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

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Table of Contents

Table of Contents

Motivation & Objectives

The Improved Deterministic Truncation of Monte Carlo (iDTMC) method

– The iDTMC method is a hybrid approach that couples **MC** with a **deterministic** solution.

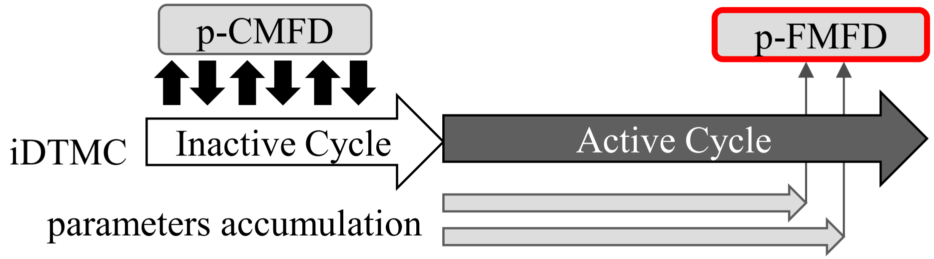


Figure 1. Schematic of the iDTMC method.

Variance estimation in the iDTMC method

1. Sample deterministic parameter sets to generate a batch of deterministic problems.
2. Solve the batch and use the variance of solutions as an estimator of the iDTMC real variance.

Sampling p-FMFD parameter sets

– The implicit Correlated Sampling (iCS) method implicitly preserves moments and correlations.

– Because the iDTMC method uses cycle-wise tallied means, statistical instability occurs in early cycles.

- To enable reliable uncertainty estimation, statistical stabilization is required.

This study proposes intra-cycle batching with iCS method for improved early-active-cycle variance estimation.

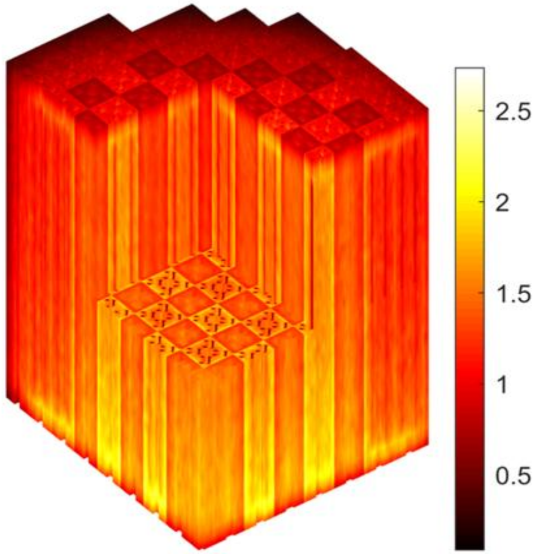
Table of Contents

The iDTMC Method

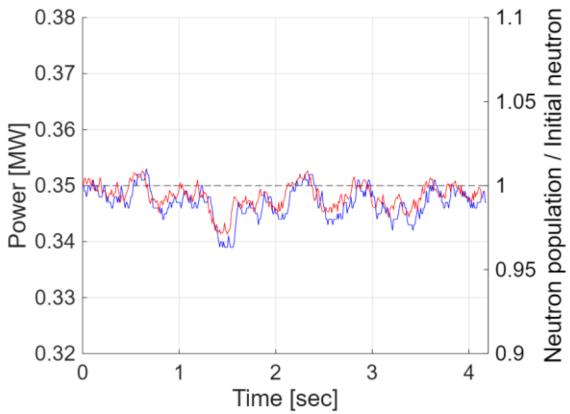
The Monte Carlo neutron transport code, iMC

- The code is under development RPTL, KAIST.
- iMC supports fundamental features of Monte Carlo:
  - Multigroup and continuous energy group structure.
  - Constructive Solid Geometry (CSG).
  - Variance reduction with iDTMC.
  - Secondary particle production and tracking.

- Various studies were conducted with iMC code:
  - Advanced reactor analysis.
    - MSR, SFR, and pebble bed reactors.
  - Multiphysics.
  - Depletion.
  - Transient with both PCQS-MC and DMC.



APR1400 whole-core
power distribution from iMC



MSR null transient result with DMC

The iDTMC method

– partial current-based **Coarse** Mesh Finite Difference method (p-CMFD)

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

$$J_s = f\left(J_s^{\pm,MC}, \phi_n^{MC}, \Sigma_{t,n}^{MC}\right)$$

$$\Sigma_{t,n}^{MC}, \Sigma_{a,n}^{MC}, \nu\Sigma_{f,n}^{MC} = f(\phi_n^{MC})$$

- In each inactive cycle, p-CMFD parameters are tallied over **assembly-sized nodes** (coarse mesh).
- The neutron balance equation (NBE) is solved, and the solution is used to update $S(\vec{r})$.

– partial current-based **Fine** Mesh Finite Difference method (p-FMFD)

- When obtaining p-FMFD solution, the same NBE is solved with **pin-sized nodes** (fine mesh).

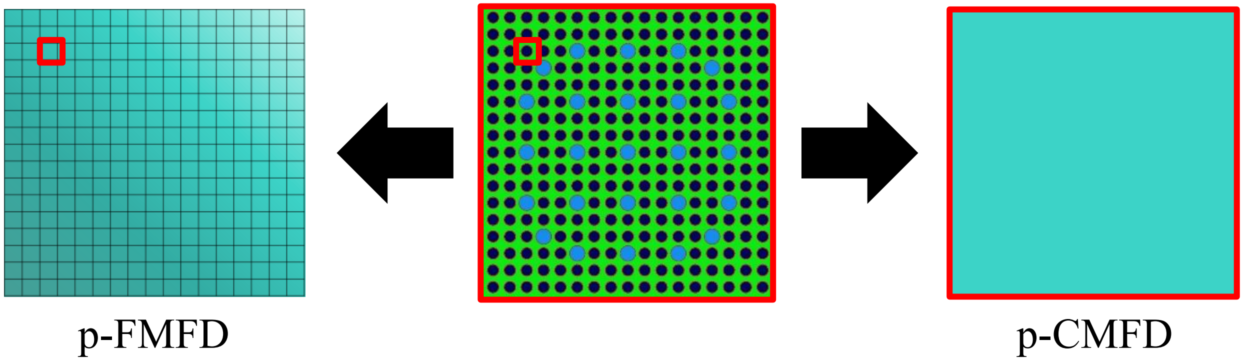


Figure 2. Difference in node configuration in p-FMFD (left) and p-CMFD (right).

The iDTMC method

1. In inactive cycles, accelerate assembly-level $S(\vec{r})$ convergence with p-CMFD.
2. In active cycles, accumulate pin-level parameters for p-FMFD.
3. Truncate the MC process and solve the p-FMFD equation to obtain k_{eff} and ϕ_n.

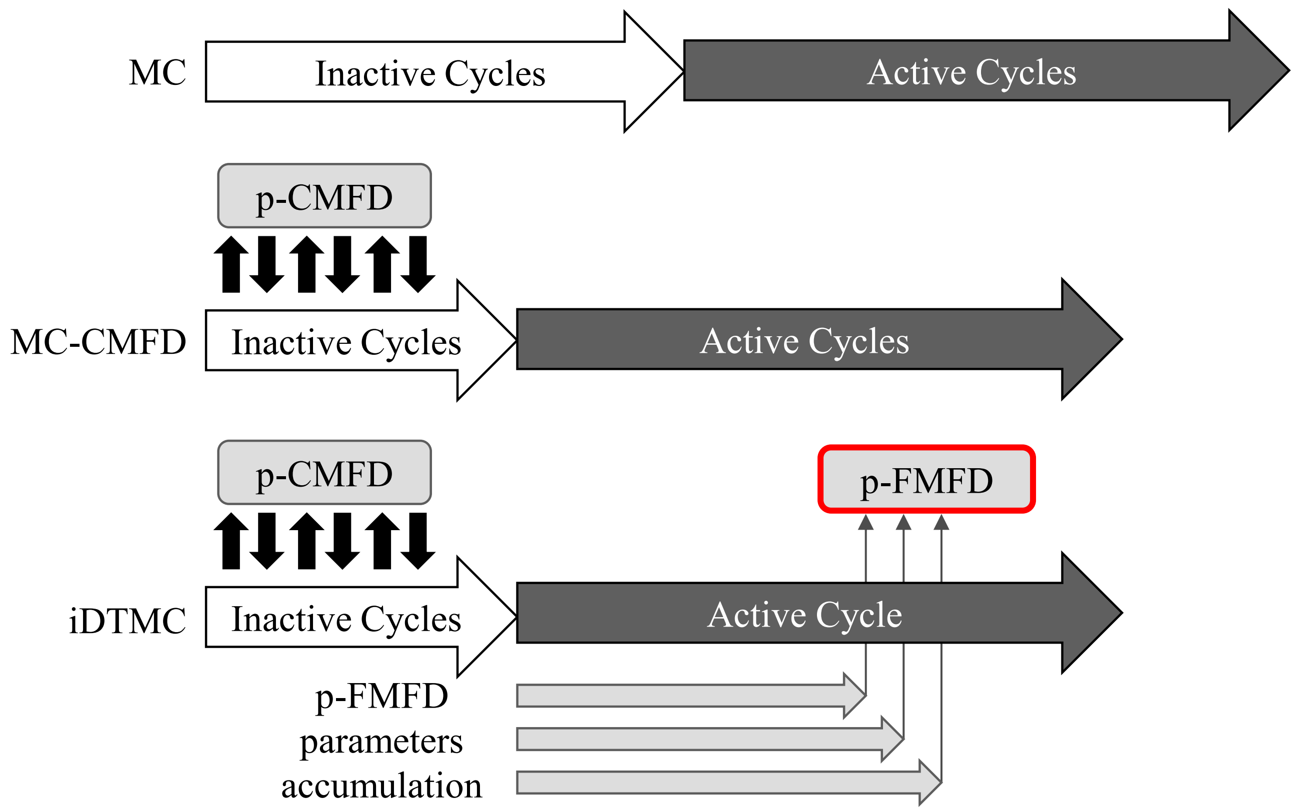


Figure 3. Difference between MC (top), MC-CMFD (mid), and iDTMC (bottom).

Figure of merit of the iDTMC method

– The advantages of the iDTMC method over the conventional MC arise from two key aspects:

- **Faster convergence of *S*** during inactive cycles.

$$H(S) = -\sum_{i=1}^{N_s} P_i \ln(P_i)$$

(where N_s is the number of meshes and P_i is the source fraction in mesh i)

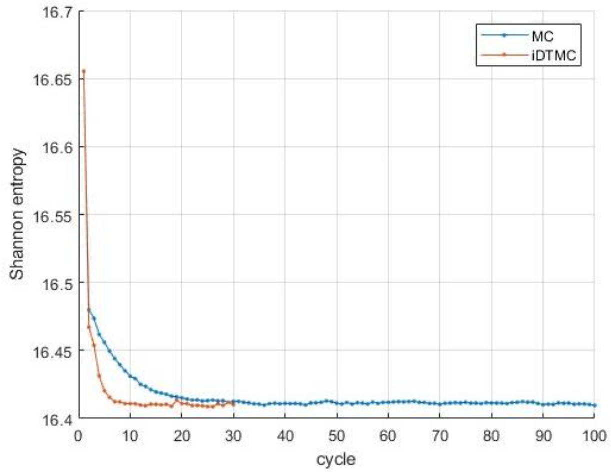


Figure 4. Shannon entropy evaluation per cycle for the conventional MC (blue) and the iDTMC method (orange).

- **Variance reduction with deterministic solution** during active cycles.

$$FOM = \frac{1}{TR^2}$$

(where T is the computing time and R is relative standard deviation)

Table of Contents

Variance Estimation in the iDTMC Method

Variance estimation in the iDTMC method

– Since p-FMFD parameters are also estimators with variance, the iDTMC solution also has uncertainty.

Estimating uncertainty of the iDTMC method

1. Sample **p-FMFD parameter** sets to generate a batch of p-FMFD problems.
2. Solve the batch and use the **variance of solutions as estimator of the iDTMC real variance.**

What parameters are sampled?

– Sampled p-FMFD parameters: total, absorption, nu-fission cross-sections, flux, and interface currents

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

$$J_s = f(J_s^{\pm,MC}, \phi^{MC}, \Sigma_t^{MC})$$

Real Variance Estimation using the Implicit Correlated Sampling Method

How can we account for all correlations?

– **Explicit modeling** of all of the parameter-wise and node-wise correlations is nearly impossible.

→ Ideally, correlations should be accounted for all **implicitly**.

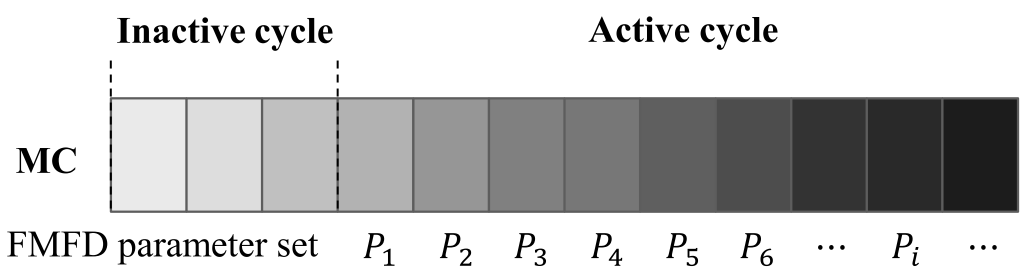


Figure 5. Accumulated p-FMFD parameter set in the iDTMC method.

– Each $P_i = \{\Sigma_a^{(i)}, \nu\Sigma_f^{(i)}, \Sigma_t^{(i)}, J^{\pm,(i)}, \phi^{(i)}\}$ in a cycle **implicitly** contains all of the correlations.

→ Directly use the accumulated parameters sets to generate new sets of p-FMFD parameters.

New method for sampling parameters

1. **Generate new parameters sets as weighted sums of the accumulated sets.**
   - The weights are randomly sampled from a Dirichlet distribution.
2. Shift the mean and variance of the generated sets to match those of the accumulated sets.

Dirichlet distribution

- Continuous multivariate generalization of the beta distribution.
- Dirichlet distribution of order $K \geq 2$ with parameter $\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_K\}$

$$f(x_1, \dots, x_K; \alpha_1, \dots, \alpha_K) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1} \ where \ B(\boldsymbol{\alpha}) = \frac{\prod_{i=1}^{K} \Gamma(\alpha_i)}{\Gamma\left(\sum_{i=1}^{K} \alpha_i\right)}$$

- For random variable $X = (X_1, \dots, X_K) \sim Dir(\boldsymbol{\alpha})$,

$$E[X_i] = \frac{\alpha_i}{\alpha_0} \ and \ Var[X_i] = \frac{\alpha_i(\alpha_0 - \alpha_i)}{\alpha_0^2(\alpha_0 + 1)} \ where \ \alpha_0 = \sum_{i=1}^{K} \alpha_i$$

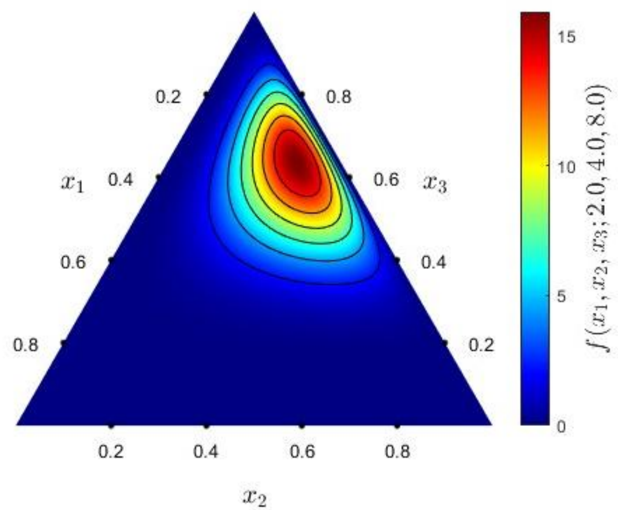


Figure 6. Probability density function of Dirichlet distribution for $\boldsymbol{\alpha} = \{2.0, 4.0, 8.0\}$.

Properties of Dirichlet distribution and symmetric Dirichlet distribution

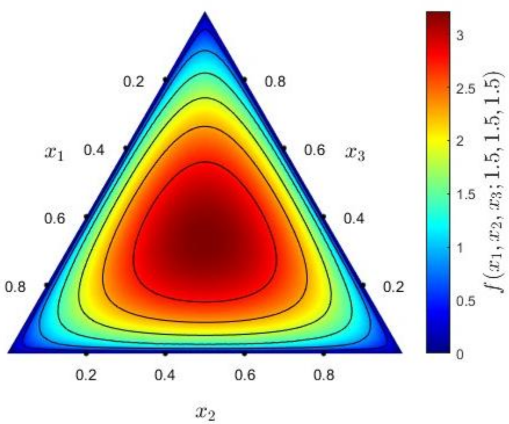
– From the PDF of Dirichlet distribution,

$$f(x_1, \dots, x_K; \alpha_1, \dots, \alpha_K) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1} \quad where\ B(\boldsymbol{\alpha}) = \frac{\prod_{i=1}^{K} \Gamma(\alpha_i)}{\Gamma\left(\sum_{i=1}^{K} \alpha_i\right)}$$

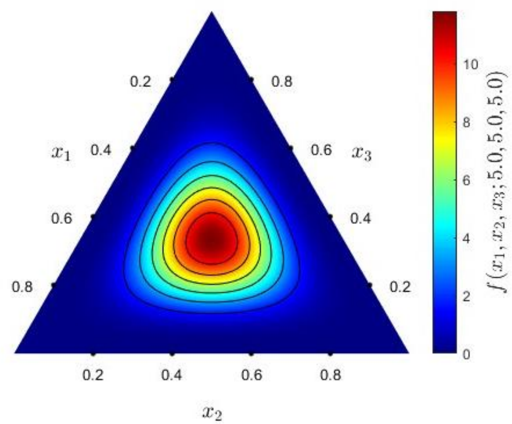
- $\sum_{i=1}^{K} x_i = 1$ and $x_i \in [0,1]$ for all $i \in \{1, \dots, K\}$

– Dirichlet distribution is symmetric when all the elements of $\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_K\}$ have the same value. (i.e. $\alpha_1 = \cdots = \alpha_K = \alpha$)

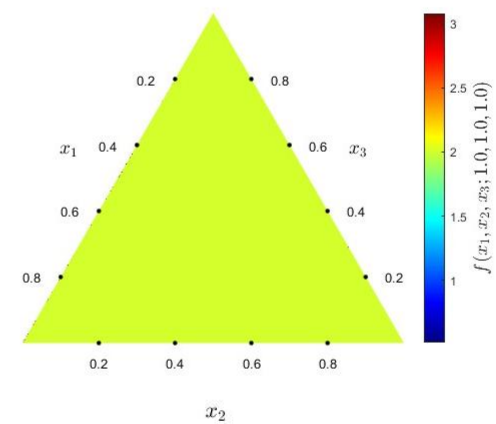
$$f(x_1, \dots, x_K; \alpha) = \frac{\Gamma(\alpha K)}{\Gamma(\alpha)^K} \prod_{i=1}^{K} x_i^{\alpha - 1}$$



$\alpha = 1.5$



$\alpha = 5.0$



$\alpha = 1.0$

Real Variance Estimation using the implicit Correlated Sampling Method

The implicit Correlated Sampling (iCS) method

1. **Mix** the accumulated p-FMFD parameter sets.
   - From N sets of accumulated p-FMFD parameter,

$$\boldsymbol{P} = \{P_1, \dots, P_N\}$$

   - To generate M sets of sampled parameters, sample

$$\omega_m = \{\omega_{m,1}, \dots, \omega_{m,N}\} \sim Dir(\alpha)$$

$$(m \in \{1, \dots, M\} \text{ and } \boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_1\}, \alpha_1 = 1)$$

   - Generate M sampled sets, $\boldsymbol{P^s} = \{P_1^s, \dots, P_M^s\}$

$$P_m^s = \boldsymbol{\omega_m} \cdot \boldsymbol{P}$$

   → **Make correlated normal distributed parameter set.**

2. **Shift** sampled parameters' mean and variance.

$$P_m = \frac{P_m^s - E[\boldsymbol{P^s}]}{Var[\boldsymbol{P^s}]} \times Var[\boldsymbol{P}] + E[\boldsymbol{P}]$$

   → **Make correlated set have accumulated mean and variance.**

➔ **Generate correlated p-FMFD parameter sets.**

<u>Variance estimation using iCS method</u>

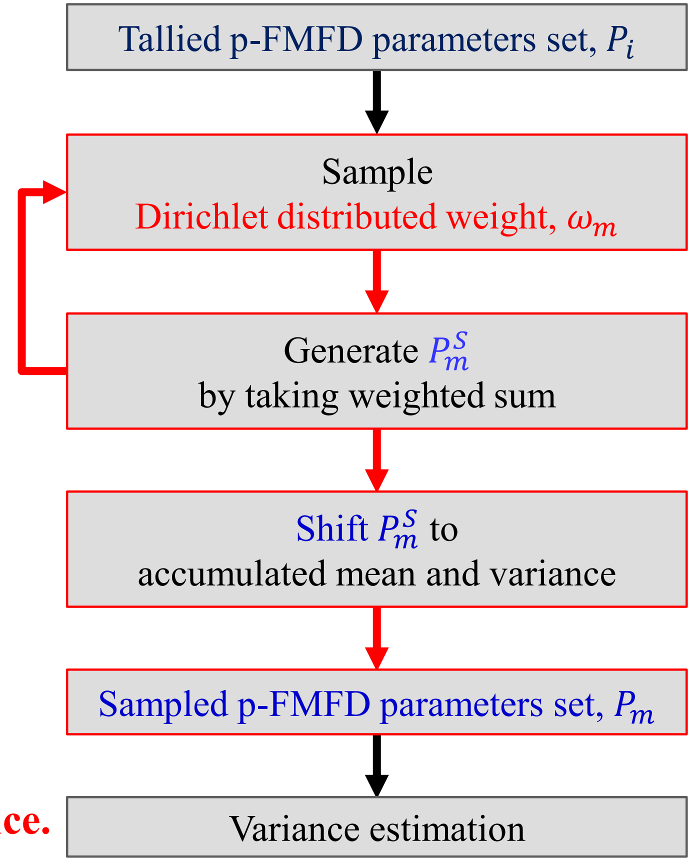
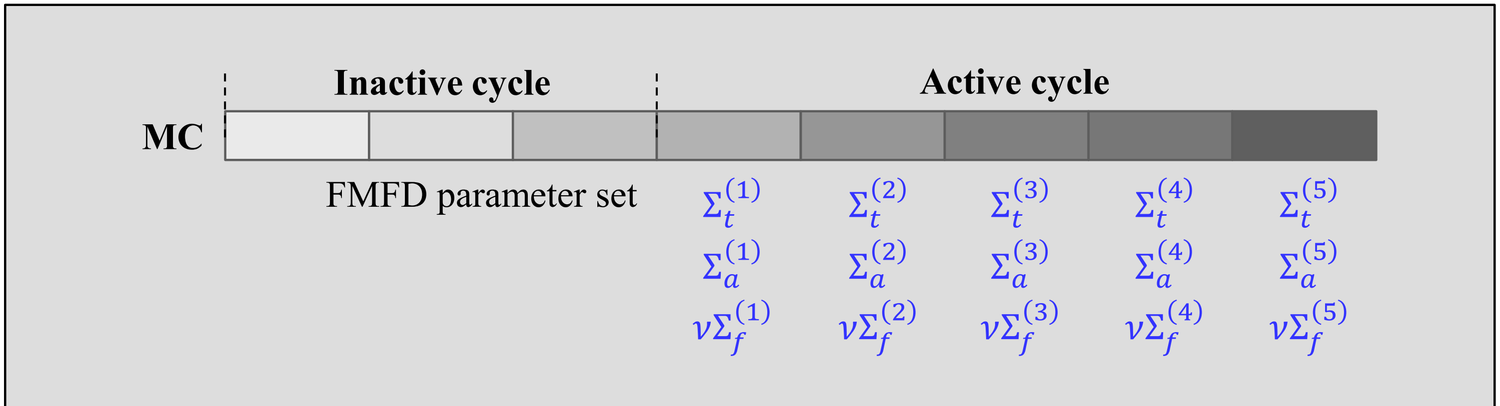


Figure 7. Schematic of variance estimation in the iDTMC method using the iCS method.

The implicit Correlated Sampling (iCS) method

– For example, only considering cross-sections: **5 active cycles**, **sample 10** parameter sets



$m = 1, \dots, 10$

Sample
Dirichlet distributed weight

$$\boldsymbol{\omega} = \{\omega_{m,1}, \dots, \omega_{m,5}\}$$

Mixing by
Dirichlet distributed weighted sum

$$\Sigma_t^{s,(m)} = \omega_{m,1}\Sigma_t^{(1)} + \cdots + \omega_{m,5}\Sigma_t^{(5)}$$

$$\Sigma_a^{s,(m)} = \omega_{m,1}\Sigma_a^{(1)} + \cdots + \omega_{m,5}\Sigma_a^{(5)}$$

$$\nu\Sigma_f^{s,(m)} = \omega_{m,1}\nu\Sigma_f^{(1)} + \cdots + \omega_{m,5}\nu\Sigma_f^{(5)}$$

Shift weighted sum to
accumulated mean and variance

$$\Sigma_t^{(m)} = \frac{\Sigma_t^{s,(m)} - E[\boldsymbol{\Sigma}_t^s]}{Var[\boldsymbol{\Sigma}_t^s]} Var[\boldsymbol{\Sigma}_t] + E[\boldsymbol{\Sigma}_t]$$

$$\Sigma_a^{(m)} = \frac{\Sigma_a^{s,(m)} - E[\boldsymbol{\Sigma}_a^s]}{Var[\boldsymbol{\Sigma}_a^s]} Var[\boldsymbol{\Sigma}_a] + E[\boldsymbol{\Sigma}_a]$$

$$\nu\Sigma_f^{(m)} = \frac{\nu\Sigma_f^{s,(m)} - E[\boldsymbol{\nu\Sigma}_f^s]}{Var[\boldsymbol{\nu\Sigma}_f^s]} Var[\boldsymbol{\nu\Sigma}_f] + E[\boldsymbol{\nu\Sigma}_f]$$

for all $m = 1, \dots, 10$

Intra-Cycle Batching with iCS Method

Intra-cycle batching method

– A methodology based on the history-based batch method to obtain statistically reliable estimates even during the early active cycles.

– Suppose there are N active cycles, each containing M particle histories.
  - At the beginning of each active cycles, the M histories are divided into N_B batches.
  - Let Q_{ij} denote the estimate of the quantity of interest Q from the j-th history in the i-th active cycle.
  - The batch-wise estimate of Q for the k-th batch is defined as,

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

  - The overall estimate of Q is then given by,

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

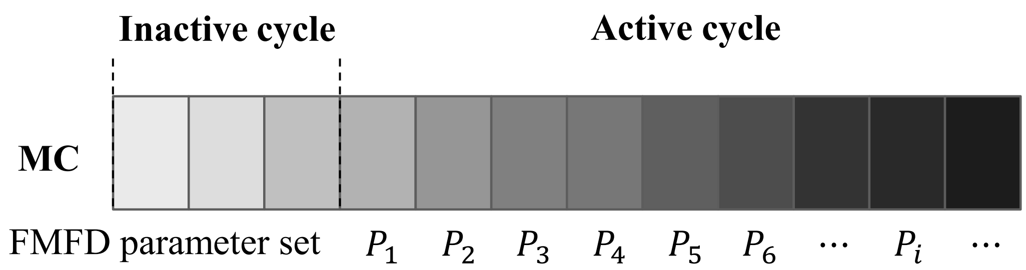
  - The variance of the mean is estimated using the standard batch-mean estimator,

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

Intra-Cycle Batching with iCS Method

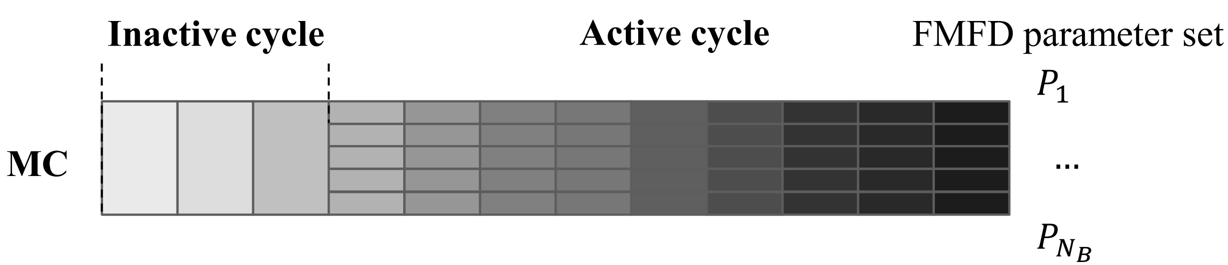
Change in uncertainty estimation in the iDTMC method

– Previously, parameters were tallied cycle-wise and the variance of the sample mean decreased as $1/N$.



- Therefore, many active cycles were required for stable uncertainty estimation.

– With intra-cycle batching, the number of batch mean is fixed at N_B.



- Consequently, the variance of the sample mean scales as $1/N_B$, which remains constant.

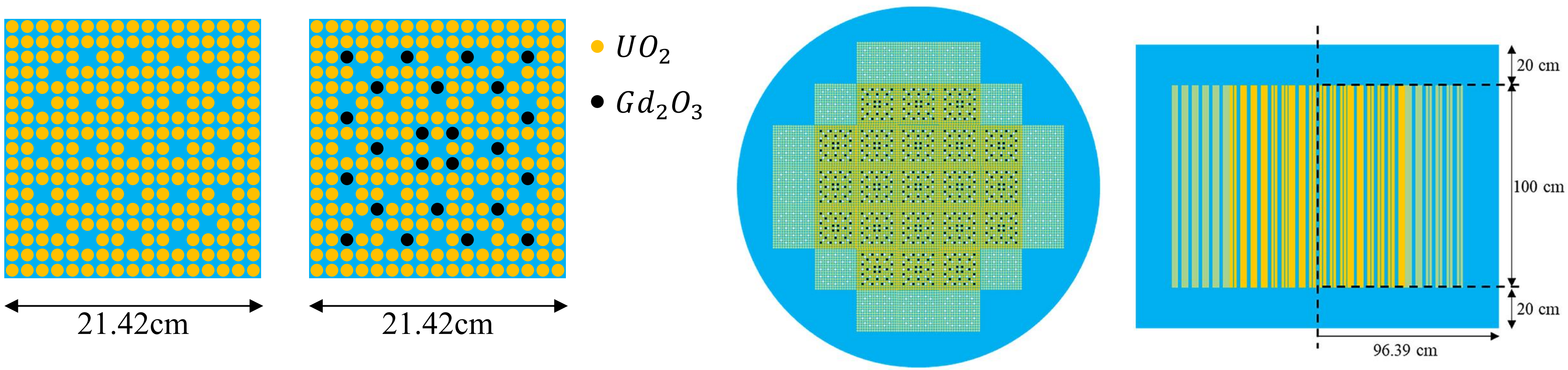
– In conclusion, intra-cycle batching **stabilizes early-cycle statistics** and **increase the effective number of samples used in the iCS weighted summation**.

Table of Contents

SMR Problem

SMR model

– Small Modular Reactor (SMR) core model was considered.
  - 7 by 7 FAs with zig-zag shape at the corner, total 37 FAs + Core surrounded by the water reflector
  - Two types of FA



Geometry Details	
Number of FA1 (with Gd_2O_3)	21
Number of FA2 (without Gd_2O_3)	16
Fuel pellet radius [cm]	0.5
Pin pitch [cm]	1.26
Cladding thickness [mm]	0.3
Reactor height [cm]	140

Material Specification	
Uranium enrichment [weight-%]	3.8
Uranium oxide density [g/cm^3]	10.4
Gadolinia weight fraction [%]	4
Gadolinia-mixed uranium oxide density [g/cm^3]	10.28
Cladding material (density) [g/cm^3]	Zircaloy (6.5)
Reflector material (density) [g/cm^3]	H_2O (0.9)

SMR Problem

Eigenvalue variance estimation using the iCS: SMR model

- 6e+06 histories/cycle, 15 inactive, 15 active with 14 p-FMFD cycles were used for the iDTMC.
- 210 independent batch calculations for the real variance calculation.
- 30 independent batch calculations for each estimation method /100 p-FMFD problems were sampled.
- Error bars represent the 99.7% confidence interval.

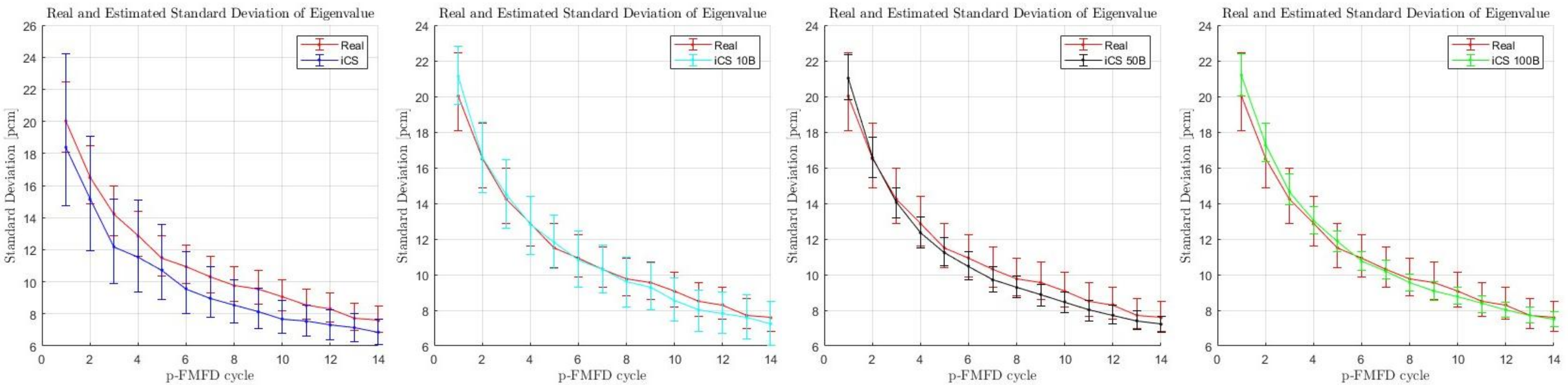


Figure 8. Mean estimation of eigenvalue standard deviation with various methods for 1 to 14 p-FMFD cycle.

Eigenvalue variance estimation using the iCS: SMR model

- 6e+06 histories/cycle, 15 inactive, 15 active with 14 p-FMFD cycles were used for the iDTMC.
- 210 independent batch calculations for the real variance calculation.
- 30 independent batch calculations for each estimation method /100 p-FMFD problems were sampled.

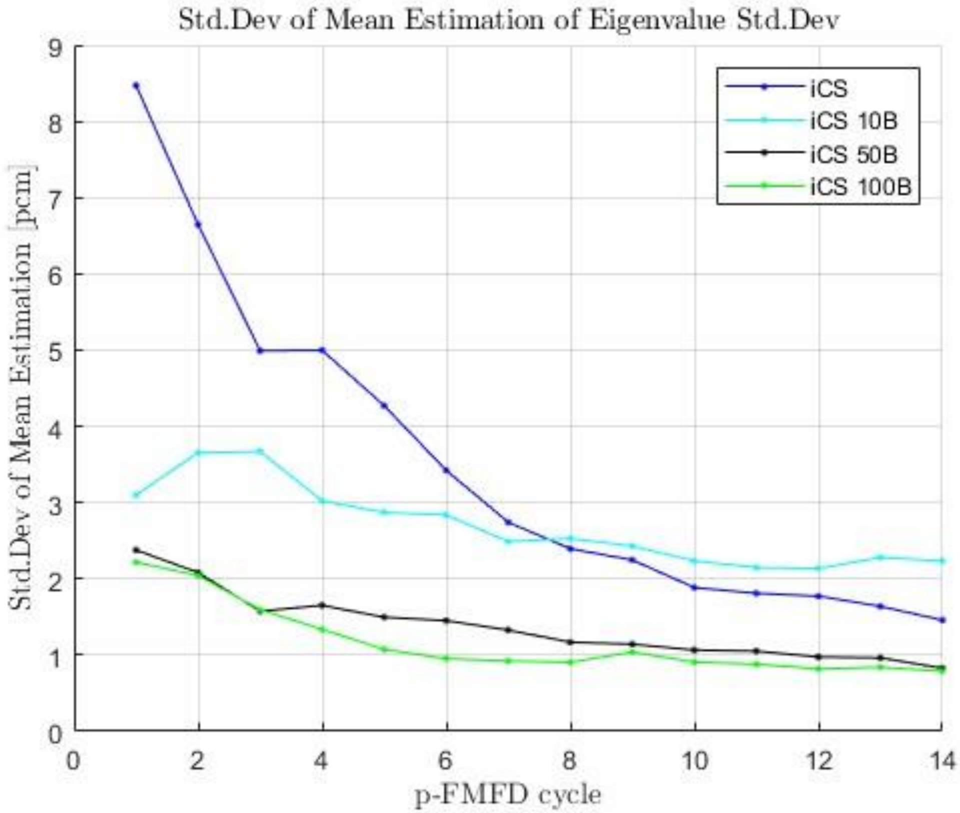


Figure 9. Standard deviation of mean estimation of eigenvalue standard deviation with various method; iCS (blue), iCS with $N_B = 10$ (cyan), iCS with $N_B = 50$ (black), and iCS with $N_B = 100$ (green).

Power distribution variance estimation using the iCS: SMR model

- 6e+06 histories/cycle, 15 inactive, 15 active with 1 p-FMFD cycles were used for the iDTMC.
- 120 independent batch calculations for the real variance calculation.
- 30 independent batch calculations for each estimation method /100 p-FMFD problems were sampled.
- Error bars represent the 99.7% confidence interval.
- The variance at the peak power pin is plotted.

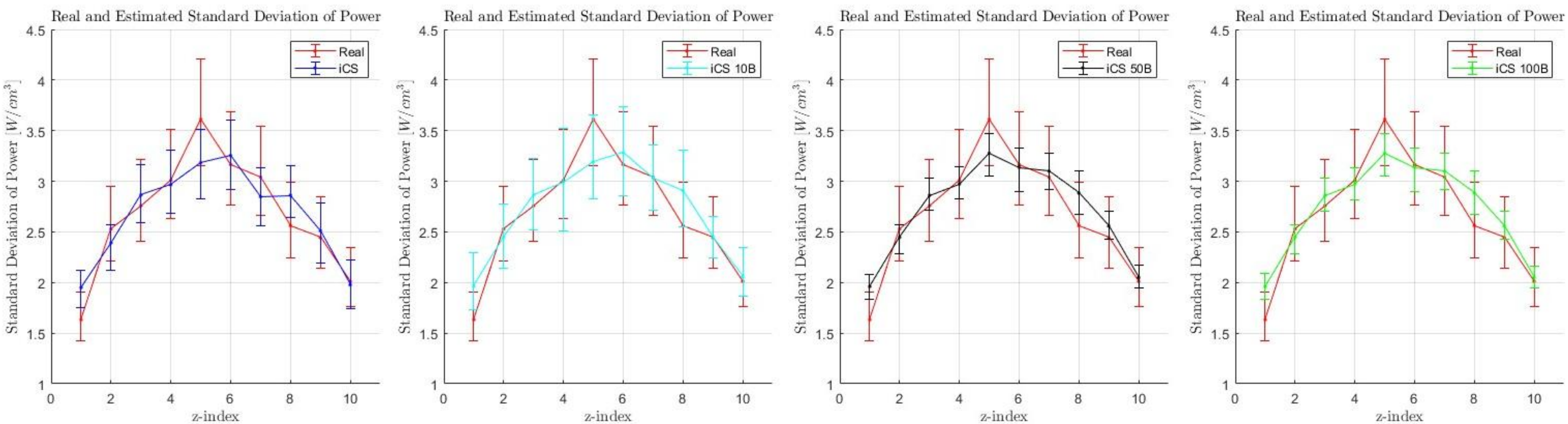


Figure 10. Mean estimation of power standard deviation with various method.

Power distribution variance estimation using the iCS: SMR model

- 6e+06 histories/cycle, 15 inactive, 15 active with 1 p-FMFD cycles were used for the iDTMC.
- 120 independent batch calculations for the real variance calculation.
- 30 independent batch calculations for each estimation method /100 p-FMFD problems were sampled.
- The variance at the peak power pin is plotted.

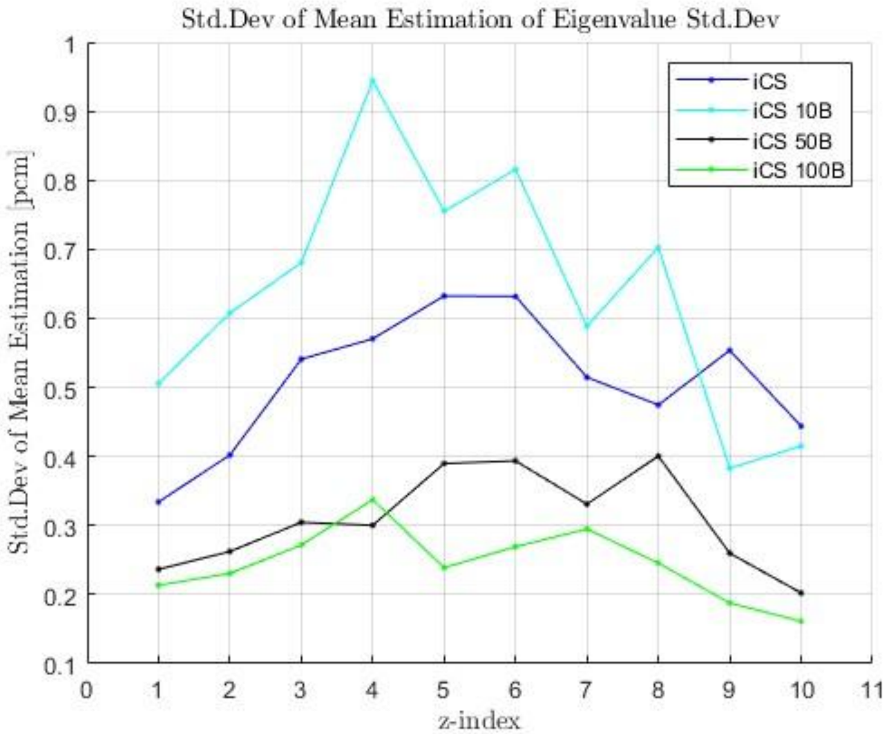


Figure 11. Standard deviation of mean estimation of power standard deviation with various method; iCS (blue), iCS with $N_B = 10$ (cyan), iCS with $N_B = 50$ (black), and iCS with $N_B = 100$ (green).

Table of Contents

Conclusions and Future Works

Summary and Conclusions

- iCS was combined with intra-cycle batching.
  - The proposed strategy enables reliable uncertainty prediction even with limited cycle statistics.

- Eigenvalue and power uncertainty estimation.
  - The estimated uncertainties were consistent with independent iDTMC reference calculations.
  - Eigenvalue and peak-pin power uncertainties were evaluated.
  - Intra-cycle batching reduced estimator fluctuation in early cycles.

- Effect of the number of batches.
  - Larger N_B generally improved estimator stability.
  - Excessively large N_B may reduce per-batch tally quality.

Future Works

- Establish an optimal N_B selection criterion and investigate adaptive batching strategies.

Thank You For Your Attention