Application of Iterative Correlated Sampling to Estimate Real Variance in the iDTMC Method

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1. Introduction

Monte Carlo neutron transport analysis is a highly accurate solution for nuclear reactor analysis. The method simulates the neutron transport and tally reactor-related quantities. However, a high-fidelity Monte Carlo solution requires numerous particle simulations, resulting in an enormous computing burden. Researchers have sought the Monte Carlo acceleration schemes. Combination with the deterministic methods is one of the acceleration methods suggested.

Improved Deterministic Truncation of Monte Carlo (iDTMC) method is a strategic combination of the deterministic and Monte Carlo solutions developed in KAIST [1-4]. The iDTMC method previously showed its advantage in acceleration and variance reduction. Furthermore, the method was modified to apply to the reactor depletion analysis, which showed good agreement with the standard Monte Carlo solutions [3].

In the Monte Carlo simulation, fission neutrons from the previous cycle are utilized for the next cycle initialization. The scheme leads to inevitable intercycle correlation. In the iDTMC method, the issue becomes more severe since the method utilizes FMFD parameters accumulated from previous cycles. The underestimation induces significant underestimation in apparent variance compared to the real. Correlated sampling was proposed and implemented to estimate the real variance of the iDTMC solution. In this paper, further improvement of the correlated sampling with an iterative approach is studied.

2. Methods

2.1 iDTMC method

iDTMC method is an acceleration and variance reduction scheme for the Monte Carlo solution. The Monte Carlo solution can provide high-fidelity solutions, while the deterministic solution is fast. The iDTMC method combines two methods to obtain a high-fidelity solution with faster computation. The procedure comprises inactive cycles with coupled p-CMFD and active cycles with decoupled p-FMFD solutions.

During the early few steps, no further calculations are performed due to the lack of convergence of FSD (Fission Source Distribution). Then, until the inactive cycle ends, the convergence of the FSD is accelerated with the p-CMFD method. [5] Based on the Monte Carlo tallies, such as neutron currents, a coarse-mesh-based deterministic solution is obtained by solving an eigenvalue problem. The solution is utilized in the next cycle of the Monte Carlo transport by adjusting the weight of the fission neutrons.

The p-FMFD method is solved in active cycles to obtain the multiplication factor and power distribution. The solution is provided with an average of p-FMFD parameters accumulated from the middle of the inactive cycles. The scheme leads to a higher precision of the iDTMC solution.

Previous studies showed that the iDTMC method could provide a highly accurate and precise solution even on the first active cycle. Since the standard Monte Carlo solution require sufficient active cycles for the precise solution, the iDTMC solution can significantly reduce the computing burden. Also, inactive cycles can be shorter than the standard Monte Carlo for the sake of the p-CMFD. Fig. 1 shows the iDTMC solution scheme.

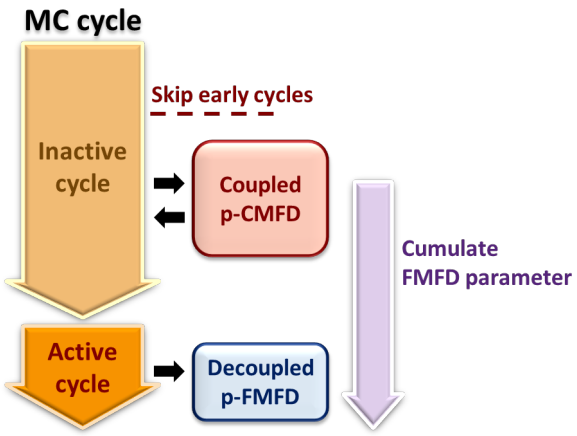

Fig 1. iDTMC scheme

2.2 Real variance estimation

Despite the advantage of the iDTMC method, the iDTMC method underestimates the variance of the solution. The issue arises from the strong inter-cycle correlation. In the current iDTMC method, FMFD parameters are accumulated from the previous inactive cycles. Therefore, the inter-cycle correlations are stronger in the iDTMC than in the standard Monte Carlo. The correlation results in severe underestimation of apparent variance compared to the real value from the multiple independent calculations.

Correlated sampling is adopted to produce the multivariate samples of FMFD parameters with proper consideration of correlation [1, 4]. The samples are used to evaluate variances of reactivity and power distribution. For each fine mesh, one-group FMFD parameters are perturbed with correlated sampling. Eq. (1) denotes the correlation matrix for each mesh.

$$\begin{bmatrix} 1 & C(\Sigma_t,\Sigma_a) & C(\Sigma_t,\nu\Sigma_f) \\ C(\Sigma_t,\Sigma_a) & 1 & C(\Sigma_a,\nu\Sigma_f) \\ C(\Sigma_t,\nu\Sigma_f) & C(\Sigma_a,\nu\Sigma_f) & 1 \end{bmatrix} \quad (1)$$

where $C(X,Y)$ denotes the correlation coefficient between quantities X and Y. Σ_t, Σ_a, $\nu\Sigma_f$ stands for one-group total, absorption, and nu-fission cross-section defined for each mesh, respectively.

The correlated sampling begins with uniform random number (URN) sampling with Latin Hypercube Sampling (LHS) [6]. The LHS is one of the URN sampling methods, resulting in well-dispersed URN with fewer samples. Fig. 2 displays the basic scheme of the LHS for 2-dimensional URN sampling with ten samples. Each domain is subdivided into equal meshes with the number of samples. The samples are chosen within the mesh where the mesh does not overlap along each direction.

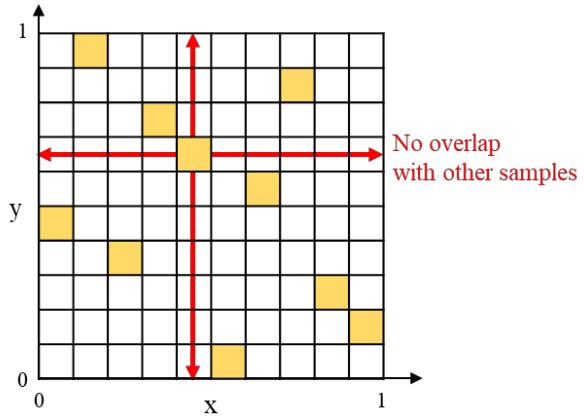

Fig 2. Sample Latin Hypercube Sampling

After the production of the URN, the URN samples are transformed into the normal distribution. The normal distribution has a mean of zero and a variance of unity. The procedure can be done with inversed CDF (Cumulative Distribution Function) of normal distribution. The normal samples need to be correlated with the given correlation matrix. Assume that the normal samples are uncorrelated. Then, the correlation matrix of the multivariate normal sample matrix X can be expressed as in Eq. (2).

$$C_0 = E[XX^T] = I_{3\times3} \quad (2)$$

where matrix $I_{3\times3}$ is a 3-by-3 square identity matrix. The diagonal and off-diagonal elements of the identity matrix are one and zero. Cholesky decomposition L of M can be written as Eq. (3) for target correlation matrix M. Note that the matrix L is a lower triangular matrix [7].

$$M = LL^T \quad (3)$$

By multiplying matrix L to X, the samples' correlation matrix can be written as Eq. (4). Multiplication of the matrix to sample X can be done with a linear combination of the multivariate samples.

$$\begin{aligned} C' = E[(LX)(LX)^T] &= E[LXX^TL^T] \\ &= LE[XX^T]L^T \\ &= LI_{3\times3}L^T = LL^T \\ &= M \end{aligned} \quad (4)$$

After the correlated multivariate normal samples are produced, the samples are converted into target distribution. In this case, the CDFs of accumulated FMFD parameters are utilized. The normal samples are changed into URN samples with CDF of normal distribution. Then the URN samples are converted into the target CDFs with inversed CDF of the target.

The correlated multivariate normal distributions are transformed into input correlation.

2.3 Iterative scheme

According to the previous studies on correlated sampling, Since the FMFD parameters' distribution are not Gaussian, the correlated sampling cannot return samples with exact correlation. However, the distributions of the FMFD parameters' CDFs cannot be expressed analytically. Therefore, an iterative approach is adopted to correlate samples accurately.

The approach extrapolates the input correlation matrix and the resulting correlation matrix. However, the matrix elements should be between -1 and 1. Therefore, sigmoid functions are utilized in the extrapolation. Sigmoid functions are functions defined within $(-\infty,\infty)$ resulting in values within [-1, 1], with a non-negative derivative. In the iterative scheme, the error function is utilized. Error function erf(x) can be defined as Eq. (5) for the real number x. Also, the inverse of the error function exists, which can be expressed as $\text{erf}^{-1}(x)$.

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x dt\ \exp(-t^2) \quad (5)$$

Given the correlation matrix of the accumulated FMFD parameters C_0. Suppose that the target correlation matrix of ith iteration is C_i, resulting in samples with a correlation matrix $C_{i,out}$. Then, the target correlation for the next iteration is perturbed by the distance between C_0 and $C_{i,out}$. The perturbation is done with the error function f(x) and its inverse function, $f^{-1}(x)$.

$$C_{i+1} = f(f^{-1}(C_i) + d_i) \quad (6)$$

where distance d_i can be calculated with Eq. (7).

$$d_i = f^{-1}(C_0) - f^{-1}(C_{i,out}) \quad (7)$$

The correlated sampling is done with the perturbed correlation matrix. In the current iDTMC scheme, five iterations are performed after the initial correlated sampling.

3. Numerical Result

3.1 Problem Description

SMR core problem is suggested as a model reactor problem. The cross-sectional view of the core is depicted in Fig. 3. The reactor core is composed of central fuel assemblies with Gadolinia fuel pins and peripheral fuel assemblies without Gadolinia fuel pins. Detailed specifications are tabulated in Table I.

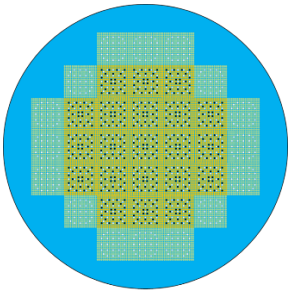

Fig 3. Cross-section view of the SMR core

Table I: Specification of the SMR core

Fuel pellet radius	0.5 cm
Pin pitch	1.26 cm
Cladding thickness	0.3 mm
Reactor height	140 cm
Uranium enrichment	3.8 weight-%
Gd_2O_3 weight fraction	4 %
Cladding	Zircaloy
Reflector	H_2O

Based on the standard Monte Carlo method, 50 inactive and 300 active cycles are utilized. The iDTMC scheme is implemented in the Monte Carlo iMC code. In this case, 30 inactive and 10 active cycles are used. To show the impact of the iDTMC method, the standard Monte Carlo was also performed with identical calculation conditions. The FMFD parameters are accumulated from the 16th cycle. For real variance estimation, 100 samples are produced to estimate the real variance with the correlated sampling. ENDF-B/VII.1 cross-section and depletion library are utilized for calculation. Additionally, real variances are evaluated from 30 independent runs.

3.2 Burnup-dependent criticality

Fig. 4 depicts the burnup-dependent criticality of the reactor core. As shown in the plot, the k_{eff} value from the iDTMC solution agrees with the standard Monte Carlo solution.

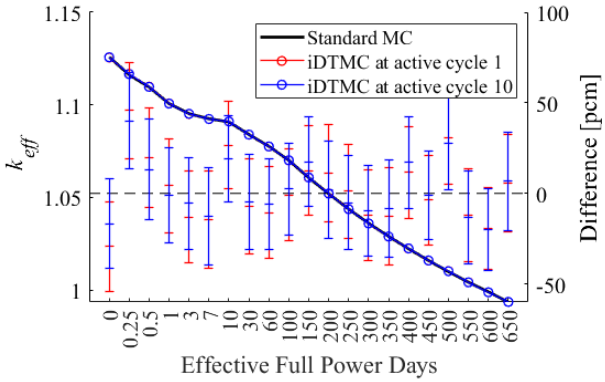

Fig 4. Burnup-dependent k_{eff}

The real variance of the criticality is estimated with the correlated sampling. Fig. 5 plots burnup-dependent estimation of the real standard deviation of k_{eff}. Fig. 6 shows the evolution of the variances on 0.25 EFPD. As mentioned in the previous section, the apparent variances of the iDTMC solution are underestimated due to inter-cycle correlation. The plot implies that the iDTMC solution shows high precision from the first active cycle and can accurately estimate the real variance.

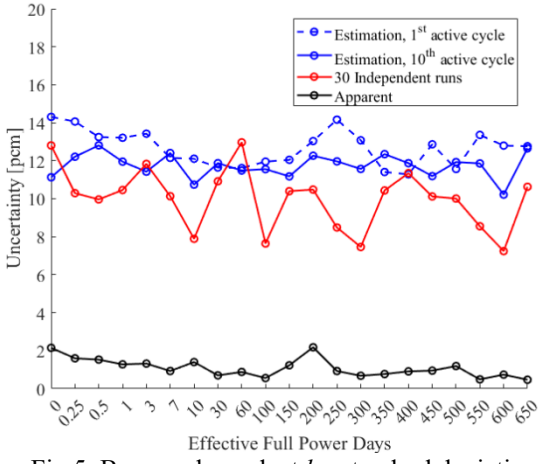

Fig 5. Burnup-dependent k_{eff} standard deviation

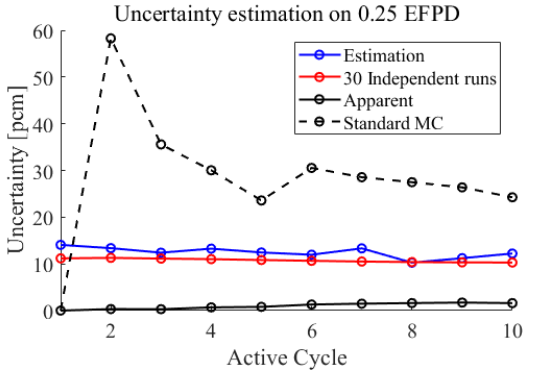

Fig 6. k_{eff} standard deviation on first burnup step

3.3 Power distribution

Fig. 7 compares the relative standard deviation from the independent runs and correlated sampling. Detailed comparison along the centerline of the core is depicted in Fig. 8. The comparisons show that the real variance of power distribution can be accurately estimated while a minor overestimation exists.

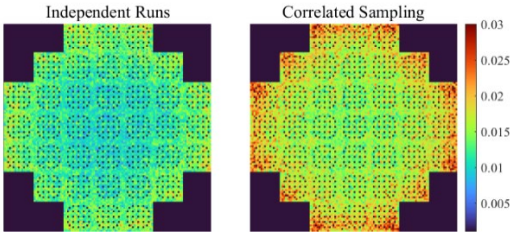

Fig 7. Relative standard deviations of power distribution on 650 EFPD from independent runs (left) and correlated sampling (right)

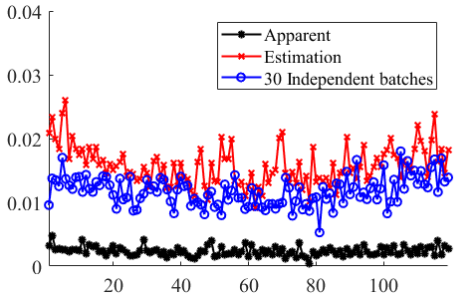

Fig 8. Comparison of relative standard deviations of power distribution along the centerline on 650 EFPD

3.4 Correlation Difference

The iterative correlation sampling method tested its impact by comparing the correlation matrix. Fig. 9 shows the axial-averaged distribution of the correlation difference on 0 EFPD. The difference in the sample correlation matrix is defined as Eq. 8, where C and C_0 stands for sample and target correlation matrices, respectively. The subscript of the matrix denotes the row and column index of an element of the correlation matrix.

$$\frac{\left|C_{12}-C_{0,12}\right|+\left|C_{13}-C_{0,13}\right|+\left|C_{23}-C_{0,23}\right|}{3} \quad (8)$$

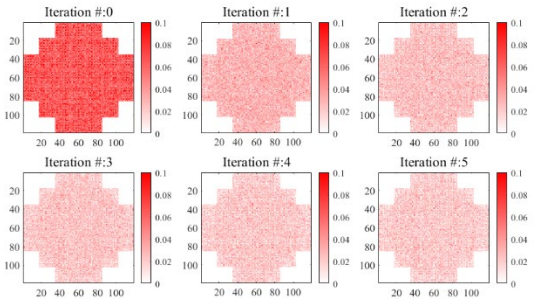

Fig 9. Correlation difference distribution on 0 EFPD

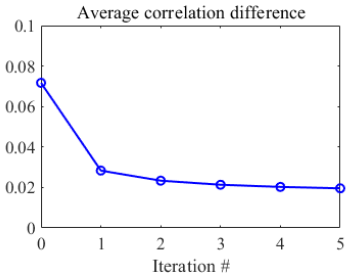

Fig 10. Average correlation difference

4. Conclusion

This work focuses on improving the real variance estimation scheme for the iDTMC method. The iDTMC-based real variance estimation showed highly accurate estimation from single calculation, which require numerous independent calculations. The iterative scheme was applied to the correlated sampling scheme. Future studies will focus on correlated sampling improvement regarding the sigmoid function, number of iterations, and overrelaxation concept.

ACKNOWLEDGEMENT

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