First-Order Perturbation for Uncertainty Quantification in the Deterministic Truncation of Monte Carlo Method

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INTRODUCTION

The Monte Carlo (MC) method is widely adopted by reactor physics and radiation transport calculations due to its tractability when handling complex geometries. However, the method requires tremendous amount of time for tracking sufficient number of particles in order to reduce its stochastic uncertainty. One of efforts to alleviate this costly computation is Coarse-mesh Finite Difference (CMFD)-assisted MC method, and widely used for acceleration of fission source distribution (FSD) [1,2]. Based on this conventional CMFD-assisted MC calculation, a deterministic truncation of MC (DTMC) is proposed by Kim and Kim [3] as a variance reduction technique, and numerically showed reduced variances compare to solution from conventional method. In this study, a new approach to evaluate uncertainty of the multiplication factor from CMFD parameters is suggested for DTMC, and the method is expected to be extended for pin-power distribution. CMFD parameters from sufficiently converged inactive cycles are used to predict uncertainties of the very first active cycle, as the ultimate purpose of DTMC is to determine the solution only with a single active cycle. As a preliminary study, standard deviation predicted from the method is compared with real standard deviation obtained from multiple independent batch calculations.

METHODOLOGY

In this section, key ideas of the DTMC method are discussed before an introduction to the new variance estimation strategy. For the variance evaluation method, two approaches are suggested to test feasibility of first order perturbation formula application.

DTMC Overview

The CMFD acceleration for MC calculation is used for faster convergence of fission source distribution (FSD) in inactive cycles. Figure 1 illustrates the basic flow of CMFD application for MC neutron transport simulation. One group CMFD parameters such as diffusion coefficient and reaction cross sections are calculated in MC simulation, and CMFD correction factor is calculated from surface net current and node-wise neutron flux from the following formula:

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

These CMFD parameters are then applied to the following deterministic eigenvalue problem equation in order to update FSD:

$$\mathbf{M}\Phi = \frac{1}{k}\mathbf{F}\Phi. \quad (2)$$

Here, **M** is a neutron migration operator and **F** is a fission source operator.

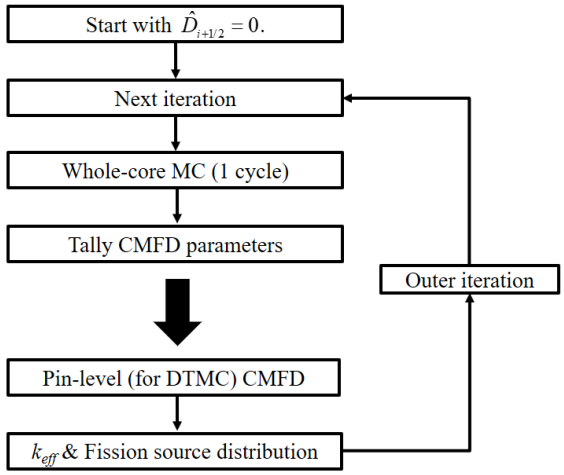

Fig. 1. CMFD accelerated MC neutron transport flow chart

In the CMFD accelerated MC, multiplication factor and reaction rates are calculated both from the MC calculation and the CMFD calculation. According to Kim and Kim [3], solution from CMFD calculation had less variance compare to MC solution, therefore use of CMFD step solution can reduce required number of active cycles to get small enough uncertainty. In DTMC method, coarse-mesh size is reduced to sub-pin level to obtain detailed reaction rate information from CMFD calculation.

Variance Estimation from CMFD Parameters

A conventional way of evaluating reactor parameters and their uncertainties from Monte Carlo calculation is the use of multiple active cycles. Here, the reactor parameters, such as multiplication factor and fission reaction rate,

directly from the MC cycles are used to calculate averages and variances. In the DTMC method, additional parameters are obtained from the MC calculation steps; CMFD parameters are calculated in every cycle. Instead of directly evaluating variances of the reactor parameters the following process can be considered:

i) Calculate variances of the CMFD parameters (From N number of MC cycles).
ii) Let the CMFD parameters have the following normal distribution [4]:

$$p(x_i) = \frac{1}{\sigma_i \sqrt{2\pi}} \exp\left(-\frac{(x_i - \mu_i)^2}{2\sigma_i^2} \right) \quad (3)$$

iii) Sample the CMFD parameters from the normal distributions (M number of samples), then calculate the reactor parameters.
iv) Calculate variances of reactor parameters which are calculated from step iii).

For step iii), a conventional eigenvalue problem can be considered for multiplication factor calculation:

$$\mathbf{M}\Phi = \frac{1}{k}\mathbf{F}\Phi, \quad (4)$$

or, the following first-order perturbation formula can be considered for faster computation:

$$\Delta\rho = \frac{\left(\Phi_0^*, [\lambda_0 \Delta\mathbf{F} - \Delta\mathbf{M}]\Phi_0\right)}{\left(\Phi_0^*, \mathbf{F}_0\Phi_0\right)}, \quad (5)$$

where, $\mathbf{M} = \mathbf{M}_0 + \Delta\mathbf{M}$ and $\mathbf{F} = \mathbf{F}_0 + \Delta\mathbf{F}$. The solution from Eq. (4) will be considered as a reference for the solution from Eq. (5) since the first-order perturbation formula can quickly calculate an approximated solution, but its error can be significant if the perturbation is not small enough.

NUMERICAL RESULTS

The suggested standard deviation (SD) methods were tested with the 3-dimensional unrodded C5G7 benchmark problem illustrated in Fig. 1 [5]. The reactor was axially divided into 3 equal meshes with pin-level radial sizes. The MC runs were simulated with 1.5 million histories and tallied CMFD parameters of D, $\hat{D}$, Σ_a, and $\nu\Sigma_f$ at each cycle. Also, 30 independent batches were used to calculate real SD (RESD) of the simulations.

Figs. 3 and 4 presents the numerical results from the simulations. The new method of SD estimation conservatively predicts SD compare to the real standard deviation (RESD). The two results from Eqs. (4) and (5) were well matched as cross section perturbation was small. Eq. (4) needed power iteration which requires significant computation time, while the use of first-order perturbation formula significantly reduced the additional computational load. In this simulation, 1000 samples were taken from the CMFD parameter distributions, and the power iteration took around 300 seconds, while solving the Eq. (5) required less than a second.

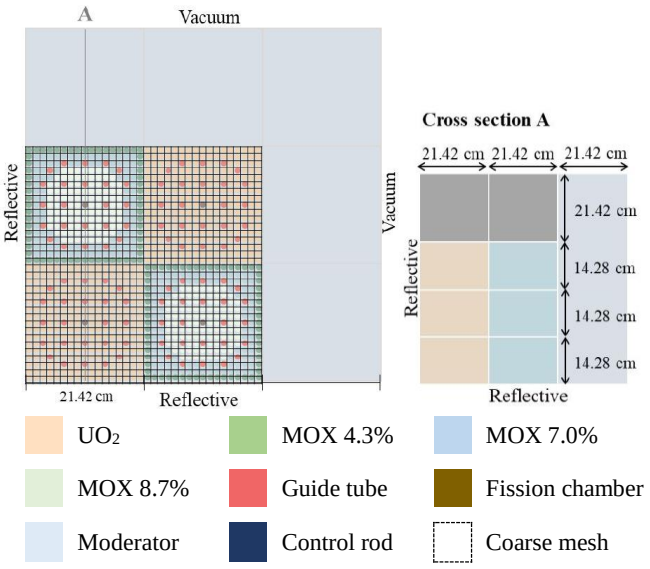

Fig. 2. Configuration of C5G7 unrodded core

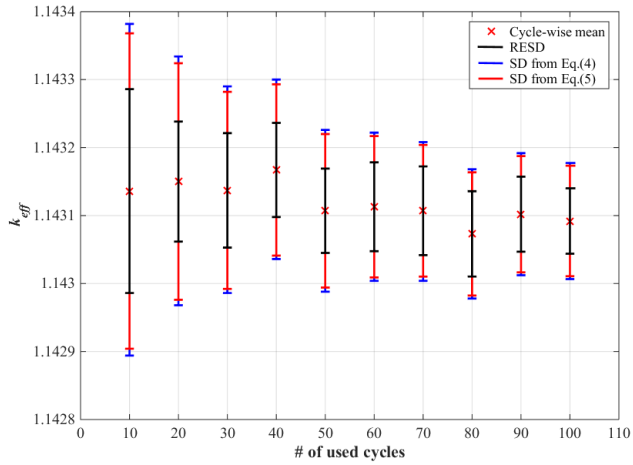

Fig. 3. Estimated k_{eff} values with SDs

The SD estimation from CMFD parameters overestimated up to 10 pcm with the use of small number of cycles. However, the discrepancy was decreased to a few pcms as more number of cycles were used to estimate the CMFD parameter distributions. The main objective of this approach is to estimate SD from sufficiently converged inactive cycles which are about several tens of cycles, so further refinement is required.

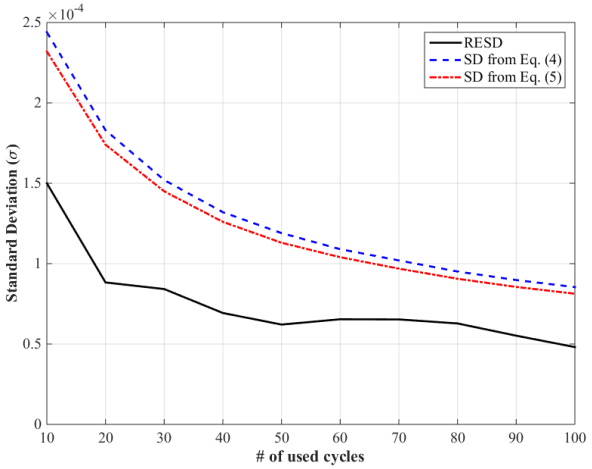

Fig. 4. Estimated RESD and SDs from the two approaches

SUMMARY

A new approach to estimate SD from uncertainties of CMFD parameters was tested. The method was able to conservatively predict RESD of the simulation based on several tens of inactive cycles. For this estimation, the first-order perturbation formula was used to replace power iteration step, which accounts for significant computation time. The first-order perturbation formula for cross sections was able to result almost identical multiplication factors from the samples, and SD was very similar. In the future, additional effort to precisely estimate RESD based on a few inactive cycles will be further studied. Also, SD estimation of pin-power distribution will be done shortly.

ACKNOWLEDGMENT

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