Application of 1-Node CMFD Acceleration in DTMC Method

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1. Introduction

The deterministic truncation of Monte Carlo (DTMC) solution method was proposed as a variance reduction technique applied in the MC simulation [1]. The previous study demonstrated that the DTMC method can decrease the stochastic uncertainty and computing time by estimating the solution with a reasonable precision even from the early active cycle [2]. The DTMC method should be further studied in the more realistic large-scale reactor model. In this case, the numerical cost paid in the deterministic calculation such as generating the group constants and solving the matrix equation can be a concern because of an amount of FMFD nodes and the corresponding matrix size. Therefore, in this study, 1-node CMFD acceleration scheme was applied to decrease the computing burden of the FMFD calculation. The numerical performance was estimated and compared in the DTMC method with and without the 1-node CMFD acceleration.

2. Methods

2.1 1-node CMFD acceleration

The 1-node CMFD method is applied to accelerate the deterministic FMFD calculation. The theory and detailed formulas are presented [3-5] in this section. The flow diagram is described in the Fig. 1. The reactor parameters such as the neutron current, flux, and group constants can be calculated from the MC simulation for the deterministic eigenvalue problem.

First, the global calculation is implemented. The typical CMFD grid is set to be fuel assembly size. The group constants are obtained by homogenizing the local parameters over the coarse node, and the correction factor is calculated on the node surfaces. The reactor parameters such as the multiplication factor, flux distribution, and the partial current can be calculated. Because the problem size is considerably decreased with the coarse mesh grid system, the computing time can be shortened.

The solution of the global calculation can update the local parameters such as the flux and partial current distribution with the modulation process. The corrected flux and partial current information can update the source information. The fission source can be updated with the flux distribution, and the current source can be updated with the partial current distribution. Because the local calculation is a fixed-source problem, the equation is independently solved at a time for each node. In turn, the local solution updates the group constants and the correction factor for the global calculation. This process is repeated until the global multiplication factor is within the tolerance (1E-9).



Fig. 1. Flow diagram FMFD with 1-node CMFD

In the 1-node CMFD formulation, the net current at the surface is represented by the surface flux and the node average flux such as

$$J_{I+1/2}^{-\varepsilon} = -\tilde{D}_{I} \left(\Phi_{I+1/2} - \Phi_{I} \right) + \tilde{D}_{I+1/2}^{-} \left(\Phi_{I+1/2} + \Phi_{I} \right), \text{ and } (1)$$

$$J_{I+1/2}^{+\varepsilon} = -\tilde{D}_{I+1} \left(\Phi_{I+1} - \Phi_{I+1/2} \right) + \tilde{D}_{I+1/2}^{+} \left(\Phi_{I+1} + \Phi_{I+1/2} \right), (2)$$

where Φ is the homogenized neutron flux of the coarse node, \tilde{D} is the interface diffusion coefficient, and \hat{D} is the correction factor. The correction factor for the global calculation can be calculated as

$$\hat{D}_{I+1/2}^{+} = \frac{\bar{J}_{I+1/2}^{ref} + \tilde{D}_{I+1}(\Phi_{I+1} - \Phi_{I+1/2})}{\Phi_{I+1} + \Phi_{I+1/2}}, \text{ and } (3)$$

$$\hat{D}_{I+1/2}^{-} = \frac{\bar{J}_{I+1/2}^{ref} + \tilde{D}_{I}(\Phi_{I+1/2} - \Phi_{I})}{\Phi_{I+1/2} + \Phi_{I}} \quad . \tag{4}$$

By the current continuity condition at the interface, the surface flux can be expressed in terms of the two neighboring average flux. Inserting the surface flux into Eqs. (1) and (2), the net current can be reformulated as

$$J_{I+1/2} = -\tilde{\delta}_{I+1/2}(\Phi_{I+1} - \Phi_{I}) + \hat{\delta}_{I+1/2}(\Phi_{I+1} + \Phi_{I}), \text{ and } (5)$$

$$J_{I-1/2} = -\delta_{I-1/2}(\Phi_I - \Phi_{I-1}) + \delta_{I-1/2}(\Phi_I + \Phi_{I-1}), \quad (6)$$

where

$$\tilde{\delta}_{I+1/2} = \frac{\tilde{D}_{I}\tilde{D}_{I+1} + \hat{D}_{I+1/2}^{+}\hat{D}_{I-1/2}^{-}}{\tilde{D}_{I} + \tilde{D}_{I+1} + \hat{D}_{I+1/2}^{+} - \hat{D}_{I-1/2}^{-}} , \text{ and } (7)$$

$$\hat{\delta}_{I+1/2} = \frac{\tilde{D}_I \hat{D}_{I+1/2}^+ + \tilde{D}_{I+1} \hat{D}_{I+1/2}^-}{\tilde{D}_I + \tilde{D}_{I+1} + \hat{D}_{I+1/2}^+ - \hat{D}_{I+1/2}^-} .$$
(8)

The group constants can be calculated in a conventional way (i.e. flux- and volume- weighted cross section). From the global calculation, the multiplication factor and the node average flux can be obtained. Because it is based on the 1-node CMFD method, the node information is not really connected to the neighboring nodes. Therefore, the data sweeping is necessary to update and improve the next iteration. The incoming partial current at the boundary surface can be updated by using the node average flux, which will give the source information in the local calculation. The global sweeping is repeated 5 times. If its eigenvalue solution is not within the tolerance, the local calculation is conducted.

The local calculation is the conventional two-node FMFD calculation, but the pin-wise source distribution can be calculated with the global solution such as

$$S_{i}^{l} = \frac{1}{k} \nu \Sigma_{f,I} \phi^{i^{*}} , \qquad (9)$$

and

$$\phi^{i^*} = \frac{\phi^i}{\sum_{j=1}^N \phi^j} \times \Phi^I \quad , \tag{10}$$

where I is the coarse node index, and i is the fine node index which belong to the node I.

Since the data is from the one-node global calculation, each surface of the coarse node is the boundary in the local calculation. Therefore, the net current between the coarse nodes should be treated with the incoming partial current. The net current with the correction factor can be expressed as

$$J_{i+1/2}^{l} = -\tilde{D}_{i}^{l}(\phi_{i+1/2} - \phi_{i}) + \hat{D}_{i+1/2}^{l-}(\phi_{i+1}^{pre} + \phi_{i}), \text{ and } (11)$$

$$J_{i-1/2}^{l} = -D_{i}^{l}(\phi_{i} - \phi_{i-1/2}) + D_{i-1/2}^{l+}(\phi_{i} + \phi_{i-1}^{pre}), \quad (12)$$

where the correction factor is obtained by

$$\hat{D}_{i+1/2}^{l-} = \frac{J_{i+1/2}^{MC} + \tilde{D}_{i+1/2}^{l}(\phi_{i+1}^{MC} - \phi_{i}^{MC})}{\phi_{i+1}^{MC} + \phi_{i}^{MC}}, \text{ and } (13)$$

$$\hat{D}_{i-1/2}^{l+} = \frac{J_{i-1/2}^{MC} + \tilde{D}_{i-1/2}^{l} (\phi_{i}^{MC} - \phi_{i-1}^{MC})}{\phi_{i}^{MC} + \phi_{i-1}^{MC}} \,. \tag{14}$$

From the diffusion approximation, the surface flux given in Eqs. (11) and (12) can be expressed in terms of the partial current as follows:

$$\phi_{i+1/2} = 4J_{i+1/2}^{l-} + 2J_{i+1/2}^{l}$$
, and (15)

$$\phi_{i-1/2} = 4J_{i-1/2}^{l+} - 2J_{i-1/2}^{l} \tag{16}$$

Inserting Eqs. (15) and (16) into (11) and (12), the final form of the net current at the boundary surface can be expressed as

$$J_{i+1/2}^{l} = -\frac{4\tilde{D}_{i}^{l}}{1+2\tilde{D}_{i}^{l}}J_{i+1/2}^{l-} + \frac{\tilde{D}_{i}^{l}+\tilde{D}_{i+1/2}^{l}}{1+2\tilde{D}_{i}^{l}}\phi_{i} + \frac{\tilde{D}_{i+1/2}^{l}}{1+2\tilde{D}_{i}^{l}}\phi_{i+1}^{pre}$$
(17)

and

$$J_{i-1/2}^{l} = +\frac{4\tilde{D}_{i}^{l}}{1+2\tilde{D}_{i}^{l}}J_{i-1/2}^{l+} - \frac{(\tilde{D}_{i}^{l} - \hat{D}_{i-1/2}^{l})}{1+2\tilde{D}_{i}^{l}}\phi_{i} + \frac{\hat{D}_{i-1/2}^{l}}{1+2\tilde{D}_{i}^{l}}\phi_{i-1}^{pre}.$$
(18)

The local calculation is a fixed source problem. Thus, the flux distribution can be obtained in a single iteration. Then, the detailed pin flux distribution can be obtained. With this information, the net current, surface flux, and outgoing partial current can be calculated for the next global iteration. Finally, the reference net current for the global calculation can be updated. This whole process is repeated until the multiplication factor converges.

Comparing to the conventional FMFD method without the 1-node CMFD acceleration scheme, the additional procedures are necessary to generate the global parameters. This can slightly increase the computing time in a single iteration. However, because the global calculation can quickly update the source information, the total number of iterations and the resulting total computing time can be substantially decreased.

3. Numerical results

In this analysis, *i*MC computer code was used, which has been developed in KAIST for the reactor analysis based on the Monte Carlo method. It can handle any complex geometry based on the multi-level universe constructive solid geometry (CSG) scheme, and continuous energy calculation with ACE format cross section library. Hybrid parallel calculation with OpenMP and MPI is available. Various variance reduction techniques are applied, and the depletion, multi-physics, and time-dependent calculation are being developed.

An SMR size core problem is solved to characterize the numerical performance and efficiency of the FMFD and DTMC method with the 1-node CMFD acceleration. The configuration of the reactor core is described in Figs. (2) and (3).



Fig. 2. Radial configuration and CMFD grid

In the radial direction, the fine mesh is set to be pin size (1.26 cm), and coarse mesh is set to be assembly size (21.42 cm). On the other hand, the axial node size for the FMFD method is 10 cm, and the coarse node covers two find nodes so as to be 20 cm. Therefore, the DTMC method can provide the detailed pin power distribution. The more detailed flux profile inside the nodes can be reproduced by coupling the high-fidelity MC solution. The total number of fine nodes is more than 100,000, while the coarse nodes are only 360. In this simulation, 3,000,000 histories per cycle is used, and 50 active cycle calculation is implemented to estimate the reactor parameters.

Fig 4. describes the convergence behavior of the FSD by the Shannon entropy, and compares between the

standard MC and the FMFD-assisted MC method. The FMFD method can substantially accelerate the convergence of the FSD particularly in the big-size problem. The FMFD methods showed similar results regardless of the 1-node CMFD application. In the SMR problem, the standard MC method requires more than 150 inactive cycles to obtain the converged FSD, while the FMFD method only requires more than 20 inactive cycles. Therefore, the corresponding computing time necessary in the inactive cycle also can be significantly decreased.



Fig. 3. Axial configuration of the SMR core



Fig. 4. Convergence behavior of the FSD

However, the computing time per cycle is inevitably increase in the FMFD method compared to the standard MC method because the additional calculation is required to generate the FMFD parameters, conduct the power iteration, and solve the matrix equation. Table I shows the cycle-wise and total computing time for each method. The FMFD and DTMC methods without the acceleration spent 80 seconds more than the standard MC method in the inactive cycle, and 20 seconds more in the active cycle on the average. This time increase is quite noticeable because it accounts for almost 30 percent of the entire time in each cycle.

Parameter			FMFD / DTMC		
		Standard	w/o	w/	
		MC	1-node	1-node	
			CMFD	CMFD	
No. of	inactive	150	20	20	
cycles	active	50	50	50	
Time per cycle (sec)	inactive	214	279	216	
	active	211	268	203	
Total time (hr)	inactive	8.9	1.5	1.2	
	active	2.9	3.7	2.8	
	total	11.8	5.3	4.0	

Table I. Comparison of the computing time

Table II. Specific computing time for FMFD and	
DTMC method with and without 1-node CMFD	

		FMFD/DTMC		
Con	puting time	w/o	w/	
for single cycle (sec)		1-node	1-node	
		CMFD	CMFD	
Inactive	MC	228.7	214.6	
	Deterministic	50.0	1.3	
Active	MC	215.4	202.0	
	Deterministic	52.7	1.3	

In the meantime, the application of the 1-node CMFD acceleration in the FMFD method can reduce the computing time of the deterministic calculation from 68 seconds to 1 second in the inactive cycle. In short, the 1-node CMFD acceleration attained over 95% speedup, and made the deterministic calculation insignificant on the entire simulation. As a result, the FMFD and DTMC methods with the 1-node CMFD acceleration spend just similar computing time with the standard MC method in the active simulation.

Even though the FMFD and DTMC methods require longer cycle-wise computing time than the standard MC method, the total computing time is still shorter in the FMFD and DTMC methods due to the significant time reduction in the inactive cycle. Furthermore, the CMFD scheme decreased the time even more by accelerating the deterministic calculation.

Table III.	Comparison	of FOM for k_{eff}	

Parameter	Standard MC	w/o 1-node CMFD		w/ 1-node CMFD	
		FMFD	DTMC	FMFD	DTMC
keff	1.50859	1.50822	1.50852	1.50831	1.50861
SD (pcm)	6.4	7.3	2.6	6.1	2.6
Time (hr)	11.8	5.3	5.3	4.0	4.0

FOM	5777	9857	78402	18786	100265
Ratio	1.0	1.7	13.6	3.3	17.4

Last, the numerical performance is compared with respect to the multiplication factor. The multiplication factor and the associated standard deviation are calculated, and the computing time and the FOM are estimated and compared. The DTMC method can decrease the stochastic uncertainty from the early cycle compared to the standard MC method. As a result, the DTMC method showed higher numerical efficiency even without the CMFD acceleration. Moreover, the numerical performance of the DTMC method is much improved with the CMFD acceleration about 15 times higher than the standard MC result.

4. Conclusions

The 1-node CMFD acceleration scheme was applied to the FMFD and DTMC methods to decrease the numerical cost for the deterministic calculation. The numerical performance of the 1-node CMFD method was validated in the benchmark problem. It decreased the computing time of the deterministic calculation over 98%, and thus increased the FOM of the multiplication factor almost 9 times more compared to the standard MC method.

This application can improve the performance more effectively in a bigger size reactor problem which has a higher dominance ratio. Furthermore, the one-node CMFD is suitable for the parallel calculation because the local calculation can be conducted independently at each coarse node. Therefore, the numerical cost can be more decreased by applying the parallel mechanism in the CMFD calculation.

REFERENCES

[1] Inhyung Kim and Yonghee Kim, "A Study on CMFD Truncation of Monte Carlo Neutron Transport Solution", Proceedings of KNS Autumn Meeting, Gyeongju, Korea, October 2017.

[2] Inhyung Kim and Yonghee Kim, "A Study on Deterministic Truncation of Monte Carlo Transport Calculation", Proceedings of Reactor Physics Meeting, Cancun, Mexico, April 2018.

[3] Seongho Song, Hwanyeal Yu, and Yonghee Kim, "One-Node and Two-Node Hybrid Coarse-Mesh Finite Difference Algorithm for Efficient Pin-by-Pin Core Calculation", Nuclear Engineering and Technology, 50:3, pp. 327-339, April 2018.

[4] Seongho Song, "Pin-by-Pin Core Calculation with NEMbased Two-Level CMFD Algorithm", Master's Thesis, KAIST, 2016.

[5] Yonghee Kim, "The One-Node CMFD Computational Framework for Highly Parallel Reactor Analysis", Proceedings of the KNS 2016 spring meeting, Daejeon, May 2016.