INVESTIGATION ON DETERMINISTIC TRUNCATION TO CONTINUOUS ENERGY MONTE CARLO NEUTRON TRANSPORT CALCULATION

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ABSTRACT

This paper presents the application and evaluation of a deterministic truncation of Monte Carlo (DTMC) solution method in a whole core reactor problem based on a continuous energy transport calculation. The DTMC method has been studied and developed as a systematic way to truncate the high-fidelity Monte Carlo (MC) solution to reduce the computational cost without compromising the essential reliability of the solution. Its feasibility and capability were preliminarily validated in several benchmark problems using a multi-group energy MC code. In this paper, further study has been conducted in the more practical application with the continuous-energy based MC calculation. The concept of the DTMC method is briefly described. Improvements to enhance the numerical stability and efficiency are specified in details. The DTMC method is applied to an SMR problem, in which reactor parameters are estimated to characterize the numerical performance and are compared to the standard MC method. Last, the computing time and corresponding figure-of-merit are evaluated.

KEYWORDS: MC, DTMC, FMFD, 1-node CMFD, m-PRUP method, Variance reduction

1. INTRODUCTION

The deterministic truncation of the MC (DTMC) solution method is one of the acceleration schemes which can be applied in the Monte Carlo (MC) simulation. Its feasibility has been verified and validated by the numerical analysis based mostly on the multi-group energy [2-3] and preliminarily on the continuous energy structure [4]. The results showed that the DTMC method can allow the fast convergence of the fission source distribution (FSD), reduce the computing time in the inactive cycle, and provide the accurate solution itself with the lower statistical uncertainties than the standard MC method [2-3].

In the meantime, for the efficient DTMC calculation, some more ideas have been developed and considered. The modified particle ramp-up (m-PRUP) method can determine the minimum generation size, the number of inactive cycles, and the final generation size in a systematic way for the efficient DTMC calculation. Moreover, the one-node CMFD acceleration scheme is implemented to decrease the deterministic eigenvalue calculation. In this study, the aforementioned methods are intimately applied in the MC calculation, and its numerical performance will be discussed in the SMR reactor problem.

2. METHODS

2.1. FMFD and DTMC methods accelerated by 1-node CMFD method

The coarse mesh finite difference (CMFD) method has been popularly applied in a MC simulation to decrease the numerical cost. The CMFD method quickly solves the cheap and simple deterministic finite difference method (FSD) with a current correction generated by a high-fidelity MC method, and refines the FSD of the MC in the next cycle by adjusting particles' weight. As a result, the CMFD method can accelerate the convergence of the FSD, and substantially reduce the computing time during inactive cycles.

In the meantime, according to the generalized equivalence theory, it is found out that the deterministic CMFD solutions also can accurately predict the expectation of the system attribute as a subset of solutions to the original MC approach. In short, the CMFD results can be used not only to speed up the source convergence, but also to provide the evidence for the solution prediction. In this regard, the DTMC method has been proposed for statistical treatment of the deterministic solutions which are equivalently truncated from the high-fidelity MC simulation.

However, because the local solution parameters in the CMFD method is obtained on the coarse mesh, the deep understanding of the reactor system may be infeasible such as the pin-wise detailed neutron behavior or more specifically. Therefore, the DTMC method should accompany with a fine mesh finite difference (FMFD) method. The FMFD method can provide the detailed pin flux and power distribution.

Once the reactor FMFD parameters such as the one-group constants, neutron flux, and surface currents are obtained, the neutron balance equation can be formulated such as:

$$\sum_{s=x,y,z} \frac{a_s}{v_i}(j_{s1} - j_{s0}) + s_a^i \phi_i = \frac{1}{k} \nu\sigma_f^i \phi_i \,, \tag{1}$$

where j is the net current, σ_a is the absorption cross section, σ_f is the fission cross section, ϕ is the neutron flux, a is the node surface area, v is the node volume, s indicates the surface index (i.e. $s1 = i + 1/2$ and $s0 = i - 1/2$), i is the node index, $\bar{S}_i = \frac{1}{k}\nu\sigma_f^i\phi_i$ is the fission source. The net current can be expressed with a correction factor as

$$j_{s1} = -\tilde{d}_{s1}(\phi_{i+1} - \phi_i) + \hat{d}_{s1}(\phi_{i+1} + \phi_i) \,, \tag{2}$$

where $\tilde{d} = \frac{2D_{i+1}D_i}{(D_{i+1} + D_i)\Delta_s}$ is the interface diffusion coefficient, D is the diffusion coefficient, Δ_s is the node size, $\hat{d}$ is the correction factor which can be written as

$$\hat{d}_{s1} = \frac{J_{s1}^{MC} + \tilde{d}_{s1}(\phi_{i+1}^{MC} - \phi_i^{MC})}{\phi_{i+1}^{MC} + \phi_i^{MC}} \quad \text{(3.a)}, \quad \text{and} \quad \hat{d}_\Gamma = j_\Gamma^{MC} / \phi_I^{MC} \quad \text{(3.b)} \tag{3}$$

at the interface and boundary surface respectively

By solving the FMFD equation (Eq. 1), the essential reactor parameters such as the multiplication factor and pin-wise flux profile can be calculated. This is utilized for predicting the expectation of the problem solution and improving the convergence of the FSD. However, because the FMFD method adopts the fine mesh, the number of nodes and associated matrix equation size can be significant especially in the large-scale reactor problem. Accordingly, the computing time also can be significant.

Therefore, 1-node CMFD method is applied to decrease the computing burden allocated to the deterministic FMFD and DTMC calculations. The 1-node CMFD method can reduce the eigenvalue problem size by grouping the pin data into the assembly data, and the corresponding computing time. From the FMFD method, the local pin parameters are condensed and homogenized into the global coarse nodes (normally

assembly size). The group constants, flux, and net current for the global calculation can be calculated by taking the average such as

$$\Sigma_\alpha^I = \frac{\sum_{i=1}^{N} \sigma_\alpha^i \phi_i}{\sum_{i=1}^{N} \phi_i} \text{ (4.a)}, \quad \Phi_i = \frac{1}{N}\sum_{i=1}^{N} \phi_i \text{ (4.b)}, \text{ and } \quad J_{s1} = \frac{1}{M}\sum_{s=1}^{M} j_{s1} \text{ (4.c)}, \tag{4}$$

where Σ_α is the α-type cross section in the coarse node, Φ and J are the neutron flux and current respectively for the global eigenvalue calculation, N and M are the number of pin nodes in a coarse node and pin surfaces on a coarse node surface. Then, the neutron balance equation can be rewritten on the coarse mesh basis such as:

$$\sum_{S=x,y,z} \frac{A_S}{V_I}(J_{s1} - J_{s0}) + \Sigma_a^I \Phi_I = \frac{1}{k} \nu \Sigma_f^I \Phi_I . \tag{5}$$

In the 1-node CMFD method, the net currents can be represented by the node average flux and surface flux at the both sides. By the continuity condition, the net current at the interface surfaces can be expressed with the two neighboring node fluxes such as :

$$J_{S1} = -\tilde{\delta}_{S1}(\Phi_{I+1} - \Phi_I) + \hat{\delta}_{S1}(\Phi_{I+1} + \Phi_I) \tag{6}$$

where

$$\tilde{\delta}_{S1} = \frac{\tilde{D}_I \tilde{D}_{I+1} + \hat{D}_{S1}^+ \hat{D}_{S1}^-}{\tilde{D}_I + \tilde{D}_{I+1} + \hat{D}_{S1}^+ - \hat{D}_{S1}^-} \text{ (7.a)}, \quad \hat{\delta}_{S1} = \frac{\tilde{D}_I \hat{D}_{S1}^+ + \tilde{D}_{I+1} \hat{D}_{S1}^-}{\tilde{D}_I + \tilde{D}_{I+1} + \hat{D}_{S1}^+ - \hat{D}_{S1}^-} \text{ (7.b)}, \tag{7}$$

and $\tilde{D}_I = \frac{2D_I}{\Delta_I}$, D_I is the diffusion coefficient, $\hat{D}_{S1}^- = \frac{J_{S1} + \tilde{D}_I(\Phi_{S1} - \Phi_I)}{\Phi_{S1} + \Phi_I}$ is the correction factor, and the net current at the interface surface can expressed similarly to Eq. (3.b). After the global parameters are obtained, the parameters needed for the local source can be modulated as the following:

$$\phi_i^{updated} = \Phi_I \times \frac{\phi_i}{\frac{1}{N}\sum_{i=1}^{N} \phi_i} \text{ (8.a) and } \quad j_{s1}^{\pm,updated} = J_{S1}^{\pm,} \times \frac{j_{s1}^{\pm}}{\frac{1}{M}\sum_{m=1}^{M} j_{s1}} \text{ (8.b)}, \tag{8}$$

where the lower case indices indicate the fine mesh index which belongs to the coarse mesh (i.e. $i \in I$ and $s \in S$). Meanwhile, it should be noted that the adjacent local solution at the node bordering the interface surface between the coarse nodes is not known before the local sweeping in the 1-node CMFD method where each coarse node is independently solved. Therefore, the net current at the interface surface can be expressed like

$$j_{s1} = -\tilde{d}_i(\phi_{s1} - \phi_i) + \hat{d}_{s1}^-(\phi_{i+1}^{pre} + \phi_i) . \tag{9}$$

where ϕ_{i+1}^{pre} is the neutron flux at the adjacent node before the local sweeping. From the diffusion approximation, the surface flux can be expressed in terms of the net and partial currents as:

$$\phi_{s1} = 4 j_{s1}^- + 2 j_{s1} . \tag{10}$$

By substituting Eq. (11) into Eq. (10), the net current at the interface surface can be rewritten in terms of the node flux and the partial current.

$$j_{s1} = O_{j,i}^- + \hat{\delta}_{s1}^- \phi_i + O_{f,i}^- , \tag{11}$$

where $O_{j,i}^-$ and $O_{f,i}^-$ are the surface and fission sources respectively given by

$$O_{f,i}^- = \frac{4\tilde{d}_i}{1 + 2\tilde{d}_i} J_{s1}^- \text{ (12.a)}, \text{ and } \quad O_{f,i}^- = \frac{\hat{d}_{s1}}{1 + 2\tilde{d}_i} \phi_{i+1}^{pre} \text{ (12.b)} \tag{12}$$

Then, the pin-wise detailed flux profile over the core can be calculated by solving the local fixed-source problem at all coarse nodes. With the flux and Eqs. 10 & 11, the net current, the surface flux, and the outgoing partial current can be obtained in turn. Finally, the reference net current can be calculated with the two opposite outgoing partial current at the interface, and update the correction factor for the global calculation. This global/local process is repeated until the multiplication factor converges. (Figs. 1 & 2)

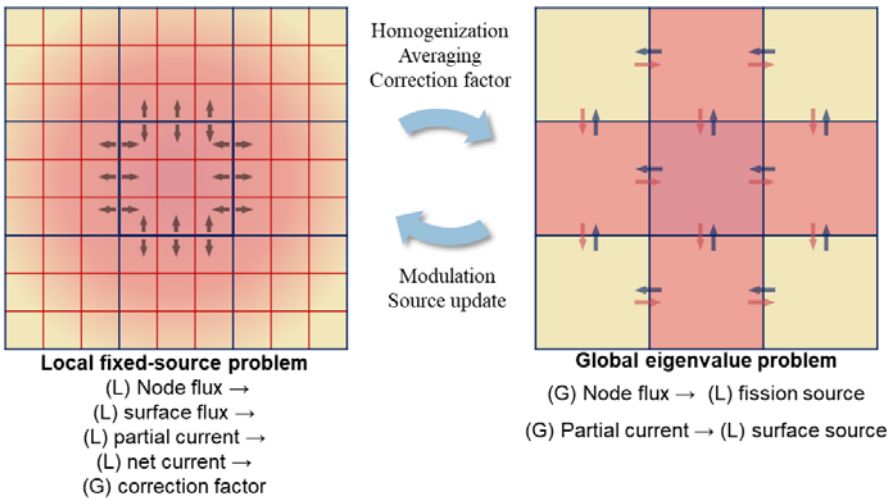

Figure 1. Diagram of FMFD method with 1-node CMFD method

2.2. m-PRUP method

The m-PRUP method can provide the proper MC calculation condition like the minimum generation size, the number of inactive cycles, and the final generation size. The proper generation size is significant particularly in the efficient FMFD and DMTC calculation because the reliability of the solutions closely depends on the reliability of the FMFD parameters.

The m-PRUP method starts with the minimum generation size, and gradually increases the generation size. The minimum generation size can be approximately estimated by taking into account the number of nodes. During the ramp-up process, the FSD convergence can be judged and determined by the convergence of the Shannon entropy [5].

In the m-PRUP method, three convergence tests are implemented to examine the proper generation size. The first one for the convergence of the FSD with the given generation size, the second one for finding the optimal generation size, and the last one for the convergence of the FSD with the optimal generation size. The convergence criteria are derived to be inversely proportional to the square root of the generation size because the Shannon entropy is also a statistical parameters and should follow the stochastic nature. (Fig. 3)

$$\varepsilon = \frac{C}{\sqrt{N}} \tag{13}$$

where the constant has been drawn and settled down from the amount of the trial and error.

Table I. Constants for the convergence and stopping criteria of the m-PRUP method.

Constant, *C*	**Standard MC**	**FMFD**
ε_1 & ε_3	1E-4	1E-3
ε_2	1E-5	1E-4

2.3. Flow diagram

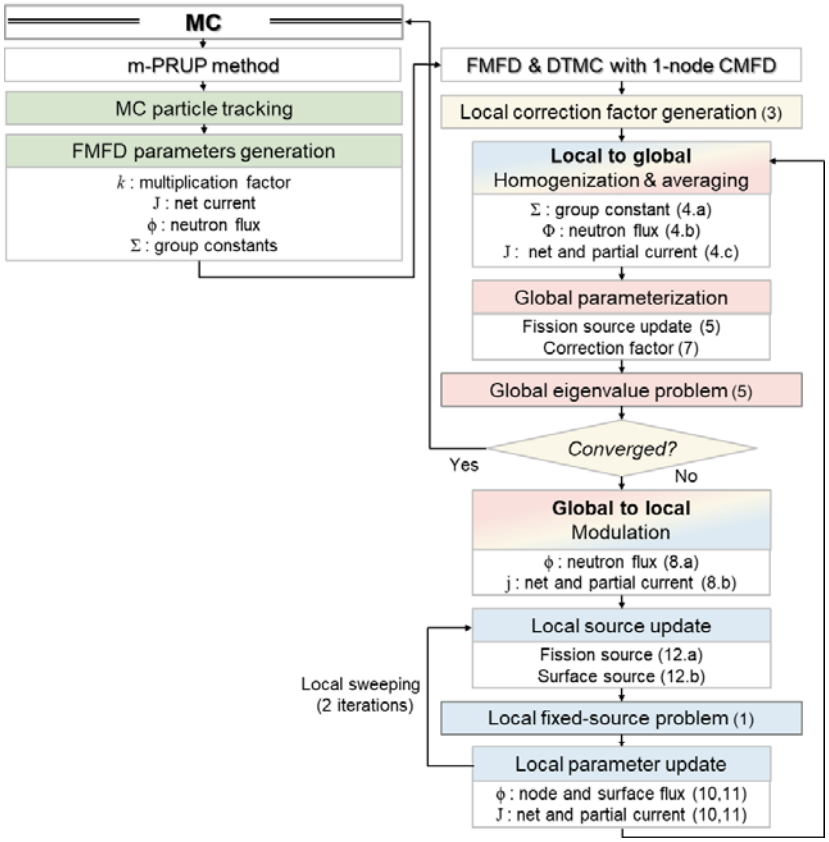

Figure 2. Flow chart of the FMFD with the 1-node CMFD method in MC simulation

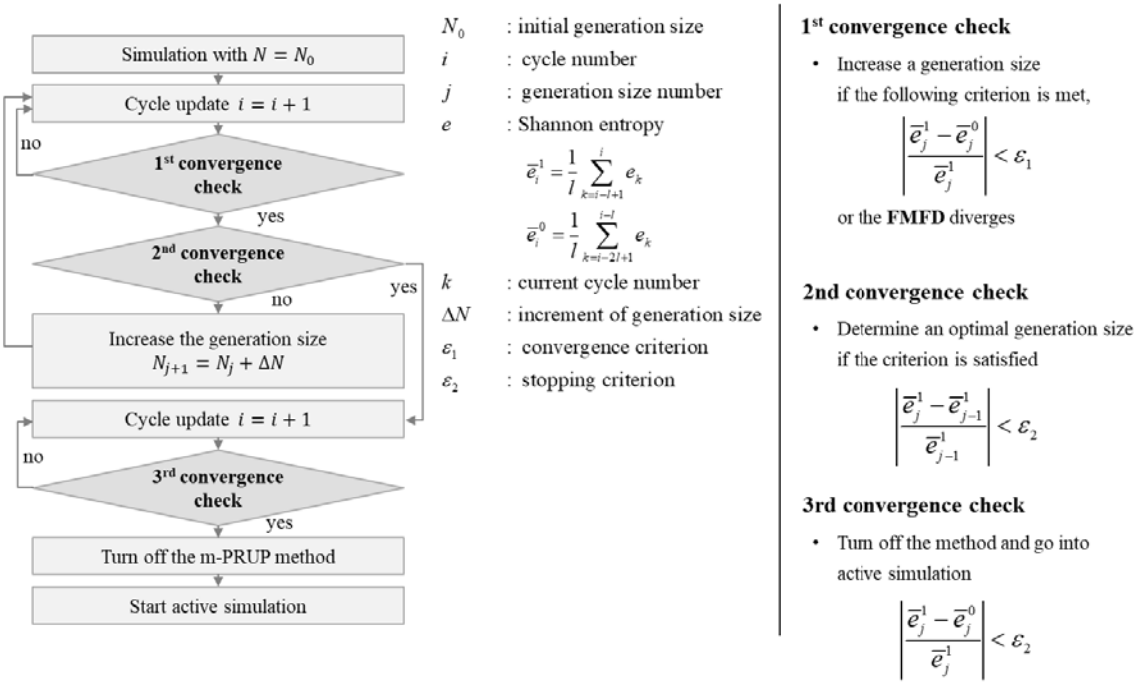

Figure 3. Algorithm of the m-PRUP method

The aforementioned methods are all intimately applied in the MC simulation. Whole calculation process is illustrated in Figures 2 and 3. The m-PRUP method first determines the generation size. It will increase the generation size until the optimal generation size is searched. Meanwhile, the MC simulation produces the FMFD parameters which can form the deterministic eigenvalue problem. The deterministic calculation is carried out with the FMFD method accelerated by the one-node CMFD method (Eq. 5), Then, the deterministic solution can update the FSD of the subsequent MC cycle as well as can be statistically processed to predict the solution.

3. NUMERICAL RESULTS

Numerical calculation has been implemented with the IMC code, which has been developed for neutronic analysis in KAIST. This code can deal with the arbitrary geometry based on the multi-level universes and the continuous energy structure with the ACE-formatted cross section library. Efficient hybrid parallel computation is provided with utilization of the MPI and OpenMP platforms. Many acceleration schemes such as the CMFD method, FMFD method, DTMC method, and m-PRUP method etc. enable a fast and efficient calculation, and T/H coupled multi-physics calculation and depletion calculation are available.

In this analysis, the continuous energy MC transport calculation was implemented by the standard MC method and the DTMC method with the 1-node CMFD acceleration. The reactor parameters were calculated and compared each other. Furthermore, numerical performance in terms of the computing time, statistical errors, and figure-of-merits (FOM) is evaluated.

3.1. Problem Description

Figures 4 and 5 describe the radial and axial configuration of an SMR reactor core. The core consists of 29 UO_2 fuel assemblies and is surrounded by the reflector. The size of the fine and coarse mesh grid are described in the figure. In the MC simulation, the number of inactive cycles and the generation size in a cycle were determined by the m-PRUP method, and 10 active cycles were used. Total 196 cores of Xeon E5-2697 with the clock speed of 2.60GHz were used for the MC calculation.

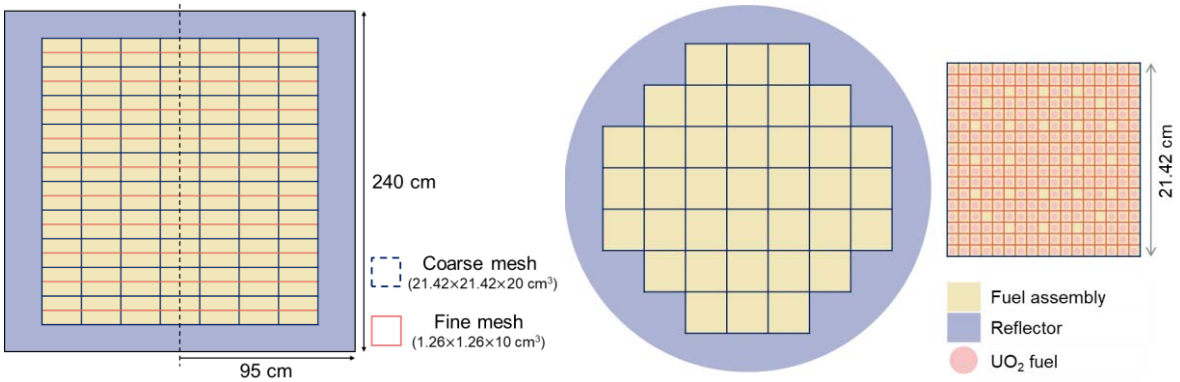

Figure 4. Reactor core configuration

3.2. Multiplication factor

Table I compares the multiplication factors and their standard deviation at the specific active cycles (i.e. 2, 3, 5, and 10). It is clear that the DTMC method had the lower standard deviation compared to the MC method. The multiplication factor of the DTMC method is quite consistent along with the simulation.

Table II. Comparison of the multiplication factor at the specific cycles

Cycle	Parameters	Standard MC	MC-FMFD	DTMC

2	k_{eff}	1.52579	1.52576	1.52675
	SD (pcm)	11.3	8.2	7.7
3	k_{eff}	1.52581	1.52576	1.52672
	SD (pcm)	9.0	5.1	6.6
5	k_{eff}	1.52581	1.52573	1.52668
	SD (pcm)	8.6	5.7	5.2
10	k_{eff}	1.52585	1.52570	1.52680
	SD (pcm)	5.9	4.4	4.0

Figure 5 depicts the cycle-cumulative real standard deviation of each method. For the calculation of the real standard deviation, 10 independent simulations have been conducted with the different random seeds. It is clear that the real standard deviation of the DTMC results was lower than that of the MC results.

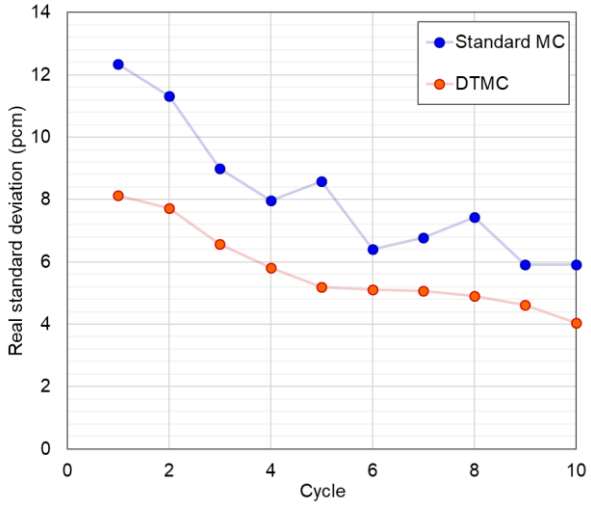

Figure 5. Cycle-cumulative standard deviation in the active cycle

3.3. Computing time and FOM

The numerical performance with regard to the variance reduction has been examined through the multiplication factor. In this section, the computing time is also compared and the corresponding FOM is estimated and compared to each method. Table III presents the number of cycles and the computing time for each method.

Table III. Comparison of the computing time

	MC	**MC-FMFD**
No. of histories per cycle	1E7	
No. of inactive cycles	100	15
No. of active cycles	10	
Inactive cycle (hr)	5.4	2.0
Active cycle (hr)	0.6	1.3
Total time (hr)	6.0	3.3

Because the standard MC method should much more inactive cycles to determine the FSD, the computing time consumed in the unnecessary calculation is significant. On the contrary, the FMFD method reduced the computing time significantly during the inactive cycle by accelerating the convergence of the FSD. The computing time in the standard MC was estimated by 5.4 hour, but reduced to 2.0 hour by the FMFD method with 1-node CMFD acceleration. However, the FMFD method consumed more time in the active cycles due to the additional deterministic calculation,

Last, the FOM for the each method was estimated and compared. Figure 6 shows the cycle-accumulated FOM. It clearly shows that the FOM of the DTMC method is much higher than that of other MC methods. It is obvious that the DTMC method can predict the solution with lower uncertainties, and also considerably reduce the computing time to obtain the converged FSD. This made it possible to have a remarkable numerical performance compared to the MC solutions.

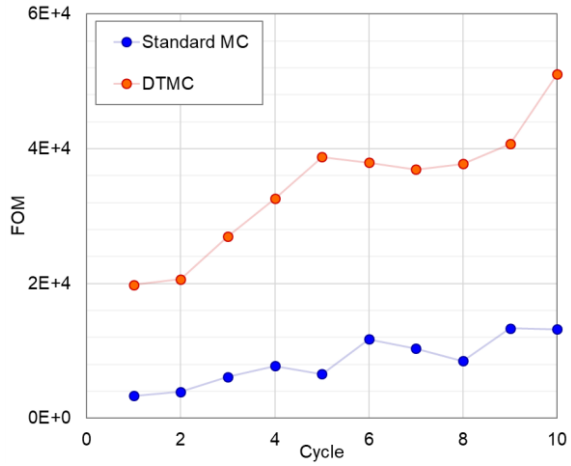

Figure 6. Cycle-cumulative FOM

4. CONCLUSIONS

For the variance reduction and acceleration of the MC simulation, the FMFD and DTMC methods are applied in conjunction with the m-PRUP method and the 1-node CMFD acceleration. The FMFD method can accelerate the convergence of the FSD. In addition, the DTMC method provided the accurate solution with lower statistical uncertainties compared to the MC solution. As a result, the DTMC method achieved mush higher numerical performance like 5 to 7 times higher FOM.

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