# Deterministic Truncation of Monte Carlo Solutions with Continuous Energy Nuclear Data

HyeonTae Kim, Yugwon Jo, Inhyung Kim, and Yonghee Kim\*

Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

\*Corresponding author: yongheekim@kaist.ac.kr

## 1. Introduction

The coarse-mesh finite difference (CMFD) method was proposed to accelerate the deterministic transport calculation [1]. As an alternative to the CMFD method, the partial current-based CMFD (p-CMFD) method, which shows an unconditionally stable convergence was proposed [2]. The CMFD and the p-CMFD method have been popularly used as an efficient acceleration method for fission source distribution convergence in Monte Carlo (MC) *k-eigenvalue* problems [3-5]. Lee et al. showed the real variance reduction of the solution as the acceleration methods were extended to the active cycles [4].

Our previous study suggested deterministically truncated MC (DTMC) solutions as a way of saving computational burden [6]. The DTMC is the deterministically obtained solution which is a subset of the continuous MC solution. In order to provide detailed power-distributions from the finite difference step, the mesh size was reduced to the pin-level, led us to call it as fine-mesh finite difference (FMFD) method. The solutions from the DTMC method was reported to have significantly reduced uncertainties both for the two major reactor parameters, the multiplication factor and the pin-power distribution [7-8]. Recently, a feasibility study to further reduce the uncertainty caused by the low particle population near vacuum was done [8]. Since the DTMC solution has smaller uncertainty, the number of active cycles can be reduced, or the required active cycles are truncated into a few.

However, the aforementioned works regarding the DTMC method have been done with multi-group nuclear data and considered not enough to thoroughly examine the method. This paper presents an extension of the DTMC method with the continuous energy nuclear data. In order to investigate the real variance reduction effect, the in-house three-dimensional continuous energy MC code McBOX [9] was used. The numerical results on the three-dimensional continuous-energy pressurized water reactor (PWR) test problem shows the improved performance of the DTMC solution, compared to the direct MC tally.

## 2. Methodology

This section describes the key features of the DTMC method. The DTMC method provides systematically truncated solutions from the FMFD assisted MC. The

high fidelity MC calculations provide the FMFD parameters such as the neutron current, flux, and reaction cross-sections, which are necessary to formulate the FMFD system matrix. By solving the matrix equation of the reactor eigenvalue problem, the major reactor parameters, the multiplication factor and the detailed power distribution, are obtained. The results are used not only to update the FSD of the subsequent MC calculation by correcting the particles' weight, but also used for statistical samples to predict the solution by themselves. (Fig. 1)



Figure 1 Flow chart of MC/FMFD (or p-FMFD) and DTMC method.

The DTMC method highly depends on accuracies of the FMFD parameters calculated from the MC simulation, but it is less sensitive to the stochastic random effect of the MC simulations because the solutions are obtained in the deterministic way. As a result, it minimizes the uncertainties of the solution and reduces the computational burden.

In order to formulate the FMFD equation, one-group cross sections are obtained as:

$$\Sigma_{\alpha,i} = \frac{F_{\alpha,i}}{\phi_i^{MC}} ,.$$
 (1)

where,  $\Sigma_{\alpha,i}$  denotes the  $\alpha$  type reaction rate at the *i*<sup>th</sup> node.

The leakage correction factor for the net current is obtained as:

$$\hat{D}_{i+1/2} = -\frac{2J_{i+1/2} + \tilde{D}_{i+1/2} \left(\phi_{i+1} - \phi_i\right)}{\phi_{i+1} + \phi_i}, \qquad (2)$$

where  $\phi_i$  is a pin-averaged neutron flux at *i*-th mesh cell and  $\tilde{D}_{i+1/2}$  is an arbitrary diffusion coupling coefficient between fine-mesh cells *i* and *i*+1, defined as:

$$\tilde{D}_{i+1/2} = \frac{2d_i d_{i+1}}{d_i + d_{i+1}},$$
(3)

$$d_i = \frac{1}{3\Sigma_i h_i}, \qquad (4)$$

with fine-mesh cell size  $h_i$ .

In the p-FMFD method, the two leakage correction factors for the incoming and outgoing partial currents are obtained, respectively, as:

$$\hat{D}_{i+1/2}^{-} = \frac{2J_{i+1/2}^{-} - \tilde{D}_{i+1/2}\left(\phi_{i+1} - \phi_{i}\right)}{2\phi_{i+1}},$$
(5)

$$\hat{D}_{i+1/2}^{+} = \frac{2J_{i+1/2}^{+} + \tilde{D}_{i+1/2}\left(\phi_{i+1} - \phi_{i}\right)}{2\phi_{i}}.$$
(6)

In this paper, the DTMC solution is obtained from the p-FMFD calculation.

#### 3. Numerical Results

The configuration of the continuous-energy threedimensional PWR test problem is shown in Figure 2. The ENDF/B-VII.0 continuous-energy library at 600K is used for the MC simulation.

On this test problem, 50 independent batch runs are performed for the real variance analysis with three different test cases; 1) the conventional MC, 2) the MC with the p-CMFD feedback (MC/p-CMFD), and 3) the MC with the p-FMFD feedback (MC/p-FMFD), where the calculational condition for each test case is shown in Table I. For the p-FMFD calculation, the fine-mesh cell is taken to be a single pin-cell size in the radial direction (1.26 cm) and equally divided into 10 in the axial direction (45.5444 cm), while the coarse-mesh cell for the p-CMFD calculation is taken to be an assembly size in the radial direction (21.42 cm) with the same axial division of the p-FMFD.

For the three test cases, both the k-eigenvalue and the one-group integrated fine-mesh flux distributions are investigated with respect to both the real standard deviation (real SD) and the bias. It is noted that the MC/p-FMFD yields two solutions; one is the direct MC tally and the other is the DTMC solution. In case of the MC/p-CMFD, the one-group fine-mesh flux distributions are estimated by the direct MC tally.



Figure 2 Configurations of continuous-energy threedimensional reactor test problem.

Table I Calculational conditions for three test cases

Calculational Conditions	Conventional MC	MC /p-CMFD	MC /p-FMFD
Number of Histories per Cycle	2,000,000	2,000,000	2,000,000
Number of Inactive Cycles	200	40	50
Number of Active Cycles	200	200	200
Number of Cycles Skipping Accumulation*	N/A	25	15

\*The MC tallies for the p-CMFD and p-FMFD parameters are accumulated to reduce both the variances and the biases in the parameters, while initial a few cycles are skipped to accumulate for faster convergence of the FSDs.

As studied in Ref. [10], the number of first-in-firstout (FIFO) accumulation cycle length (*L*) of the MC tallies for the p-CMFD (or p-FMFD) parameters can significantly affect the real SDs. With varying accumulation length *L*, the real SDs in one-group integrated fine-mesh flux distributions are investigated as Fig. 3. The flux weighted average of the real SDs in the MC/p-CMFD becomes minimum at the accumulation length L = 10, while the minimum appears at the accumulation length L = 2 in the MC/p-FMFD.



Figure 3 Flux weighted average of real SDs in one-group integrated fine-mesh flux distributions, where the FIFO accumulation cycle length L = 0 indicates the results from the conventional MC.

Table II compares the real SD and the bias of the keigenvalue for the three test cases at their optimum accumulation lengths as found above (L = 10 for MC/p-CMFD, L = 2 for MC/p-FMFD). The direct MC tally from the MC/p-CMFD shows 1.37 times smaller real SD in the k-eigenvalue than that of the conventional MC, while the DTMC solution from the MC/p-FMFD shows 1.22 times smaller real SD. It is noted that the bias in the DTMC solution from the MC/p-FMFD is 0.61 times of the real SD, while the bias in the direct MC tally from the MC/p-FMFD is 3.08 times of the real SD which is not negligible.

	k-eigenvalue	Conventional MC	MC/p-CMFD $(L = 10)$		MC/p-FMFD (L = 2)	
		Direct MC Tally	Direct MCTally	DTMC Solution	Direct MC Tally	DTMC Solution
	Average of Sample Mean	1.264607	1.264611	1.264609	1.264784	1.264637
	Real SD	0.000061	0.000045	0.000055	0.000057	0.000050
	Bias*	-	0.000004	0.000002	0.000177	0.000030
	Ratio of Bias* to Real SD	-	0.08	0.03	3.08	0.61
I	Real SD Improvement**	1.00	1.37	1.10	1.06	1.22

Table II Comparisons of real SD and bias of the k-eigenvalue for three test cases

\* Bias is estimated by the difference of the average sample mean with respect to that of conventional MC.

\*\*Real SD improvement is estimated by the ratio of the real SD to that of the conventional MC.

Figure 4 compares the real SDs of the one-group finemesh flux distributions for the three test cases at their optimum accumulation lengths. It is shown that the peak real SDs appearing in the conventional MC are suppressed in the both the MC/p-CMFD and the MC/p-FMFD.



Figure 4 Comparisons of real SDs in one-group fine-mesh flux distributions for three test cases.

Table III compares the flux weighted averages of the real SDs and the biases in the one-group fine-mesh flux distributions for the three test cases. The DTMC solution of the MC/p-FMFD shows the best performance in terms of the real SDs in the one-group fine-mesh flux distributions among the test cases, where the absolute bias is 0.25 times of the real SD.

### 4. Summary and Conclusions

In the continuous-energy PWR test problem, the DTMC solution obtained from the MC/p-FMFD was compared with the direct MC tallies obtained from 1) the conventional MC, 2) the MC/p-FCFD, and 3) the MC/p-FMFD. For the one-group integrated flux distributions, the DTMC solution shows the smallest real variance.

As a further study, the DTMC method will be investigated in the three-dimensional continuous-energy large-scale reactor problem (e.g., commercial PWR reactor problem). In addition, utilization of the DTMC solution from the initial few active cycles will be investigated.

Table III Comparisons of flux weighted averages of re-	al SDs
and absolute biases in one-group fine-mesh flux distrib	outions
for three test cases	
	-

Flux Weighted	Conventional MC	$\frac{\text{MC/p-CMFD}}{(L=10)}$	MC/p-FMFD $(L = 2)$	
Quantities	Direct MC Tally	Direct MC Tally	Direct MC Tally	DTMC Solution
Real SD	3.37E-07	2.53E-07	2.43E-07	2.42E-07
Absolute Bias*	-	4.67E-08	2.28E-07	2.60E-07
Ratio of Absolute Bias* to Real SD	-	0.17	0.26	0.25
Real SD Improvement**	1.00	1.33	1.39	1.39

\* Absolute bias is estimated by the absolute difference between the average sample mean and that of conventional MC.

\*\*Real SD improvement is estimated by the ratio of the real SD to that of the conventional MC.

#### 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," Ann. Mtg. Atomic Energy Soc. Japan, Sasebo, Japan, March 27–29, 2003.

[3] 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.

[4] M.J. Lee et. al., "Coarse mesh finite difference formulation for accelerated Monte Carlo eigenvalue calculation", Ann. Nucl. Energy, 65, 101-113, 2014.

[5] E. Wolters et. al., "Hybrid Monte Carlo CMFD Methods for Accelerating Fission Source Convergence", Nucl. Sci. Eng., 174, pp-286-299, 2013.

[6] I. Kim and Y. Kim, "A Study on CMFD Truncation of Monte Carlo Neutron Transport Solution", Trans. Kor. Nucl. Soc. Autumn Meeting, Gyeongju, Korea, October 25-27, 2017

[7] I. Kim and Y. Kim, "A Study on Deterministic Truncation of Monte Carlo Transport Solution", PHYSOR 2018, Cancun, Mexico, 2018.

[8] I. Kim and Y. Kim, "A Study on Optimization of Albedo Boundary Conditions for the Deterministic Truncation of Monte Carlo Solutions", Trans. Kor. Nucl. Soc. Spring Meeting, Jeju, Korea, May 17-18, 2018.

[9] Y.G. Jo and N. Z. Cho, "Users' Manual for McBOX – A Nuclear Reactor Analysis Monte Carlo Code Version 2," NURAPT-2018-05, Korea Advanced Institute of Science and Technology, Korea (May 2018).

[10] Y.G. Jo and N. Z. Cho, "Acceleration and Real Variance Reduction in Continuous-Energy Monte Carlo Whole-Core Calculation via p-CMFD Feedback," Nucl. Sci. Eng., 189, 26-40 (2018).