Application of the History-based Batch Method to the iDTMC Method for Reliable Real Variance Estimation

Reactor Physics & Transmutation Lab.

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Motivation & Objectives

Improved Deterministic Truncation of Monte Carlo (iDTMC) method

– A hybrid stochastic/deterministic MC acceleration method
  - Accelerates convergence of fission source distribution **(p-CMFD)**
  - Obtains pin-wise solution **(p-FMFD)**

  → **Correlation becomes stronger in iDTMC than conventional MC**

  → **Even more underestimation of the variance!**

– Estimating the real variance

1) **Estimate** p-FMFD parameters' **distribution** & **sample** the parameters

2) **Solve** p-FMFD or use 1^{st}-order perturbation theory and **estimate real variance**

History-Based Batch Method

– Batch-wise calculated p-FMFD parameters can be obtained

In this work, new methods for estimating the real variance of iDTMC method are studied: using History-Based Batch Method

The current iDTMC Method

The iDTMC method

– p-CMFD: Accelerates convergence of fission source distribution
  1) The one-group neutron balance equation is solved using the higher-order MC solution
  2) Update fission source distribution of MC
– p-FMFD: Obtains pin-wise solution
  1) Solving same equation as p-CMFD do, with finer meshes

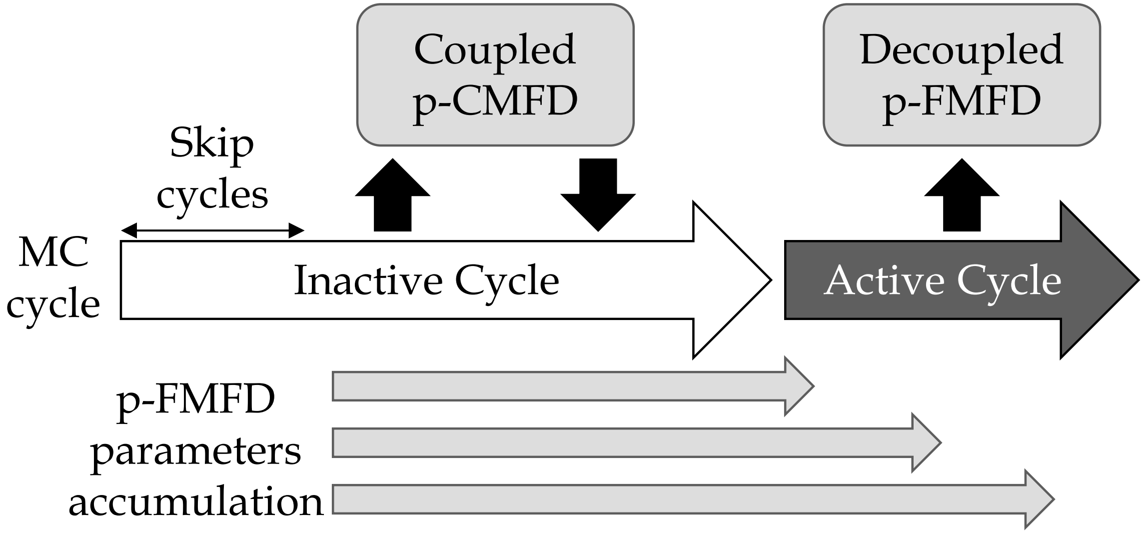


Figure 1. Schematic diagram of iDTMC method

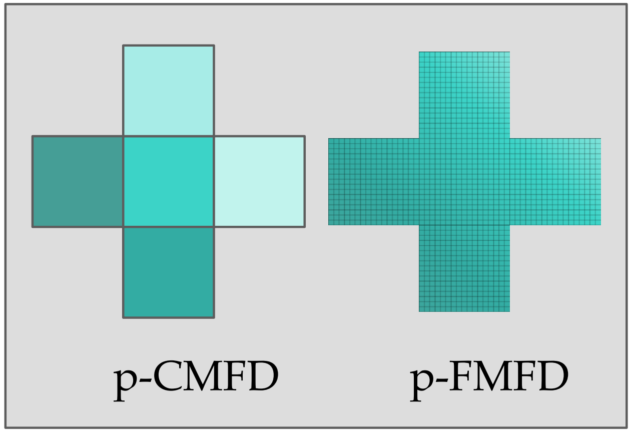


Figure 2. Mesh configuration for p-CMFD and p-FMFD calculations

The iDTMC method

– Figure of merit of the iDTMC method compare with MC with CMFD acceleration

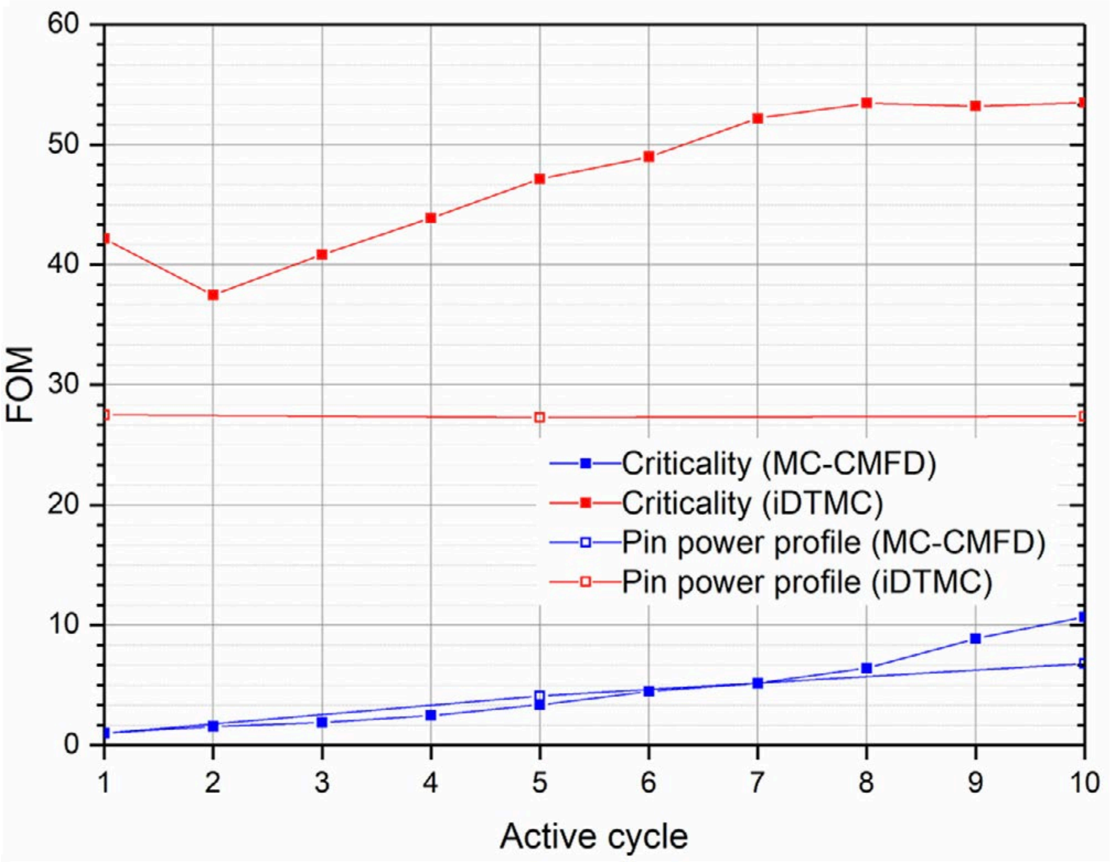


Figure 3. Figure of merit of the iDTMC method
and the MC with CMFD acceleration in SMR problem

The current iDTMC Method

Determining uncertainty

1) Using the accumulated parameters from previous cycles, **additional parameters are sampled.**

   → XSs, initial flux distribution etc.

2) The same neutron balance equation is solved multiple times using these new parameters and **the variance of theses solutions is used as the uncertainty for the iDTMC method**

What parameters are sampled?

– p-FMFD; total, absorption, nu-fission cross-sections, flux, and interface current

$$\sum \frac{A_s}{V_{i,j,k}}\left\{-\left(\tilde{D}_{s0}+\hat{D}_{s0}^{+}\right)\phi_{n-1}+\left(\tilde{D}_{s0}+\hat{D}_{s0}^{-}+\tilde{D}_{s1}+\hat{D}_{s1}^{+}\right)\phi_n-\left(\tilde{D}_{s1}+\hat{D}_{s1}^{-}\right)\phi_{n+1}\right\}+\Sigma_a^{i,j,k}\phi_{i,j,k}=\frac{1}{k_{eff}}\nu\Sigma_f^{i,j,k}\phi_{i,j,k}$$

$$where\ \tilde{D}_{s0}=\frac{2D_nD_{n-1}}{(D_n+D_{n-1})/\Delta}\ and\ \hat{D}_{s0}=\frac{J_{s0}^{MC}+\tilde{D}_{s0}\left(\phi_n^{MC}-\phi_{n-1}^{MC}\right)}{\phi_n^{MC}+\phi_{n-1}^{MC}}$$

→ How are the new parameters sampled?

New variance estimation scheme for the iDTMC Method

New method for sampling parameters

– **Cycle-wise uncorrelated parameters** are sampled for the variance estimation

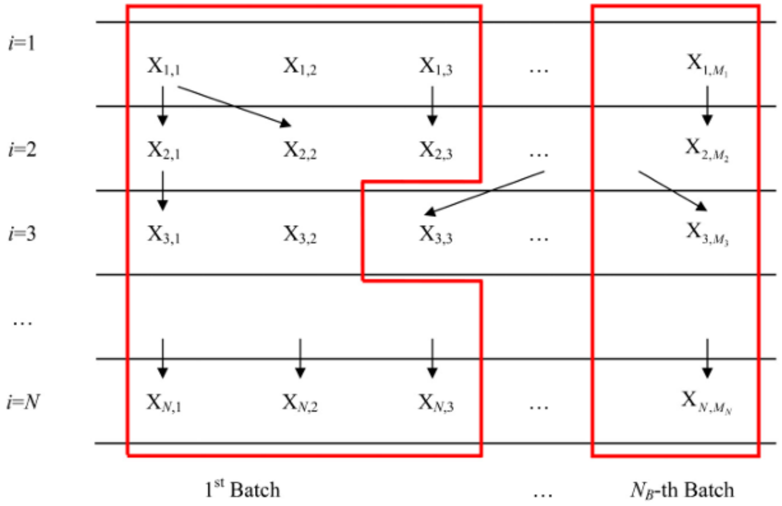
History-Based Batch Method

– Tow sources for mutual dependency of tallied value in MC simulation

1) Genealogical dependency of particle histories

2) Normalization scheme of fission source neutrons' weight

→ Regard as N_B independent MC runs on N active cycles with M/N_B histories per cycle (instead of N active cycles with M histories per cycle)



Batch-avg MC tally:

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

Estimation of batch-wise MC tally:

$$\bar{Q}_{HB} = \frac{1}{NM} \sum_{i=1}^{N} \sum_{k=1}^{N_B} \sum_{j\in k} f_i^k Q_{ij}$$

Associated variance:

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

New variance estimation scheme for the iDTMC Method

New Method: The History-based Batch Sampling

– Minor difference exists to **conserve the conventional MC simulation**
  - Normalization of weight does not apply for each history-based batch

    → Same weight normalization process as conventional MC do
  - To conserve number of histories per batch, weight correction considered at banking:

$$n = \left\lfloor w_i \left(\frac{\nu\sigma_f}{\sigma_t}\right)\left(\frac{1}{k_{eff}}\right) f_i^k + \xi \right\rfloor$$

  - Only for the variance calculation, when we tally, weight correction considered:

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

$$\bar{Q}_{HB} = \frac{1}{NM} \sum_{i=1}^{N} \sum_{k=1}^{N_B} \sum_{j\in k} f_i^k Q_{ij} \ \ and \ \sigma^2[\bar{Q}_{HB}] = \frac{1}{N_B(N_B-1)} \sum_{k=1}^{N_B} \left(Q^k - \bar{Q}_{HB}\right)^2$$

– For the iDTMC calculation, accumulated parameters without weight correction is used

→ With this method, we can **calculate iDTMC result** without bias

and also, we can estimate the real variance of each parameters

New variance estimation scheme for the iDTMC Method

New Method: The History-based Batch Sampling

- From the HBM, cycle-wise independent parameters' variance are estimated:

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

- For parameter sampling, we use estimated variance and accumulated mean
- For the Σ_t, Σ_a, and $\nu\Sigma_f$, correlated sampling was used

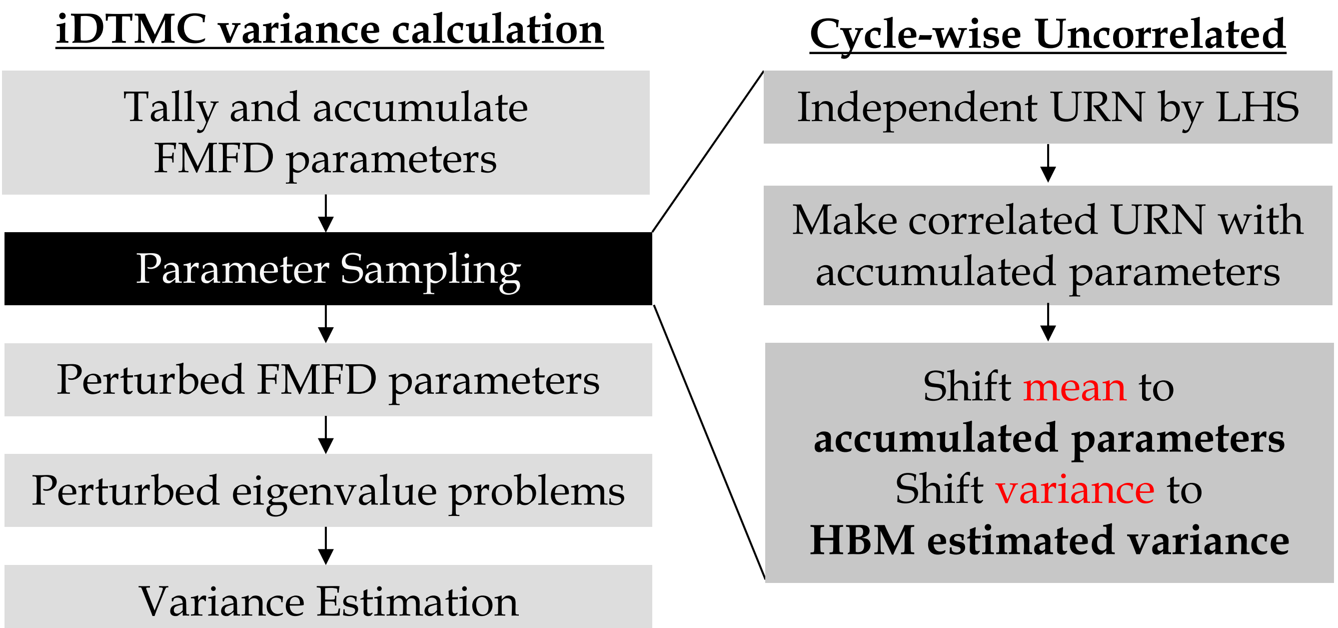


Figure 4. Schematic of real variance estimation using History-based Batch method to produce cycle-wise uncorrelated parameters in IDTMC method

Numerical Results

Problem description: SMR model

SMR model

- SMR model
  - FA1: 17-by17 FA, Gd+U oxide
  - FA2: 17-by-17 FA, U oxide
  - 10 axial nodes
- 30 inactive and 10 active cycles
- First 15 inactive cycles are skipped

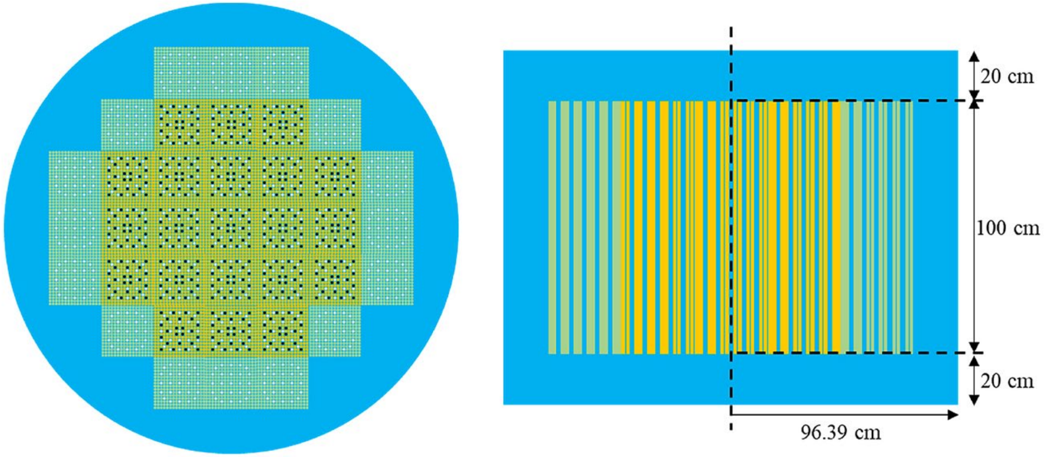


Figure 5. Cross-sectional (left) and side (right) view of the SMR model

Geometry Detail	
Number of FA1	16
Number of FA2	21
Fuel pellet radius	0.5cm
Pin pitch	1.23cm
Cladding Thickness	0.3mm

Material Specification	
U enrichment , U oxide density	3.8 w/o, 10.4 g/cm^3
Gd weight fraction, Gd+U oxide density	4%, 10.28 g/cm^3
Cladding material (density)	Zircaloy (6.5 g/cm^3)
Reflector material (density)	H_2O (0.9 g/cm^3)
Temperature	294 K

Result from History-based Batch Sampling

Estimation Result for Real Variance of Eigenvalue (1^{st}-order perturbation)

- 1.5E+06 histories were used
- Real eigenvalue from 149 batch calculation: 1.12593±10.96pcm

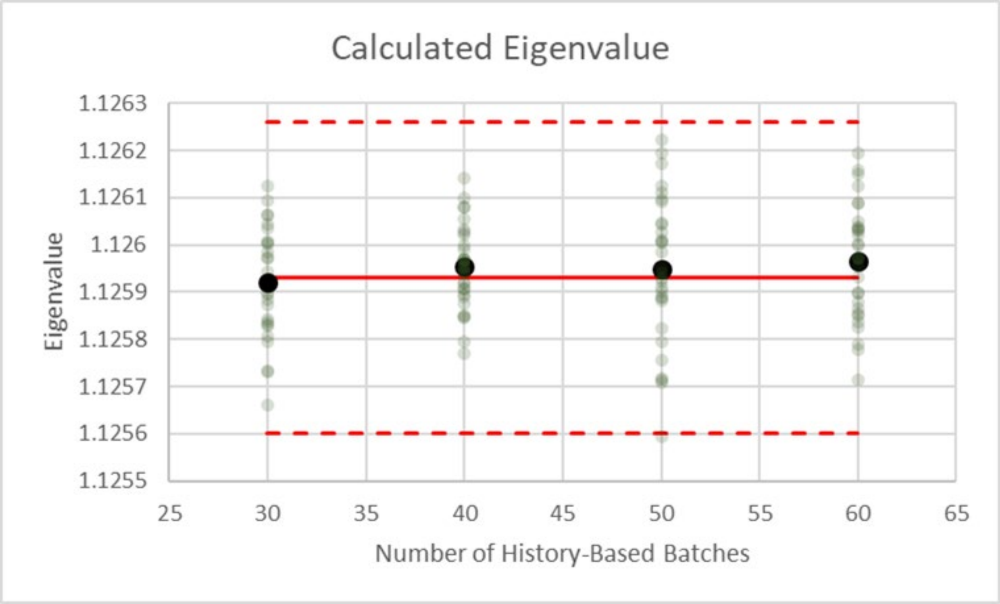


Figure 6. Calculated eigenvalue for various number of history-based batches at 10^{th} active cycle

- 30, 40, 50, and 60 history-based batches (HB) are tested
- For each number of history-based batches, 30 independent batch calculation was done
- **All eigenvalues are in the boundary of 3σ (red dotted line)**

Result from History-based Batch Sampling

Estimation Result for Real Variance of Eigenvalue (1st-order perturbation)

– 1.5E+06 histories were used

– Real eigenvalue from 149 batch calculation: 1.12593±10.96pcm

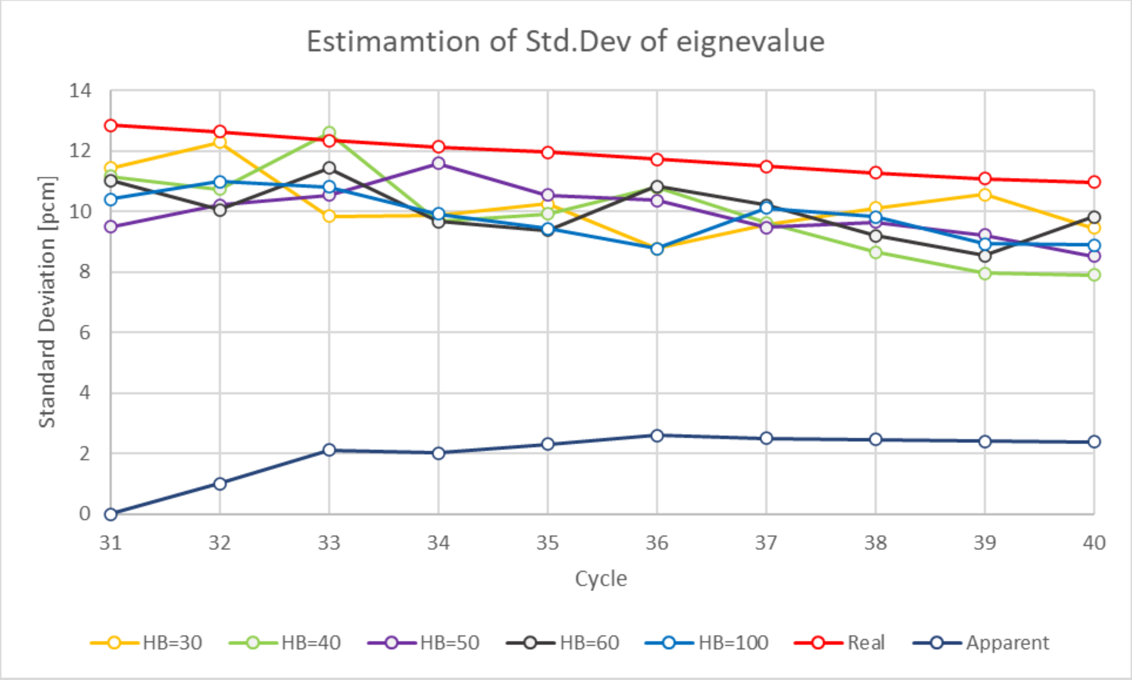


Figure 7. Independent batch averaged estimated variance and real variance (red), 'HB' represents number of history-based batches

Method	Estimated Std.Dev [pcm]	Relative Error [%]
HB=30	9.46	13.69
HB=40	7.9	27.92
HB=50	8.53	22.17
HB=60	9.83	10.31
HB=100	8.89	18.89
Apparent	2.40	78.10

– Small underestimation compare with the real variance

– Smaller relative error compared with apparent variance regardless of number of HB

Result from History-based Batch Sampling

Estimation Result for Real Variance of Eigenvalue (1^{st}-order perturbation)

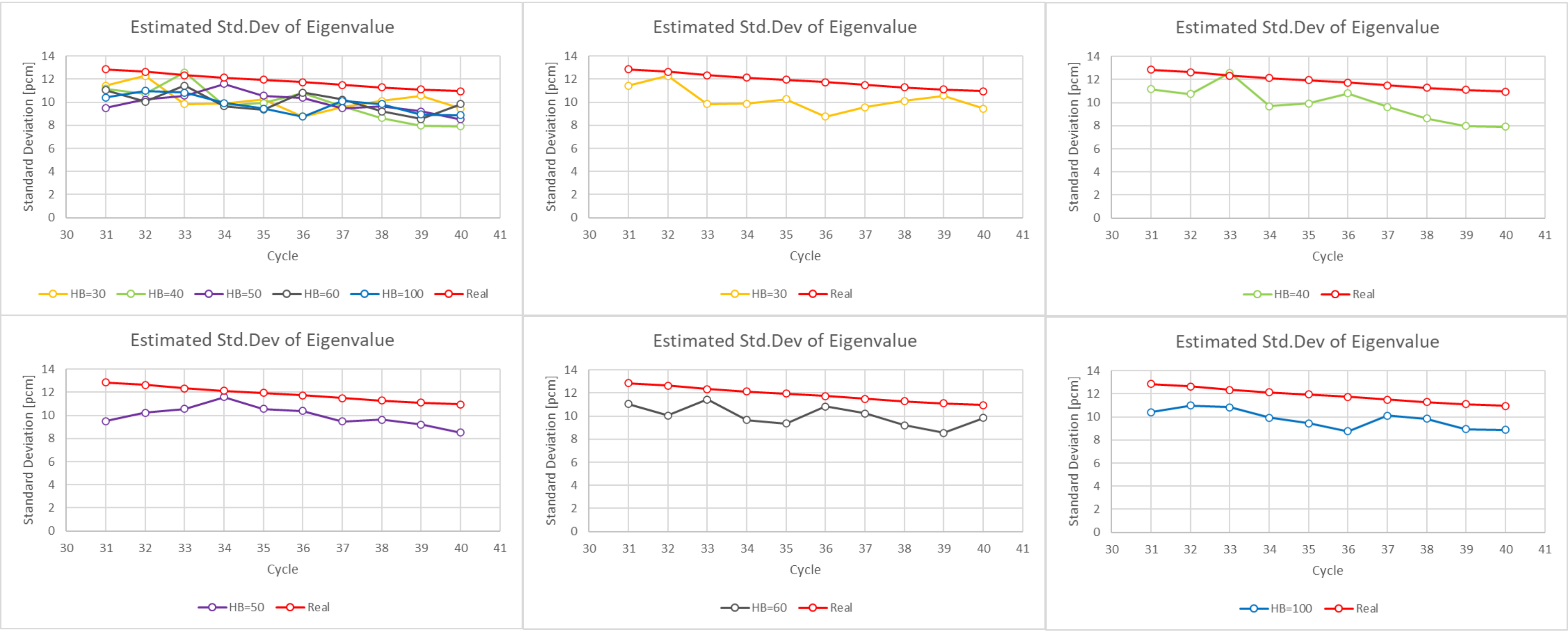


Figure 8. Estimated variance for each number of history-based batches

Result from History-based Batch Sampling

Estimation Result for Real Variance of Eigenvalue (solving p-FMFD)

- 1.5E+06 histories were used
- Real eigenvalue from 149 batch calculation: 1.12593±10.96pcm
- At 10th active cycle:

Number of HB	Estimated $\sigma_{k_{eff}}$ [pcm]		Relative error [%]	
	1st-order	p-FMFD	1st-order	p-FMFD
30	9.46	9.49	13.69	13.40
40	7.9	7.83	27.92	28.54
50	8.53	8.36	22.17	23.73
60	9.83	9.60	10.31	12.38
100	8.89	8.88	18.89	18.96

- Similar result when we use 1st-order perturbation theory

Result from History-based Batch Sampling

Estimation Result for Real Variance of Power Distribution

- 1.5E+06 histories were used

$$\bar{\sigma}_p = \frac{1}{N_{pins}} \sum_{i=1}^{N_{pins}} \sigma_i \ where\ \sigma_i = std.dev\ of\ fule\ pin\ i$$

- Real variance from 45 batch calculation: **3.913pcm**

Method	$\bar{\sigma}_p$ [pcm]	Relative Err [%]
HB=30	3.811	2.6
HB=40	3.815	2.5
HB=50	3.822	2.3
HB=60	3.825	2.3
HB=100	3.854	1.5
Apparent	0.648	83.5

- When we average the relative error of variance estimation for each pin, for all HB, average error was within 10% (7.7~9.1%)

Estimation Result for Real Variance of Power Distribution

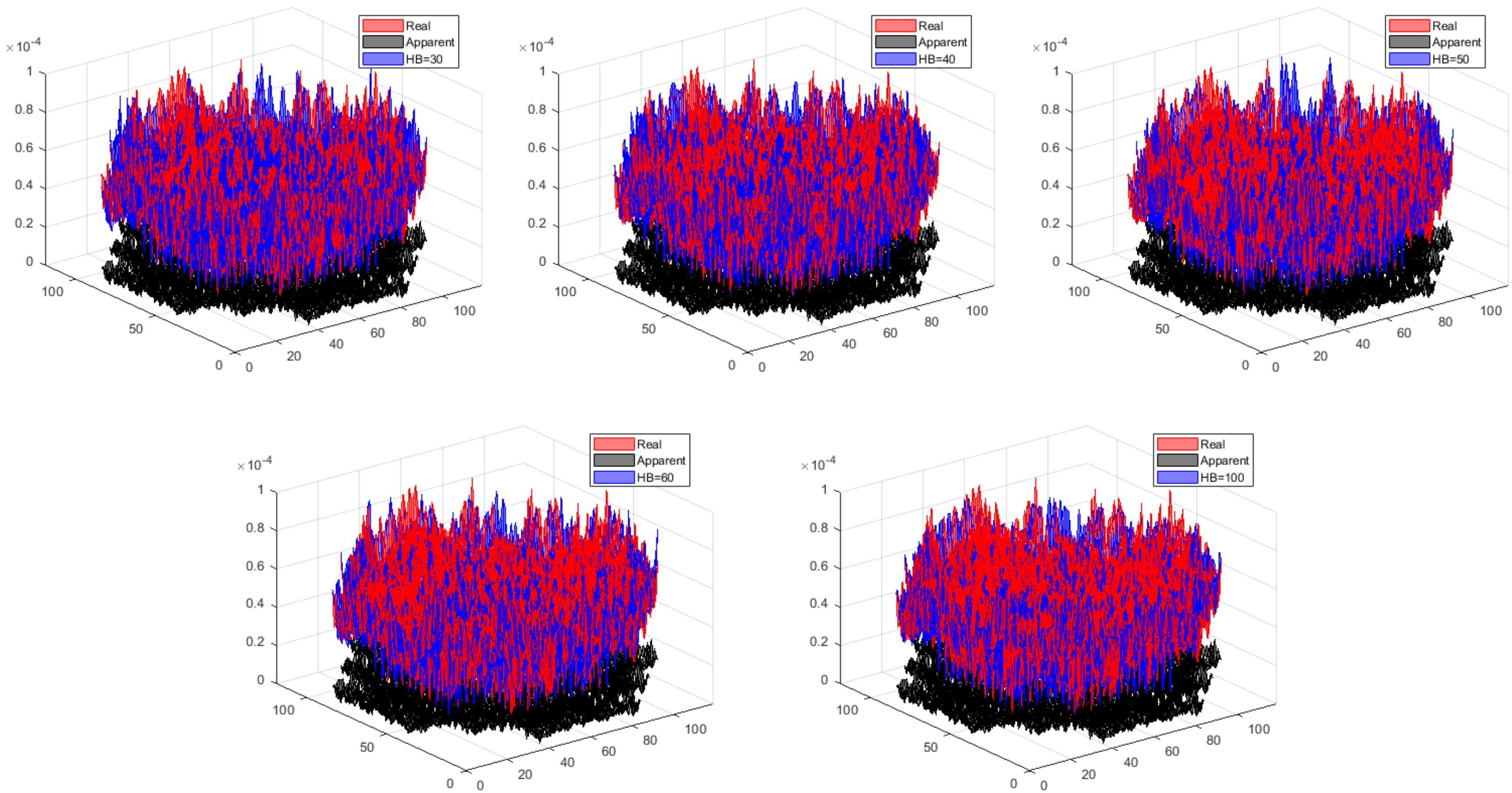


Figure 9. Estimated variance of power distribution
for each number of history-based batches at the midplane

Estimation Result for Real Variance of Power Distribution

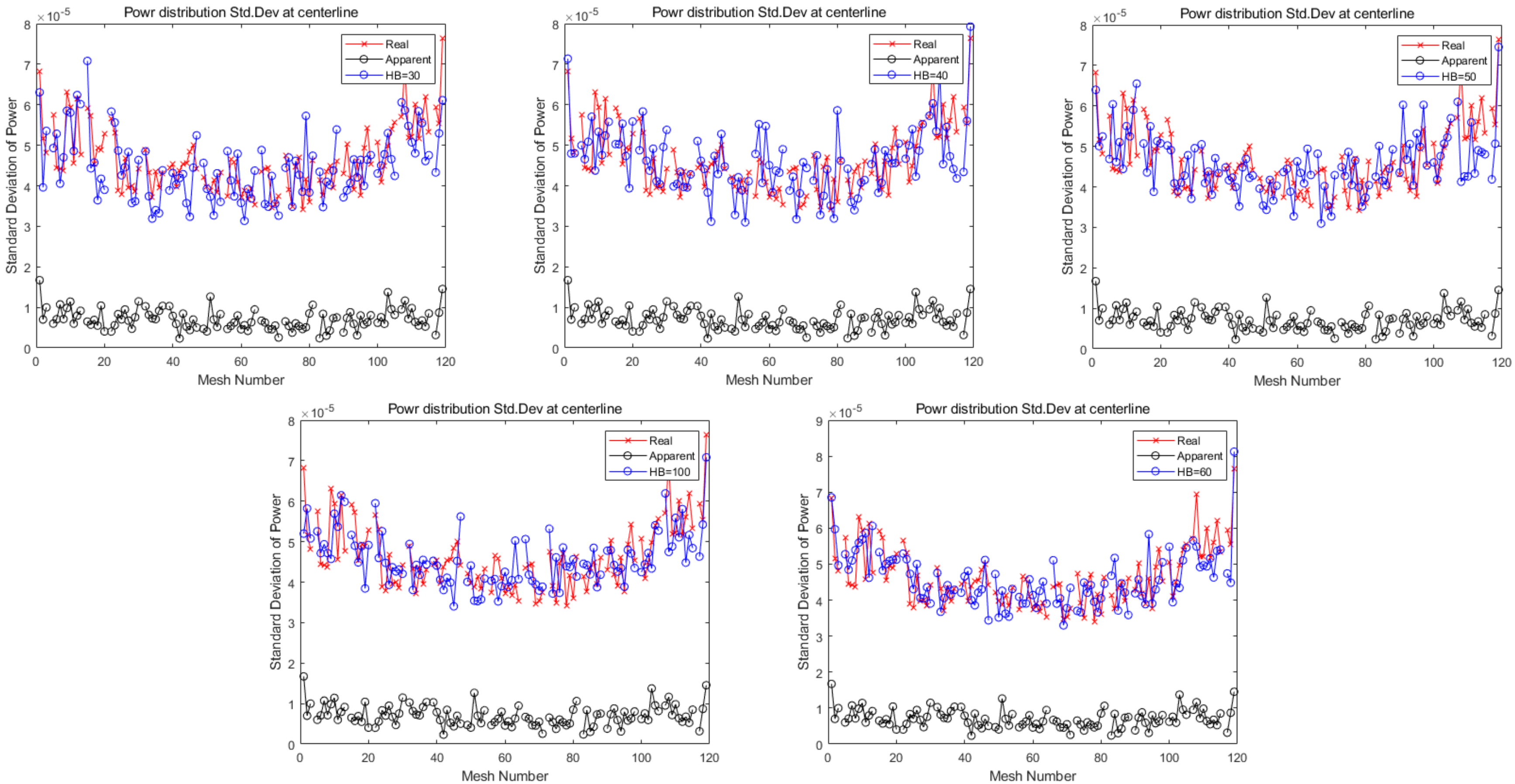


Figure 10. Estimated variance of power distribution
for each number of history-based batches at the centerline

Conclusion and Future Work

Conclusion

– Independent batch calculation was done with History-Based Batch Sampling
  - For 30, 40, and 60 history-based batches, 30 batch calculation were done for each
  - All eigenvalues are in the boundary of 3σ, which shows there were non-significant bias

– Variance estimation of eigenvalue with HBM was done
  - For overall active cycle, estimation was slight underestimating the real one
  - Estimations show at least 50% higher accuracy compare with the apparent Std.Dev

– Variance estimation of power distribution with HBM was done
  - Estimations show at least 80% higher accuracy compare with the apparent Std.Dev

Future Work

– Batch calculation for the estimation must be done to see variance of the estimation

– Node-wise correlation and correlation between cross-sections & flux must be dealt with

Thank you for listening

Questions?

Backup Slides

History-Based Batch Method

Limitation of Conventional Monte Carlo Simulation

– Tow sources for mutual dependency of tallied value in MC simulation

1) Genealogical dependency of particle histories

2) Normalization scheme of fission source neutrons' weight

– Let MC simulation with N active cycles with M histories per cycle

– Define Q_{ij} as MC estimate of a tally Q form the j'th history at active cycle i

- Real Variance:

$$\sigma^2[\bar{Q}] = \frac{1}{NM}\sigma^2[Q_{ij}] + \frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j} cov[Q_{ij}, Q_{i',j'}]$$

- Apparent Variance:

$$\sigma_A^2[\bar{Q}] = \frac{1}{NM}\sigma^2[Q_{ij}] - \frac{1}{(NM)^2(NM-1)}\sum_{i,j}\sum_{i',j'\neq i,j} cov[Q_{ij}, Q_{i',j'}]$$

– There is a bias between two variance

→ Let us regard the MC simulation as

N_B independent MC runs on N active cycles with M/N_B histories per cycle

How History-Based Batch Method Works

- Let M_i^k as the number of fission source of the k'th history-based batch at cycle i

$$\sum_{k=1}^{N_B} M_i^k = M_i$$

- The normalization process giving a weight to k'th history-based batch at cycle i, w_i^k

$$w_i^k = \frac{M/N_B}{M_i^k}$$

- Then, batch-average MC tally, Q^k is

$$Q^k = \frac{1}{N(M/N_B)} \sum_{i=1}^{N} \sum_{j \in k} f_i^k Q_{ij} \;\; where \;\; f_i^k = \frac{w_i^k}{w_i} = \frac{M_i/N_B}{M_i^k}$$

- Now, estimating the sample mean and variance as

$$\bar{Q}_{HB} = \frac{1}{N_B} \sum_{k=1}^{N_B} Q^k = \frac{1}{NM} \sum_{i=1}^{N} \sum_{k=1}^{N_B} \sum_{j \in k} f_i^k Q_{ij} \;\; and \;\; \sigma^2[\bar{Q}_{HB}] = \frac{1}{N_B(N_B-1)} \sum_{k=1}^{N_B} \left(Q^k - \bar{Q}_{HB}\right)^2$$