

For a small queue length (L = 1, 3, or 5), the accumulation of the coarse-mesh MC tallies is desirable to reduce both the stochastic errors and the biases from the ratio-type estimator [20] in the p-CMFD parameters. However, for a long queue length (L = 40, 160, or 420), the inter-iteration correlations increase in the p-CMFD solutions. Therefore, we have to use the optimum queue length for the p-CMFD feedback for the real variance reduction during active iterations.

Acknowledgements

This work was supported in part by KUSTAR-KAIST Institute (KKI), Korea, under the R&D program (N1117dd0014) supervised by KAIST. This work was also supported in part by a National Research Foundation grant funded by the Korean government (Ministry of Science, ICT and Future Planning) (No. 2015M2B2A9029928).

References

[1] K.S. Smith and J.D. Rhodes, III, "CASMO Characteristics Method for Two-Dimensional PWR and BWR Core Calculation," *Trans. Am. Nucl. Soc.*, **83**, 294 (2000).

[2] N.Z. Cho et al., "On a New Acceleration Method for 3D Whole-Core Transport Calculations," *Annual Meeting of the Atomic Energy Society of Japan*, Sasebo, Japan, Mar. 27-29, 2003.

[3] N.Z. Cho et al., "Partial Current-Based CMFD Acceleration of the 2D/1D Fusion method for 3D Whole-Core Transport Calculations," *Trans. Am. Nucl. Soc.*, **88**, 594, 2003.

[4] N.Z. Cho, "The Partial Current-Based CMFD (p-CMFD) Method Revisited," *Trans. Kor. Nucl. Soc.*, Gyeongju, Korea, Oct. 25-26, 2012.

[5] S. Yun and N.Z. Cho, "Acceleration of Source Convergence in Monte Carlo k-Eigenvalue Problem via Anchoring with a p-CMFD Deterministic Method," *Ann. Nucl. Energy*, **37**, 1649-1658 (2010).

[6] Y.G. Jo and N.Z. Cho, "Fission and Surface Source Iteration Scheme with Source Splitting in Domain Decomposition Monte Carlo Calculation," *Trans. Kor. Nucl. Soc.*, Pyeongchang, Korea, Oct. 30-31, 2014

[7] Y.G. Jo and N.Z. Cho, "Fission and Surface Source Iteration Method for Domain Decomposed Monte Carlo Whole-Core Calculation," *Nucl. Sci. Eng.*, **182**, 181-196 (2016).

[8] Y.G. Jo and N.Z. Cho, "Performance Analysis of Fission and Surface Source Iteration Method for Domain Decomposed Monte Carlo Whole-Core Calculation," *Trans. Kor. Nucl. Soc.*, Jeju, Korea, May 12-13, 2016.

[9] Y.G. Jo, et al., "Continuous-energy Monte Carlo Method for Reactor Transient Analysis Based on Quasi-Static Methods," *ANS MC2015*, Nashville, TN, April 19-23, 2015.

[10] Y.G. Jo, et al., "Nuclear Reactor Transient Analysis by Continuous-Energy Monte Carlo Calculation Based on Predictor-Corrector Quasi-Static Method," *Nucl. Sci. Eng.*, **183**, 229-246 (2016).

[11] M.J. Lee et al., "Investigation of CMFD Accelerated Monte Carlo Eigenvalue Calculation with Simplified Low Dimensional Multigroup Formulation," *PHYSOR 2010*, Pittsburgh, PA, USA, May 9-14, 2010.

[12] H. Lee and D. Lee, "Application of CMFD on Continuous Energy Monte Carlo Simulation for Eigenvalue Problems," *Trans. Kor. Nucl. Soc.*, Oct. 31-31, 2014, Pyeongchang, Korea.
[13] B.R. Herman, et al., "Progress toward Monte Carlothermal hydraulic coupling using low-order nonlinear diffusion acceleration methods," *Ann. Nucl. Energy*, 84, 63-72 (2015).

[14] Y.G. Jo and N.Z. Cho, "Stabilization of Monte Carlo Fission Source Distribution in p-CMFD Acceleration Method," *Trans. Kor. Nucl. Soc.*, Gyeongju, October 24-25, 2013.

[15] X-5 MONTE CARLO TEAM, "MCNP - A General N-Particle Transport Code, Version 5 - Volume I: Overview and theory," LA-UR-03-1987, Los Alamos National Laboratory (2003).

[16] N. Horelik, et al., "Benchmark for evaluation and validation of reactor simulation (BEAVRS)," *Proc. M&C 2013*, Sun Valley, USA, May 5-9, 2013.

[17] Y.G. Jo and N.Z. Cho, "Users' Manual for McBOX-A Monte Carlo Code Version 1," Korea Advanced Institute of Science and Technology, NURAPT-2016-03 (April 2016).

[18] H.J. Shim, et al., "Real Variance Estimation by Grouping Histories in Monte Carlo Eigenvalue Calculations," *Nucl. Sci. Eng.*, **176**, 58-68 (2014).

[19] F.B. Brown, "On the use of Shannon entropy of the fission distribution for assessing convergence of Monte Carlo criticality calculation," *PHYSOR 2006*, Vancouver, Canada, September 10-14, 2006.

[20] Y.G. Jo and N.Z. Cho, "Unbiased Ratio Estimator for k-Eigenvalue in Monte Carlo Criticality Calculations," *Trans. Am. Nucl. Soc.*, **115**, 1234-1237 (2016).