Improved Early-Active-Cycle Variance Estimation in the iDTMC Method Using Intra-Cycle Batching with implicit Correlated Sampling Method

Jaehyeong Jang[1], Inyup Kim[1] and Yonghee Kim[1*]
[1]*Department of Nuclear & Quantum Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea*
[*]*Corresponding author: yongheekim@kaist.ac.kr*

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1. Introduction

The Monte Carlo (MC) method provides highly accurate reactor solutions but is limited by high computational cost. The improved Deterministic Truncation of Monte Carlo (iDTMC) method addresses this by coupling MC simulations with deterministic-like solutions to accelerate fission source distribution (FSD) convergence and obtain pin-wise solutions within a few active cycles. Although the final solution is obtained deterministically, it is constructed from MC-tallied parameters that inherently contain statistical uncertainty, and the iDTMC solution therefore retains uncertainty. An implicit Correlated Sampling (iCS) method was previously proposed to estimate the real variance of iDTMC solutions. This study enhances variance estimation during early active cycles, where limited statistics lead to unstable uncertainty predictions. An intra-cycle batching method is introduced to partition source particles into sub-groups and evaluate the variance of batch means, enabling stable and reliable variance estimation even at the early active cycles.

2. Methodology

2.1 The iDTMC Method

The iDTMC method is a hybrid framework developed to improve the computational efficiency of conventional MC simulations while preserving high-fidelity, pin-wise resolution [1]. In standard eigenvalue MC calculations, inactive cycles converge the FSD, followed by active cycles that accumulate tallies. This process is computationally demanding, and iDTMC addresses this limitation through two strategies.

During inactive cycles, a partial current-based Coarse Mesh Finite Difference (p-CMFD) method accelerates FSD convergence. Assembly-wise homogenized parameters are tallied and used to solve the one-group neutron balance equation (NBE),

$$\sum_s \frac{A_s}{V_n}(J_{s1} - J_{s0}) + \Sigma_{a,n}^{MC}\phi_n = \frac{1}{k_{eff}} \nu\Sigma_{f,n}^{MC}\phi_n. \qquad (1)$$

Here, A_s and V_n denote the surface area and node volume, ϕ and J represent the flux and current, and Σ and k_{eff} represent the cross section and effective multiplication factor. The resulting solution updates the FSD weight, reducing the required inactive cycles.

During active cycles, a partial current-based Fine Mesh Finite Difference (p-FMFD) method solves the same NBE on a fine mesh from accumulated parameters, enabling deterministic truncation while preserving fidelity. The workflow is illustrated in Figure 1.

Through deterministic acceleration and truncation, iDTMC reduces computational cost while maintaining accuracy.

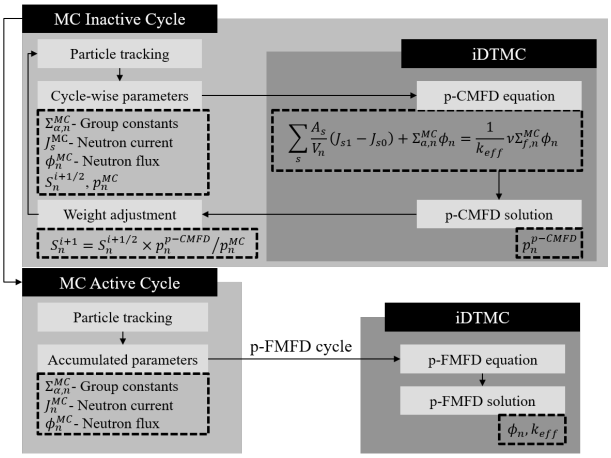


Figure 1. Schematic of the iDTMC method.

2.2 implicit Correlated Sampling Method

To estimate the uncertainty of iDTMC solutions, multiple p-FMFD parameter sets are statistically sampled, and the corresponding p-FMFD equations are constructed and solved. The variance of these deterministic solutions serves as an estimator of the iDTMC uncertainty. For the estimation to be physically meaningful, both the marginal distributions and the correlations of the tallied reactor parameters must be preserved. To satisfy this requirement, the iCS method was previously proposed [2].

In the iDTMC framework, p-FMFD reactor parameters, such as total, absorption, and production cross sections, neutron fluxes, and partial currents, are accumulated at each active cycle. Let the tallied parameter vector at the k-th active cycle be denoted as P_k where $k = 1,2, \ldots, N$, and N is the number of active cycles. Instead of explicitly constructing a high-dimensional covariance matrix, the iCS method generates statistically consistent samples through linear combinations of the cycle-wise tallies

$$P^{(s)} = \sum_{k=1}^{N} \omega_k^{(s)} P_k \tag{2}$$

where the non-negative weights $\omega_k^{(s)}$ satisfy $\sum_{k=1}^{N} \omega_k^{(s)} = 1$. The weights are drawn from a Dirichlet distribution with parameters α_k, which control the concentration of the distribution. In this study, a symmetric Dirichlet distribution with $\alpha_k = 1$ is adopted to ensure equal treatment of all active cycles and numerical stability.

Although this linear combination preserves the correlation structure embedded in the tallied parameters, the sampled set may not exactly reproduce the original mean and variance. Therefore, each sampled parameter is rescaled using the tallied mean and variance so that the marginal statistics remain consistent with those directly estimated from the simulation. The overall procedure of the iCS method is illustrated in Figure 2.

Previous studies have demonstrated that this approach reproduces the uncertainty obtained from independent batch iDTMC calculations, confirming that the statistical characteristics of the tallied parameters are effectively preserved within the iCS framework.

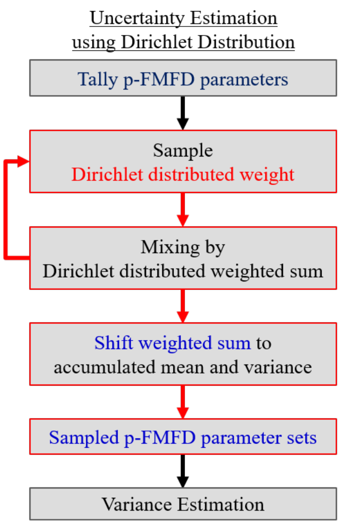


Figure 2. Schematic of the iCS method.

2.3 Intra-Cycle Batching

Although the iCS method provides accurate uncertainty estimation when sufficient statistics are accumulated, its performance deteriorates during early active cycles due to limited tally statistics. Because the iCS method relies on the mean and variance estimated from cycle-wise MC tallies, insufficient statistics in the early-stage lead to unstable variance estimates.

To address this limitation, an intra-cycle batching approach inspired by the history-based batch method is introduced [3]. In each active cycle, source particles are divided into several sub-groups, and reactor parameters are independently estimated for each sub-group. These sub-group estimates are then used to improve the statistical robustness of parameter moment estimation, enabling more stable variance evaluation even during early active cycles.

Assume a simulation consisting of M particle histories per cycle and N active cycles. In the proposed intra-cycle batching scheme, the source particles at the beginning of each active cycle are divided into N_B batches. Independent tallies are then performed for each batch, resulting in N_B estimates of the quantity of interest per active cycle.

Let Q_{ij} denote the estimate of the quantity of interest Q from the j-th history in the i-th active cycle. The tally estimate of Q for the k-the batch is defined as

$$Q^k = \frac{1}{N(M/N_B)} \sum_{i=1}^{N} \sum_{j\in k} Q_{ij} \tag{3}$$

where the inner summation is taken over histories belonging to batch k. The overall estimate of Q is then given by the average of the batch means,

$$\bar{Q} = \frac{1}{N_B} \sum_{k=1}^{N_B} Q^k \tag{4}$$

and the variance of the mean is estimated using the standard batch-mean estimator,

$$\sigma^2[\bar{Q}] = \frac{1}{N_B(N_B-1)} \sum_{k=1}^{N_B} (Q^k - \bar{Q})^2 . \tag{5}$$

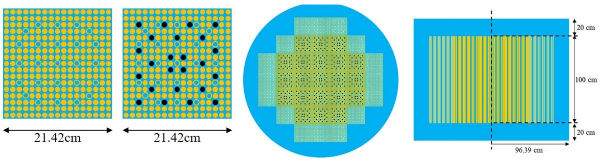
During early active cycles, limited cycle-wise samples lead to large statistical fluctuations in moment estimation. In contrast, intra-cycle batching provides multiple samples within each cycle, effectively increasing the number of samples and improving the stability of the estimated mean and variance.

Accordingly, in the iCS framework, cycle-wise parameter sets can be replaced with batch-wise sets, and the variance of the mean can be estimated from batch-wise samples, resulting in more stable uncertainty estimation in early active cycles.

In addition, the proposed intra-cycle batching approach differs fundamentally from the conventional history-based batch method. The HBM method requires internal modifications, such as re-normalization to preserve the number of particles in each history batch, whereas the proposed approach can be directly applied within each active cycle without such modifications. This feature enables a more straightforward implementation while maintaining reliable uncertainty estimation within a single active cycle.

3. Numerical Results

To assess the performance of the proposed uncertainty estimation framework, a Small Modular Reactor (SMR) problem is considered [4]. For spatial discretization, the coarse-mesh grid is defined at the assembly level in the radial direction with 5 equally spaced axial nodes, whereas the fine-mesh grid is defined at the fuel-pin level radially with 10 axial nodes. Detailed geometric and material specifications are shown in Figure 3.



Geometry Details		Material Specification	
Number of FA1	16	Uranium enrichment [w/o]	3.8
Number of FA2	21	Uranium oxide density [g/cm^3]	10.4
Fuel pellet radius [cm]	0.5	Gadolinia weight fraction [%]	4
Pin pitch [cm]	1.26	Gadolinia-mixed uranium oxide density [g/cm^3]	10.28
Cladding thickness [cm]	0.3	Cladding material (density) [g/cm^3]	Zircaloy (6.5)
Reactor height [cm]	140	Reflector material (density) [g/cm^3]	H_2O (0.9)

Figure 3. Assembly types (left), radial (middle), and axial (right) core configuration, and geometric and material specification (bottom) of the SMR problem.

All calculations employed 15 inactive cycles, 15 active cycles, and 6,000,000 particle histories per cycle. For the intra-cycle batching approach, $N_B = 10, 50,$ and 100 were tested.

For the eigenvalue analysis, the last 14 active cycles were used as p-FMFD cycles. The real variance was obtained from 210 independent iDTMC calculations. For each estimation method, 30 independent calculations were performed, and error bars represent the 99.7% confidence interval.

Figure 4 presents the real and mean estimated $\sigma_{k_{eff}}$ with corresponding error bars. To directly compare estimator stability, Figure 5 shows the standard deviation of the estimated $\sigma_{k_{eff}}$ for each method. The results show that intra-cycle batching generally reduces the fluctuation of the $\sigma_{k_{eff}}$ estimation during the early p-FMFD cycles. This improvement becomes less pronounced as more cycle-wise samples are accumulated.

For the power distribution, only the final active cycle was used as the p-FMFD cycle. The real variance was evaluated from 120 independent calculations, and 30 independent calculations were performed for each estimation method. Error bars again correspond to the 99.7% confidence interval.

Figure 6 shows the real and mean estimated σ of the axial pin power at the peak power location. Figure 7 compares the standard deviation of the estimated power σ for each method. A similar tendency is observed for the power uncertainty estimation: the batching-based iCS method provides a more stable estimator in the early stage, whereas its relative advantage diminishes once sufficient cycle-wise statistics are accumulated.

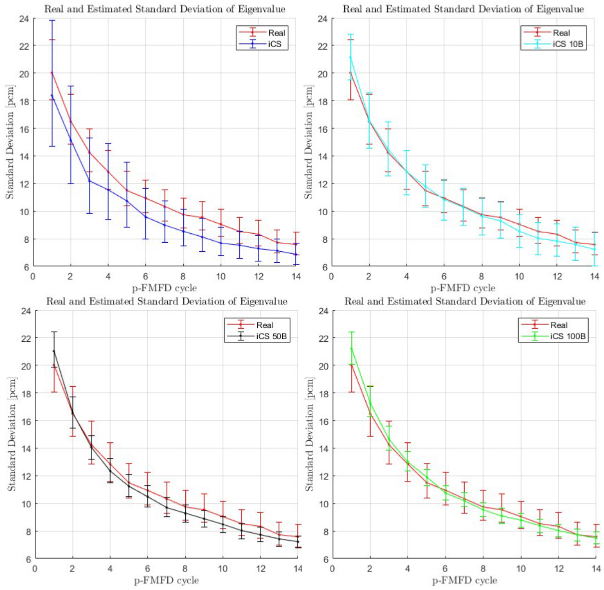


Figure 4. Comparison of the real and estimated $\sigma_{k_{eff}}$ using iCS only and iCS with intra-cycle batching.

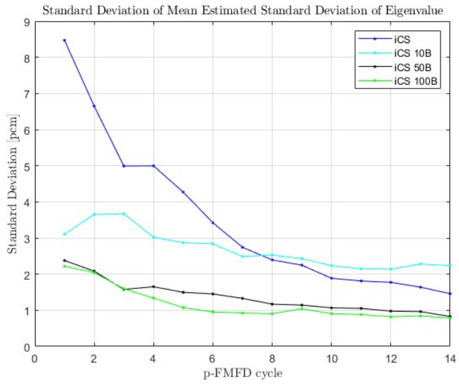


Figure 5. Standard deviation of $\sigma_{k_{eff}}$ estimator for iCS only and iCS with intra-cycle batching.

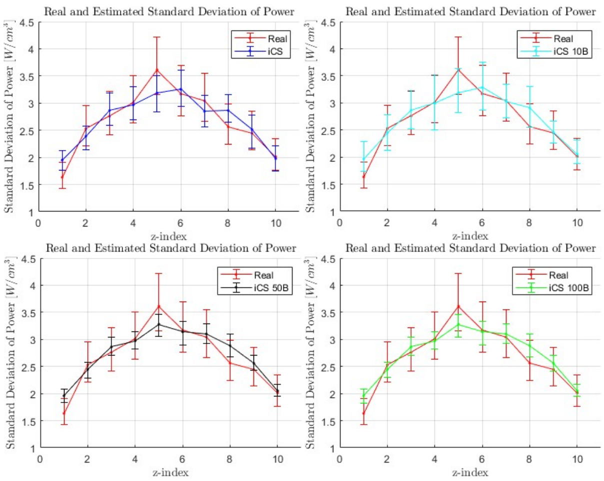


Figure 6. Comparison of real and estimated power σ using iCS only and iCS with intra-cycle batching.

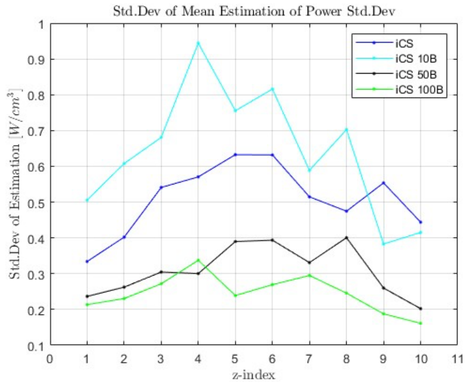


Figure 7. Standard deviation of power σ estimator for iCS only and iCS with intra-cycle batching.

The conventional iCS approach relies on cycle-wise tallied parameters, which provide limited samples in the early stage and lead to unstable moment estimation. In contrast, intra-cycle batching provides N_B sub-samples within each cycle, effectively increasing the number of samples used for estimating parameter moments and improving statistical robustness during the initial p-FMFD cycles.

However, when $N_B = 10$ is used, a different trend is observed after approximately the 9th p-FMFD cycle. While intra-cycle batching yields smaller variance during the initial cycles, the conventional iCS method begins to exhibit lower estimator variance once the number of accumulated active cycles exceeds N_B. This occurs because the conventional iCS approach continuously increases the number of cycle-wise parameter sets as the simulation proceeds, whereas the batching method maintains a fixed number of N_B sub-samples. This behavior is more evident in the power uncertainty analysis, where only the final active cycle is used as the p-FMFD cycle. In this case, the conventional iCS method utilizes all 15 accumulated cycle-wise parameter sets, while the batching approach with $N_B = 10$ is restricted to ten sub-samples. Consequently, the batching-based estimator exhibits relatively larger variance than the conventional iCS method.

As N_B increases, the width of the error bars decreases, indicating improved estimator stability. However, N_B must be chosen carefully. If N_B is too small, statistical stabilization is insufficient. If N_B is too large, the number of histories per batch becomes too small, degrading tally accuracy. Therefore, an optimal range of N_B exists that balances estimator stability and per-batch statistical quality.

4. Conclusions

This study proposed an enhanced variance estimation framework for the iDTMC method by incorporating intra-cycle batching into the iCS approach. The proposed method was developed to address the instability of uncertainty estimation during early active cycles, where limited cycle-wise statistics degrade the reliability of moment estimation.

Numerical results for both eigenvalue and power distribution demonstrated that intra-cycle batching significantly improves estimator stability in the early active cycles by effectively increasing the number of samples used for parameter moment estimation. The improvement is particularly evident when the number of accumulated active cycles is small. As the simulation proceeds and sufficient cycle-wise samples are accumulated, the advantage of batching diminishes, especially for small N_B. This behavior confirms that the primary benefit of the proposed method lies in stabilizing early-stage uncertainty prediction.

The results also showed that increasing N_B reduces estimator fluctuation. However, excessively large N_B may deteriorate per-batch tally accuracy due to insufficient particle histories per batch. Therefore, an appropriate balance between statistical stability and per-batch sampling quality is required.

Future work will focus on extending the proposed framework to single active cycle uncertainty estimation, where no cycle-wise accumulation is available and intra-cycle batching is expected to provide substantial benefit. In addition, a systematic criterion for selecting the optimal N_B will be developed based on effective sample size and statistical efficiency considerations. Further investigation into adaptive batching strategies and their impact on parameter correlation preservation will also be conducted to enhance the robustness of the iDTMC uncertainty estimation framework.

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REFERENCES

[1] I. Kim, Development of a Deterministic Truncation of Monte Carlo Solution for a Pin-Resolved Nuclear Reactor Analysis, Ph.D. Dissertation, Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea, 2021.

[2] J. Jang, I. Kim, and Y. Kim, Uncertainty Estimation of the Improved Deterministic Truncation of Monte Carlo Method Using the Dirichlet Distribution, Frontiers in Energy Research, Vol. 14, Article 1744345, 2026. doi:10.3389/fenrg.2026.1744345.

[3] H. J. Shim, S. H. Choi, and C. H. Kim, Real Variance Estimation by Grouping Histories in Monte Carlo Eigenvalue Calculations, Nuclear Science and Engineering, Vol. 176, No. 1, pp. 58-68, 2014.

[4] I. Kim and Y. Kim, Real Variance Estimation in iDTMC-Based Depletion Analysis, Nuclear Engineering and Technology, Vol. 55, No. 11, pp. 4228-4237, 2023.