Evaluation of Deterministic Truncation of Monte Carlo (DTMC) Solutions with Partial Currents Fine-Mesh Finite Difference Formulations

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1. Introduction

A deterministic truncation of Monte Carlo (DTMC) solution method is one of numerical schemes developed for the acceleration of a Monte Carlo (MC) simulation and the variance reduction of the solutions. The DTMC method proceeds a statistical treatment of the deterministic solutions truncated by the fine mesh finite difference (FMFD) method in the MC calculation. The DTMC method can significantly decrease the computing time by accelerating the convergence of the fission source distribution (FSD) during inactive cycles, and also decrease the statistical errors of the reactor parameters from the early active cycles [1,2].

The DTMC method has adopted the FMFD method to truncate the MC solutions. However, in this study, the partial current based FMFD (pFMFD) method is applied to improve the numerical stability of the DTMC method. Furthermore, a decoupled DTMC scheme is newly attempted to get rid of the possible bias in the FMFD-assisted MC solutions. In this paper, the numerical performance of the pDTMC method is characterized and compared to the standard MC method in a SMR problem. The multiplication factor, pin power distribution, and its statistical uncertainties are evaluated depending on the cycle accumulation length for the generation of the FMFD parameters. Last, the computing time and figure-of-merit (FOM) are also assessed.

2. Methods and Results

2.1 DTMC and pDTMC methods

The DTMC approaches can be considered as an effort to combine the versatile MC method and the efficient deterministic method in an optimal way [1,2]. The flow diagram of the DTMC methods is described in Fig. 1. From the MC calculation, the reactor parameters necessary for the deterministic FMFD calculation can be obtained over a fine mesh grid. Then, the deterministic eigenvalue problem can be subordinately derived with the FMFD parameters. The diffusion-like equation is formulated with a correction of the net current for the FMFD method and the partial currents for the pFMFD method. By solving the matrix equation with the power method, the deterministic solutions like the multiplication factor and the pin power distribution can be determined.

These solutions can be used not only to update the FSD of the subsequent MC cycle, but also to predict the system solution. The FSD correction accelerates the source convergence; thus, it can decrease the computing time of the inactive cycles. Meanwhile, the DTMC solutions can provide accurate solutions equivalent to the high-fidelity MC solutions, while having lower statistical uncertainties because the deterministic computation is rather free from the random process.

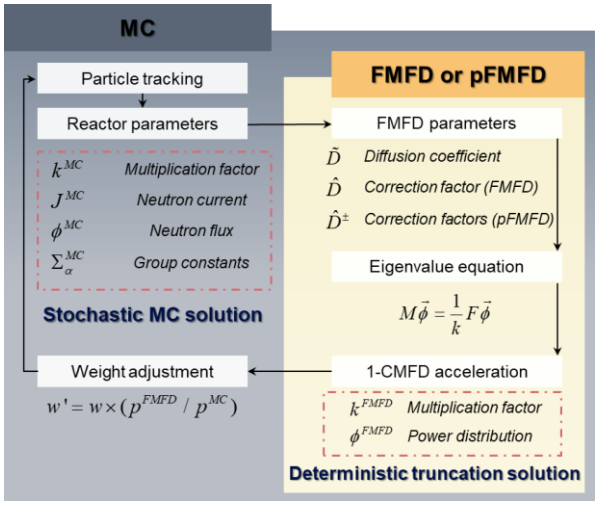

Fig. 1. Diagram of the FMFD and DTMC methods

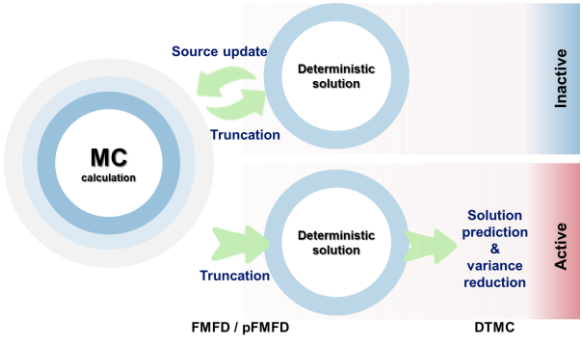

Fig. 2. Decoupled DTMC scheme

Previously, the feedback process has been applied over the whole simulation including the inactive and active cycles. However, considering the possible bias assigned to the FMFD-assisted MC calculation, the decoupled DTMC scheme is considered. As shown in Fig. 2, the FSD of the MC is only adjusted by the FMFD solutions in the inactive cycles to accelerate the convergence of the source distribution. In the active cycles, the deterministic solutions are statistically handled, but not applied back to the MC simulation. In this way, the MC calculation can run without the

deterministic contamination, and the unbiased MC solutions can be truncated.

2.2 FMFD and pFMFD methods

Given the FMFD parameters generated from the MC simulation, the one-group diffusion-like neutron balance equation can be expressed on the node i as

$$\frac{1}{V_i}\sum_{s=i,j,k} A_s(J_{s+1/2}-J_{s-1/2})+\Sigma_a^i\phi_i=\frac{1}{k_{eff}}\nu\Sigma_f^i\phi_i, \quad (1)$$

where s indicates the surface index, V is the node volume, A is the node surface area, Σ_a is the absorption cross section, J is the net current, ϕ is the neutron flux, k_{eff} is the multiplication factor, and $\nu\Sigma_f$ is the number of neutrons per fission reaction times the fission cross section. The FMFD parameters are accumulated over several contiguous cycles to be stable and reliable.

In the FMFD method [3], the net current in the *x*-direction can be written as

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

where $\tilde{D}_{i+1/2}=\frac{2D_{i+1}D_i}{(D_{i+1}+D_i)\Delta_i}$, D is the diffusion coefficient, Δ is the node size, and $\hat{D}_{i+1/2}$ is the correction factor:

$$\hat{D}_{i+1/2}=\frac{J_{i+1/2}^{MC}+\tilde{D}_{i+1/2}(\phi_{i+1}^{MC}-\phi_i^{MC})}{\phi_{i+1}^{MC}+\phi_i^{MC}}. \quad (3)$$

On the other hand, in the pFMFD method [3], the two partial currents at the interface surface are preserved, and thus the net current can be written in terms of the partial currents:

$$J_{i+1/2}=J_{i+1/2}^{+}-J_{i+1/2}^{-} \quad (4)$$

where the partial currents can be presented as

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

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

Then, the net current can be rewritten by

$$J_{i+1/2}=-\tilde{D}_{i+1/2}(\phi_{i+1}-\phi_i)+\hat{D}_{i+1/2}^{+}\phi_i-\hat{D}_{i+1/2}^{-}\phi_{i+1} \quad (7)$$

where $\hat{D}_{i+1/2}^{\pm}$ is the correction factors:

$$\hat{D}_{i+1/2}^{+}=\frac{J_{i+1/2}^{+,MC}+0.5\tilde{D}_{i+1/2}(\phi_{i+1}^{MC}-\phi_i^{MC})}{\phi_i^{MC}}, \text{ and} \quad (8)$$

$$\hat{D}_{i+1/2}^{-}=\frac{J_{i+1/2}^{-,MC}-0.5\tilde{D}_{i+1/2}(\phi_{i+1}^{MC}-\phi_i^{MC})}{\phi_{i+1}^{MC}} \quad (9)$$

The two correction factors at each interface surface would consolidate the nodal equivalence with one more degree of freedom contrary to the FMFD method [4].

2.3 m-PRUP and 1-CMFD methods

To enhance the numerical stability, the modified particle ramp-up (m-PRUP) method has been developed. It can determine the inactive cycle size and the generation size in a systematic way and also provide additional acceleration [1,5]. Furthermore, the one-node CMFD acceleration scheme has been also considered to speed up the deterministic FMFD calculation [2]. The details will not be discussed in this paper.

2.4 Apparent and real standard deviations

In the MC calculation, the reactor parameters should be statistically treated to understand the average behavior. The parameters are averaged over cycles, and its reliability is estimated by the standard deviation. However, due to the cycle correlation, the standard deviation estimated from a single MC run, so called apparent standard deviation (σ_a), could be under-estimated. Therefore, the real standard deviation (σ_r) should be calculated by accounting for numerous independent batches with the different random seeds.

The apparent standard deviation (SD) of the multiplication factor at the specific batch *b* can be calculated by

$$\sigma_a^b=\sqrt{\frac{1}{N_c(N_c-1)}\sum_{c=1}^{N_c}(\bar{k}^b-k_c^b)^2} \quad (10)$$

where *c* is the active cycle index, *b* is the batch index, N_c is the number of active cycles, k_c^b is the multiplication factor at the cycle *c* of the batch *b*, and

$$\bar{k}^b=\frac{1}{N_c}\sum_{c=1}^{N_c}k_c^b. \quad (11)$$

In the meantime, the real SD can be calculated with the amount of the independent batches.

$$\sigma_r=\sqrt{\frac{1}{N_b-1}\sum_{b=1}^{N_b}(k^*-\bar{k}^b)^2} \quad (12)$$

where N_b is the number of batches, and

$$k^*=\frac{1}{N_b}\sum_{b=1}^{N_b}\bar{k}^b \quad (13)$$

For the power distribution, the apparent and real SDs are calculated at each node similarly to Eqs. (10) and (12). Therefore, the apparent SD is estimated by

$$\sigma_{a,(i,j,k)}^b=\sqrt{\frac{1}{N_c(N_c-1)}\sum_{c=1}^{N_c}(\bar{p}_{(i,j,k)}^b-p_{c,(i,j,k)}^b)^2} \quad (14)$$

and the real SD is estimated by

$$\sigma_{r,(i,j,k)}=\sqrt{\frac{1}{N_b-1}\sum_{b=1}^{N_b}(p_{(i,j,k)}^*-\bar{p}_{(i,j,k)}^b)^2} \quad (15)$$

where $p_{c,(i,j,k)}^b$ is the normalized power value at the node (*i*,*j*,*k*) at the cycle *c* of the batch *b*,

$$\bar{p}_{(i,j,k)}^b=\frac{1}{N_c}\sum_{c=1}^{N_c}p_{c,(i,j,k)}^b \quad (16)$$

and

$$p_{(i,j,k)}^*=\frac{1}{N_b}\sum_{b=1}^{N_b}\bar{p}_{(i,j,k)}^b \quad (17)$$

Last, the node-wise SDs are averaged over the whole nodes:

$$\sigma = \frac{1}{N_n}\sum_{i,j,k}\sigma_{(i,j,k)} \quad (18)$$

where N_n is the total number of fine nodes.

2.5 Problem description

A SMR problem is considered for the evaluation of the pDTMC method. The core consists of 7 by 7 UO_2 fuel assemblies with the zig-zag shape at the corner and is surrounded by a water reflector (Fig. 3).

Neutronic analysis is implemented with an in-house MC code named iMC. In the simulation, the number of inactive cycles (see Table II) and histories (i.e. 5E+6 histories per cycle) were determined by the m-PRUP method [5], and 10 active cycles were considered. For the real standard deviation, 60 samples for the MC and 40 samples for the DTMC methods were surveyed.

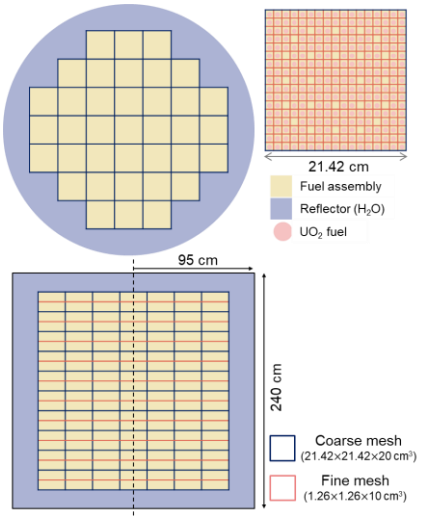

Fig. 3. Core configurations

2.5 Neutronic analysis

The statistical reliability of the reactor parameters such as the multiplication factor and pin power distribution is compared with respect to the standard deviations (SD), and the computing time and associated figure-of-merit (FOM) are evaluated.

Figures 4 presents the real SD of the multiplication factor for the conventional and decoupled pDTMC methods (i.e. pDTMC and pDTMC-d, respectively). The decoupled pDTMC approach showed similar numerical performance with the conventional DTMC approach. The pDTMC methods attain much lower real SDs compared to the standard MC method because the pDTMC method can rigorously constrain a neutron balance for the production and loss to be identical in the steady-state condition. The real SD of the pDTMC method seems decreasing with increasing the cycle accumulation length although the more cases should be sampled to reduce the uncertainty. However, the real to apparent SD ratio is definitely lower with the less cycle accumulation (Fig. 5). For the single cycle (l=1), the SD ratio is quite close to the unity.

The similar behavior is observed in the pin power distribution (Figs. 6 & 7). The pDTMC methods also demonstrate higher reliability than the MC method though the decrement is not significant as much as that of the multiplication factor. However, it is clearly observed that the real SD of the pDTMC methods is decreasing with increasing the accumulation length.

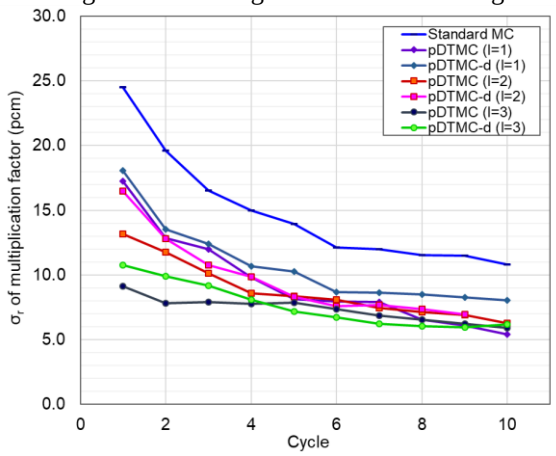

Fig. 4. Real SD of k_{eff}

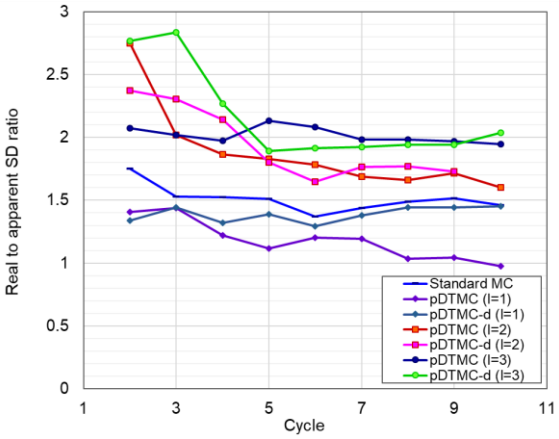

Fig. 5. Real to apparent SD ratio for k_{eff}

Table II specifies the computing time consumed for neutronic analysis with the MC code depending on the methods. Total 56 cores of Xeon E5-2697 with clock speed of 2.60 GHz were used. It should be noted that the computing time of the both MC and pFMFD methods is already shorten by the m-PRUP method. Therefore, both cases are still faster than the standalone MC simulation.

Because the pFMFD method can significantly decrease the number of inactive cycles necessary to obtain the converged FSD, the computing time can be accordingly reduced. Due to the additional deterministic calculation, the pFMFD method should pay a little bit more numerical cost in the active cycle, but the total computing time is still less than the standard MC method.

As a result, the pDTMC approach can achieve the much higher FOMs in both multiplication factor and

power distribution (Figs. 8 & 9). The DTMC methods have roughly 3-5 times higher FOM for the multiplication factor and 40% to 400% higher FOM for the power profile. The higher FOMs also can be observed with the more accumulation length particularly in the power distribution.

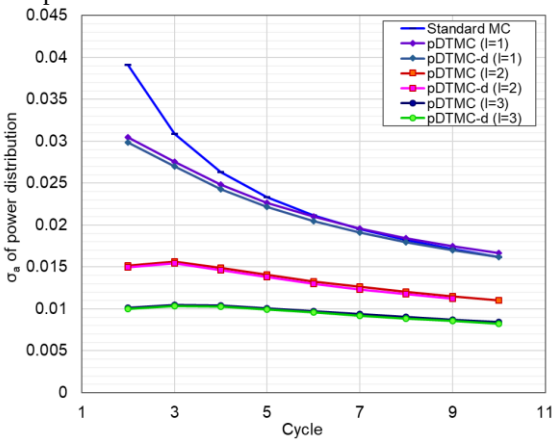

Fig. 6. Apparent SD of power distribution

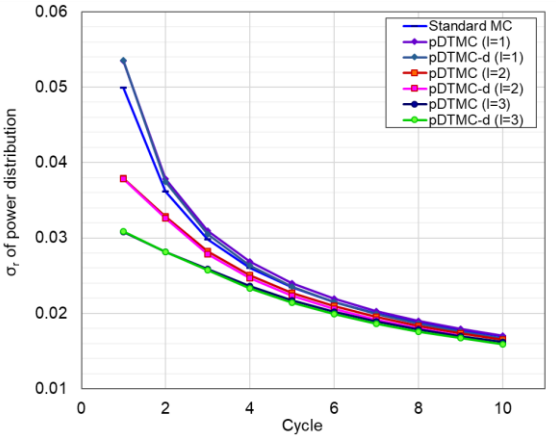

Fig. 7. Real SD of power distribution

Table II. Computing time of each method

Time	MC	pFMFD
No. of inactive cycles	44	7
Inactive cycle (min.)	59	31
Active cycle (min.)	37	39
Total (hr.)	1.6	1.2

3. Conclusions

A decoupled DTMC scheme based on the pFMFD corrections has been proposed to get rid of the possible bias in the FMFD-coupled MC solutions, and the decoupled pDTMC solutions turn out to be similar to the conventional DTMC solutions in terms of the statistical uncertainties and computing time. The pDTMC method consistently provides smaller real SD of the multiplication factor compared with the standard MC approach. The pDTMC solutions are sensitive to the accumulation length of the active MC cycle. The real-to-apparent SD ratio of the k_{eff} value is close to 1 when the FMFD equation is formulated independent every cycle, i.e., l=1. Meanwhile, a bigger accumulation length results in a clearly reduced real SD in the pin-wise power distribution, whereas the apparent SDs become clearly smaller than the real ones. A further study to determine the optimal accumulation length is underway to maximize the benefits of the DTMC method.

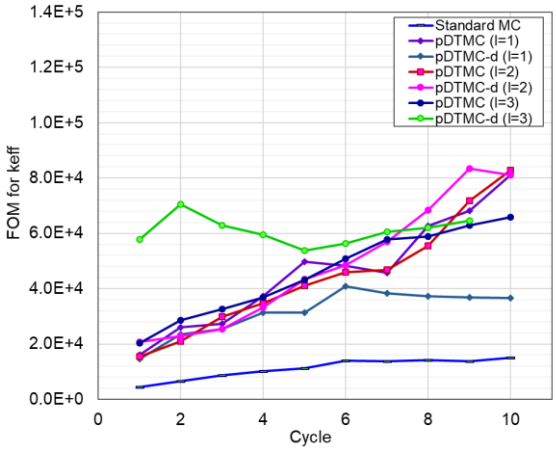

Fig. 8. FOM for k_{eff}

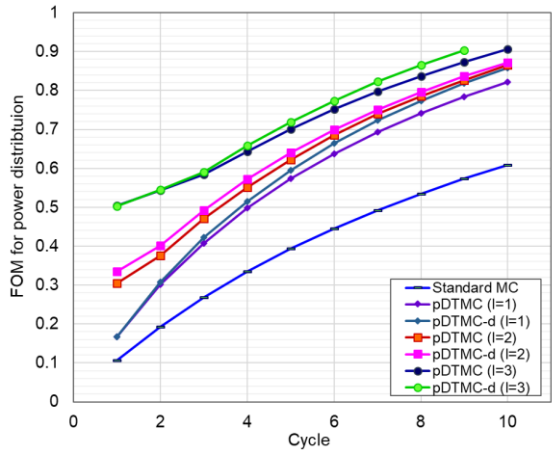

Fig. 9. FOM for power distribution

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