Real Variance Estimation in iDTMC method using Spectral Analysis Method and Autoregressive (1) Model

October 25, 2024

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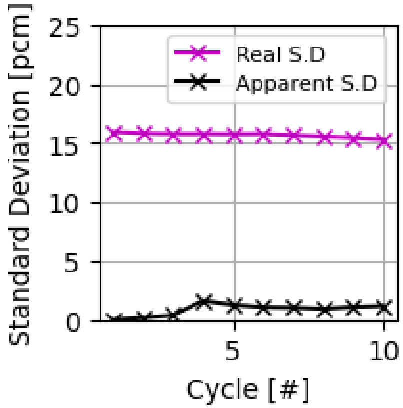
Motivation & Objectives

The Monte Carlo (MC) method

– Simulates neutron transport in a stochastic manner to obtain a solution with some uncertainty (variance)

→ Samples are inherently correlated cycle-wise in MC methods

→ **Causes underestimation of the variance**



Improved Deterministic Truncation of Monte Carlo (iDTMC)

– A hybrid stochastic/deterministic MC acceleration method
- Partial Current-based Coarse Mesh Finite Difference (**p-CMFD**) method
  - ✓ Accelerates convergence of fission source distribution (FSD)
- Partial Current-based Fine Mesh Finite Difference (**p-FMFD**) method
  - ✓ Obtains pin-wise solution

→ **Correlation becomes stronger in iDTMC**

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

In this work, new methods for estimating the real variance of iDTMC method are studied: using the Spectral Analysis method and Autoregressive (1) model

The iDTMC method

- p-CMFD: Accelerates convergence of FSD
- p-FMFD: Obtains pin-wise solution

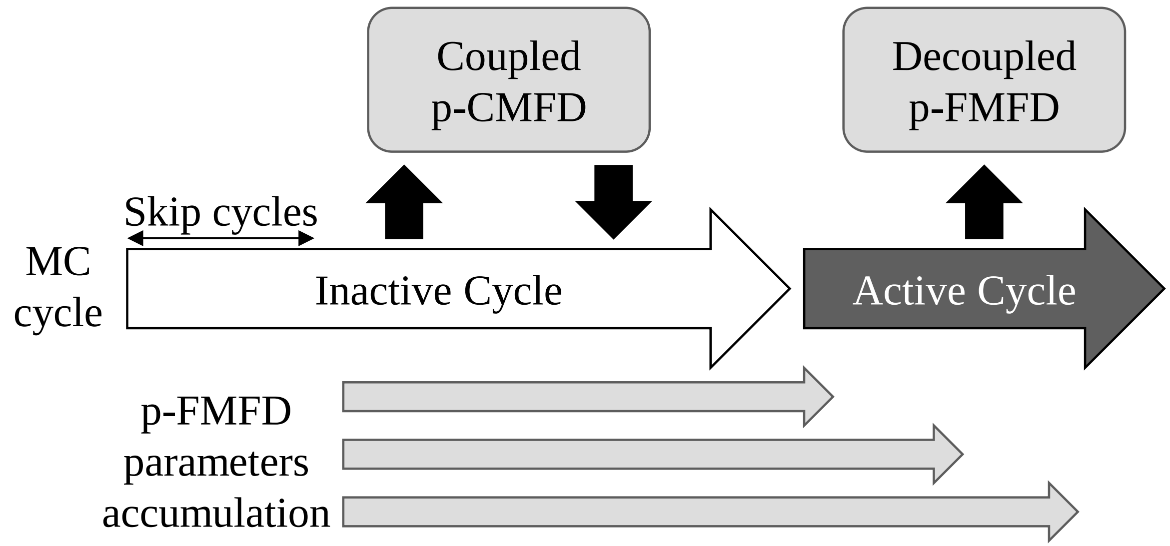


Figure 1. Schematic diagram of iDTMC method

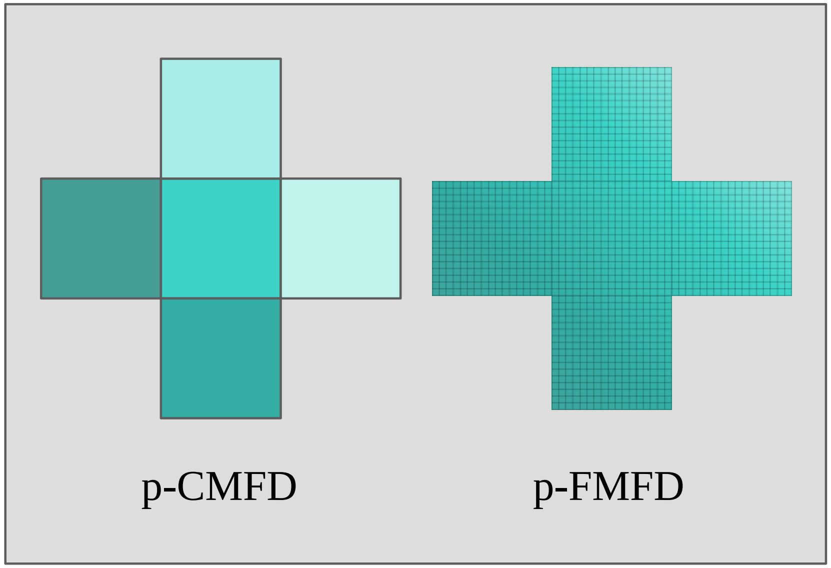


Figure 2. Mesh configuration for
p-CMFD and p-FMFD calculations

The iDTMC method

- p-CMFD: Accelerates convergence of FSD

1) The one-group neutron balance equation is solved using constants from the higher-order MC solution

$$\sum_{s}\frac{A_s}{V_i}(J_{s1}-J_{s0})+\Sigma_a^i\phi_i=\frac{1}{k_{eff}}\nu\Sigma_f^i\phi_i$$

$$J_{s1}=J_{s1}^{+}-J_{s1}^{-}=-\widetilde{D}_{s1}(\phi_{i+1}-\phi_i)+\widehat{D}_{s1}^{+}\phi_i-\widehat{D}_{s1}^{-}\phi_{i+1}$$

$$\widetilde{D}_{s1}=\frac{1}{\Delta_i}\frac{2D_iD_{i+1}}{D_i+D_{i+1}},\ \widehat{D}_{s1}^{\pm}=\frac{J_{s1}^{MC\pm}\pm\widetilde{D}_{s1}(\phi_{i+1}^{MC}-\phi_i^{MC})/2}{\phi_{i+\frac{1}{2}\pm\frac{1}{2}}^{MC}}$$

2) Update FSD of MC

$$w_i'=w_i\times\left(\frac{p_i^{p-CMFD}}{p_i^{MC}}\right)$$

The current iDTMC Method

The iDTMC method

- p-FMFD: Obtains pin-wise solution

$$\sum_s \frac{A_s}{V_i}(J_{s1} - J_{s0}) + \Sigma_a^i \phi_i = \frac{1}{k_{eff}} \nu\Sigma_f^i \phi_i$$

- Determining uncertainty

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

   → XSs, diffusion coefficients, 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 solution**.

➔ **How are the new parameters sampled?**

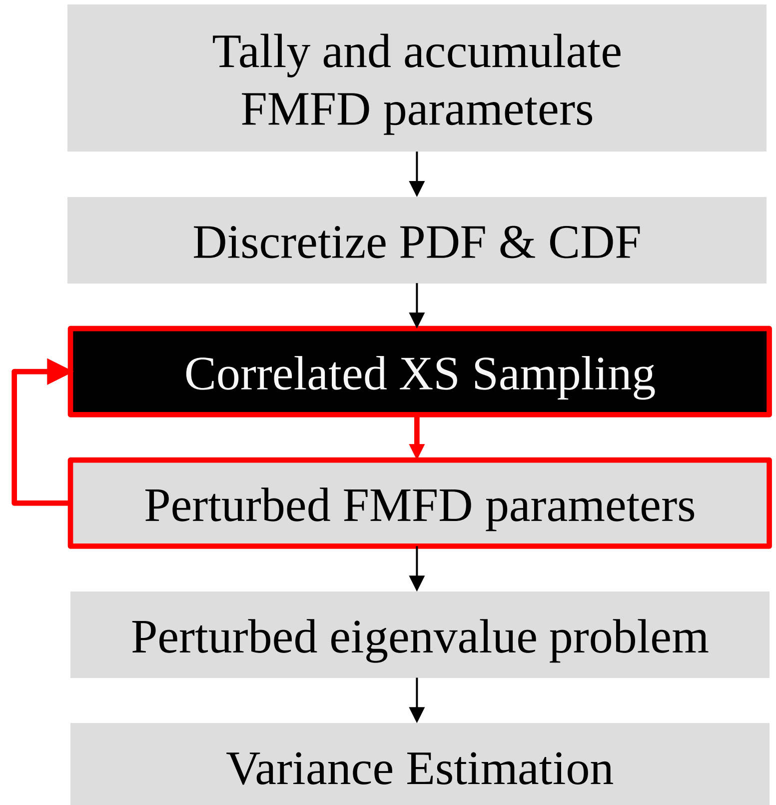
The current iDTMC Method

Current method for sampling parameters

→ **Correlated sampling**

– p-FMFD parameters (e.g., XSs) have strong correlation by reaction type, cycle, cell etc.

iDTMC variance calculation



1) **Sample p-FMFD parameters** from probability density functions using correlated sampling

<Correlation Matrix>

$$C = \frac{1}{\sigma_X \sigma_Y} \begin{bmatrix} 1 & Cov(\Sigma_t, \Sigma_a) & Cov(\Sigma_t, \nu\Sigma_f) \\ Cov(\Sigma_t, \Sigma_a) & 1 & Cov(\Sigma_a, \nu\Sigma_f) \\ Cov(\Sigma_t, \nu\Sigma_f) & Cov(\Sigma_a, \nu\Sigma_f) & 1 \end{bmatrix}$$

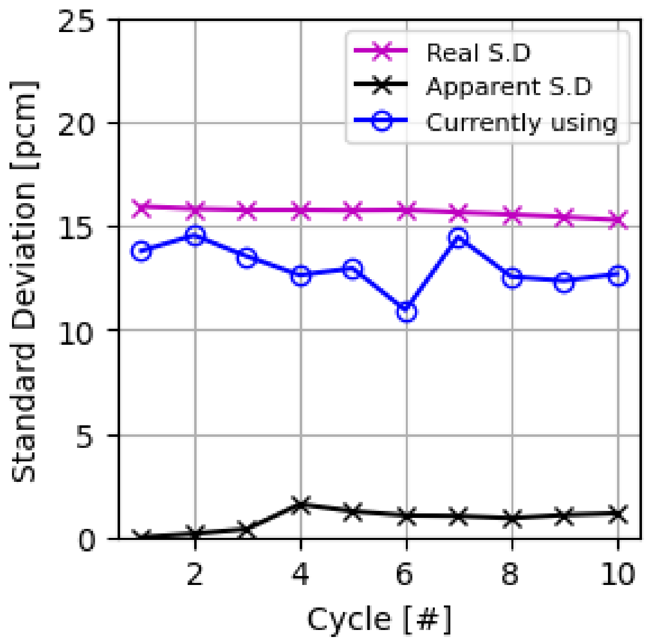
2) **Generate perturbed eigenvalue problems** (**iteration** is needed to match the correlation matrix)

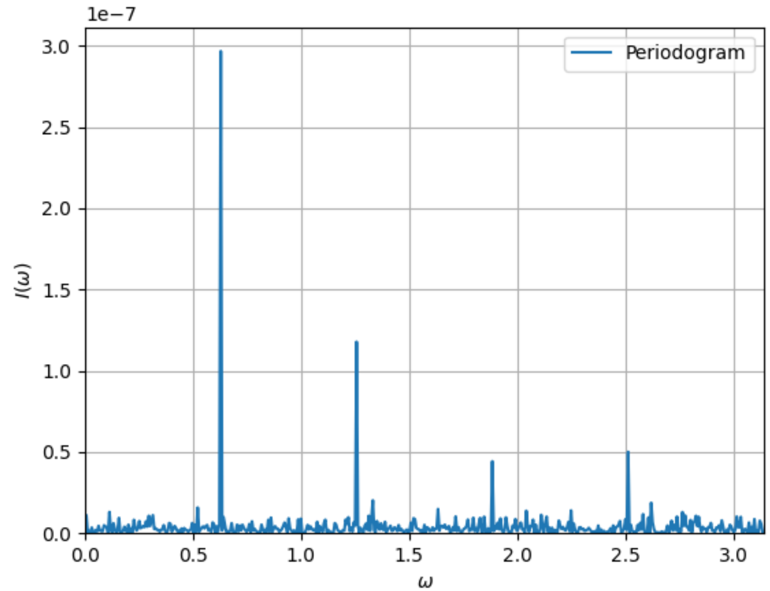
3) **Estimate real variance** by either solving the perturbated problems or using 1st -order perturbation theory

Limitations of the current iDTMC Method

Limitations of the current method

– While the estimated variance is closer to the real variance, **significant cycle-wise correlation of the sampled parameters is observed** from Spectral Analysis Method (SAM) based analysis.





→ Cycle-wise correlation is the main factor behind underestimation of the variance in MC methods!

New variance estimation scheme for the iDTMC Method

New method for sampling parameters

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

Autoregressive (1) model

– Samples of X taken from **consecutive cycles** $(\ldots, X_{t-1}, X_t, X_{t+1}, \ldots)$ can be seen as an Autoregressive (AR) process

– **First-order** AR model (AR (1)) of X

$$(X_t - \mu) = \phi(X_{t-1} - \mu) + Z_t(0, \sigma^2)$$

- μ: the **mean** of X
- ϕ: the **correlation coefficient** for the samples
- σ^2: the **variance** of the Gaussian white noise Z_t

New variance estimation scheme for the iDTMC Method

Autoregressive (1) model

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- μ: the **mean** of X
- ϕ: the **correlation coefficient** for the samples
- σ^2: the **variance** of the Gaussian white noise Z_t

– AR (1) model parameter estimators:

- Least Square Estimator (LSE)

1) Assume σ^2 is small
2) Needs large number of samples

➔ **Not appropriate for iDTMC!**

- Maximum Likelihood Estimator (MLE)

➔ **Can be used with fewer samples**

New variance estimation scheme for the iDTMC Method

Autoregressive (1) model

$$(X_t - \mu) = \phi(X_{t-1} - \mu) + Z_t(0, \sigma^2)$$

- μ: the mean of X
- ϕ: the correlation coefficient for the samples
- σ^2: the variance of the Gaussian white noise Z_t

$<$Parameter Estimation with MLE$>$

– For MLE, for parameter $\theta = (\mu, \phi, \sigma^2)$, likelihood function is:

$$logL(\theta) = -\frac{1}{2}\log\left(\frac{2\pi\sigma^2}{1-\phi^2}\right) - \frac{\left(Y_1 - \frac{c}{1-\phi}\right)^2}{\frac{2\sigma^2}{1-\phi^2}} - \frac{\mathrm{T}-1}{2}\log(2\pi\sigma^2) - \sum_{t=2}^{T}\frac{(Y_t - c - \phi Y_{t-1})^2}{2\sigma^2}$$

$$c = (1-\phi)\mu$$

– With the likelihood function, we may estimate parameters $\hat{\theta}$:

$$\frac{d(logL(\hat{\theta}))}{d\hat{\theta}} = 0$$

– The bisection method is used to obtain the parameters that satisfy the above equation

New variance estimation scheme for the iDTMC Method

New method: real variance estimation using AR (1) model

- From the AR (1) model, t[th] cycle parameter could be estimated with accumulated parameters as:

$$X_t - \mu = \phi(X_{t-1} - \mu) + Z_t(0, \sigma^2)$$

- When we set ϕ to 0, we can sample cycle-wise uncorrelated parameters **without iteration**:

$$X_t^{uncorr} = \mu + Z_t(0, \sigma^2)$$

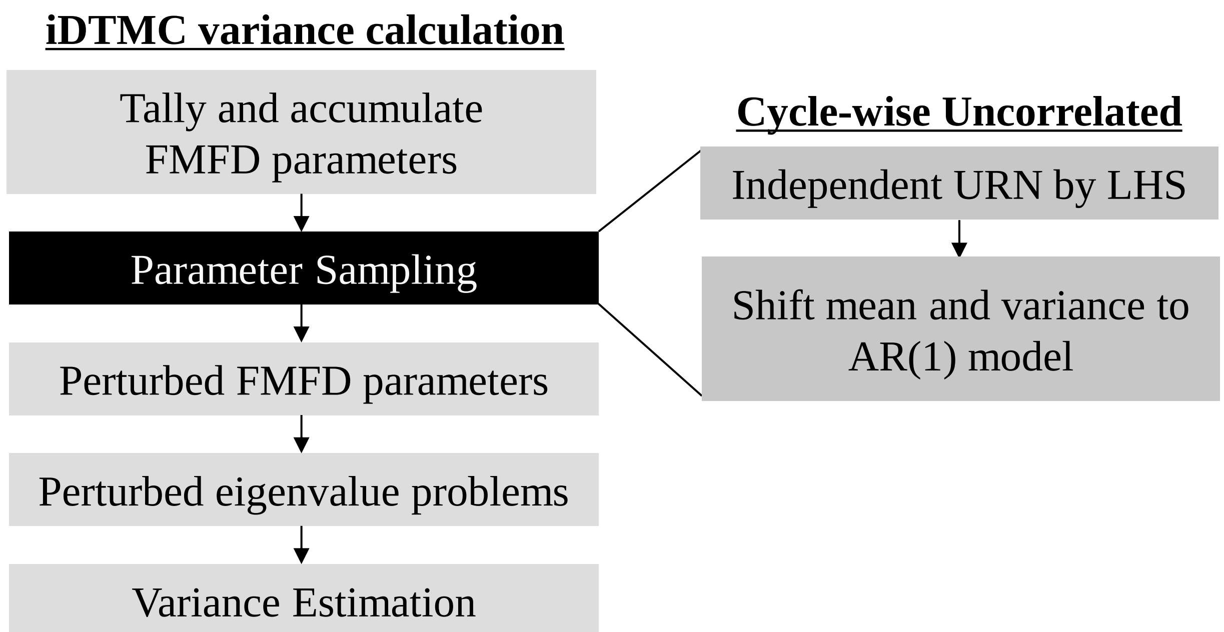


Figure 9. Schematic of real variance estimation using AR(1) model to produce cycle-wise uncorrelated parameters in IDTMC method

Numerical Results

SMR model

– SMR model
  - FA1: 17-by-17 FA, Gd+U oxide
  - FA2: 17-by-17 FA, U oxide
  - 10 axial nodes
– 1.5e+6 histories
– 30 inactive and 10 active cycles
– First 15 inactive cycles are skipped

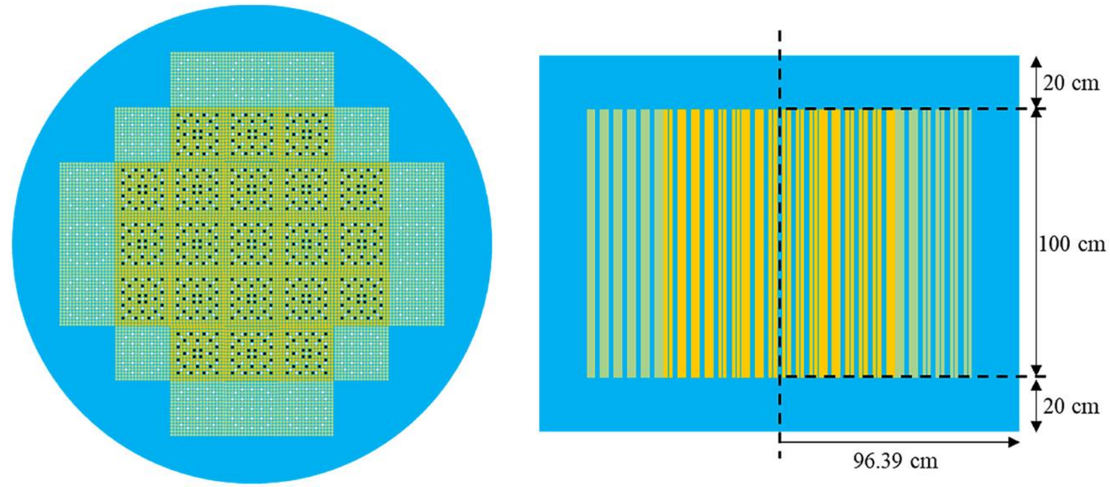


Figure 9. Cross-sectional (left) and side (right) view of the SMR model

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

Cycle-wise Correlation Coefficient

– Correlation coefficients obtained from AR (1) model

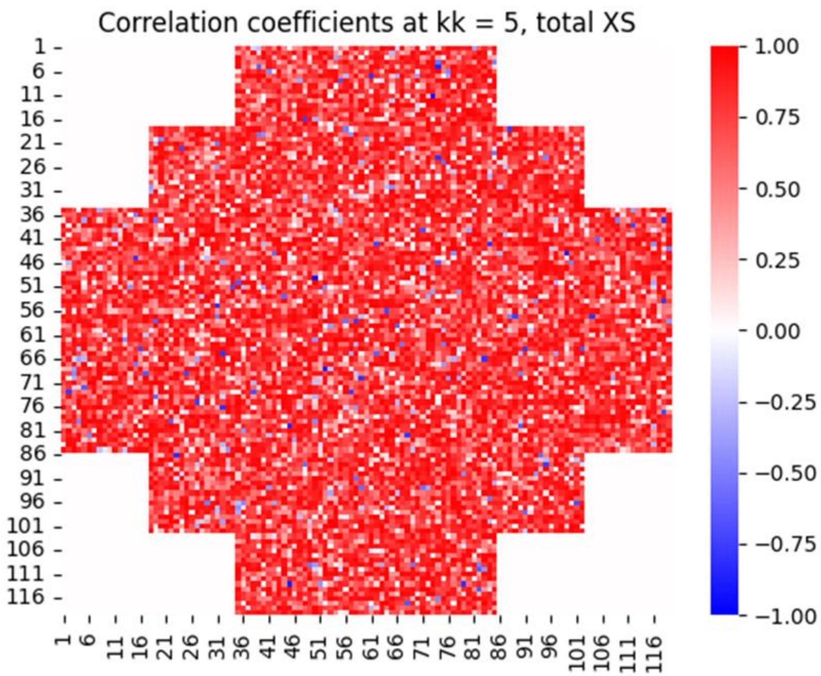


Figure 10. Correlation coefficient of total cross-section for each node at 5th axial plane

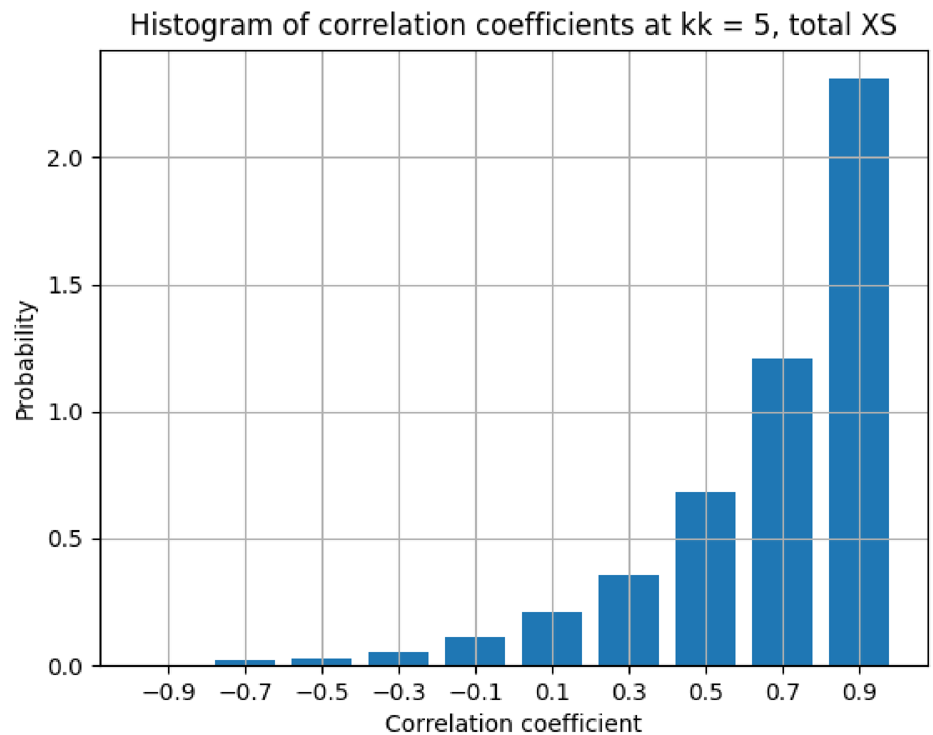


Figure 11. Histogram of correlation coefficient of total cross-section at 5th axial plane

Real variance estimation using AR (1) model

Cross-section distribution by estimated AR (1) model

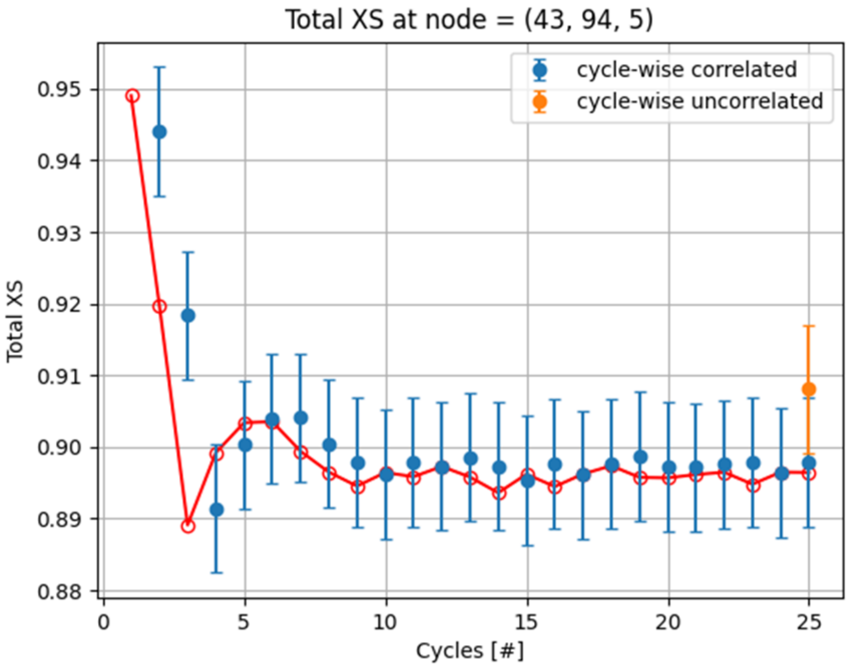


Figure 12. Accumulated total cross-section at (43, 94, 5) and AR (1) model estimation at 10th active cycle

[AR (1) parameters]
ϕ : 0.8787
μ : 0.9081
σ^2 : 8.0389e-5

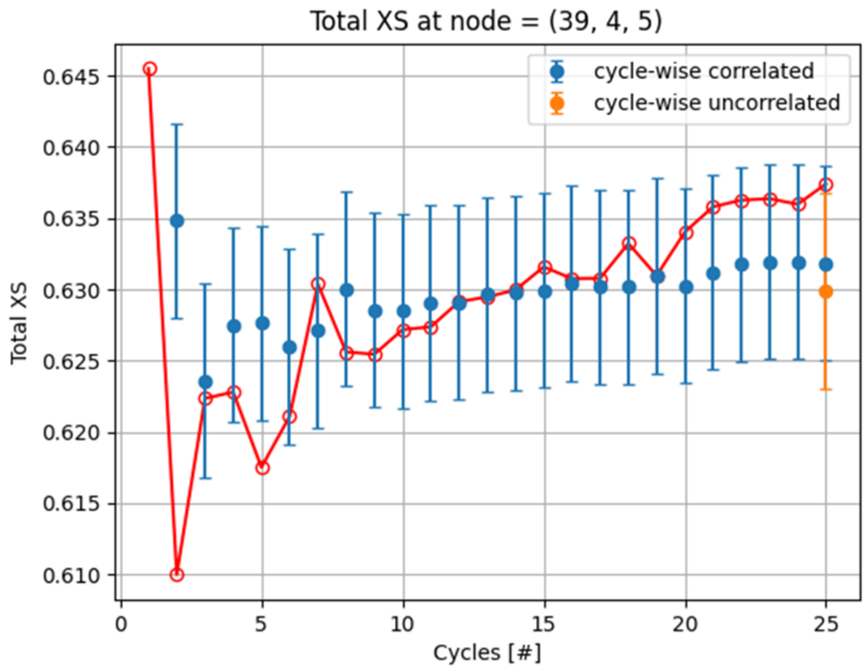


Figure 13. Accumulated total cross-section at (39, 4, 5) and AR (1) model estimation at 10th active cycle

[AR (1) parameters]
ϕ : 0.3169
μ : 0.6299
σ^2 : 4.6713e-5

Cross-section distribution by estimated AR (1) model

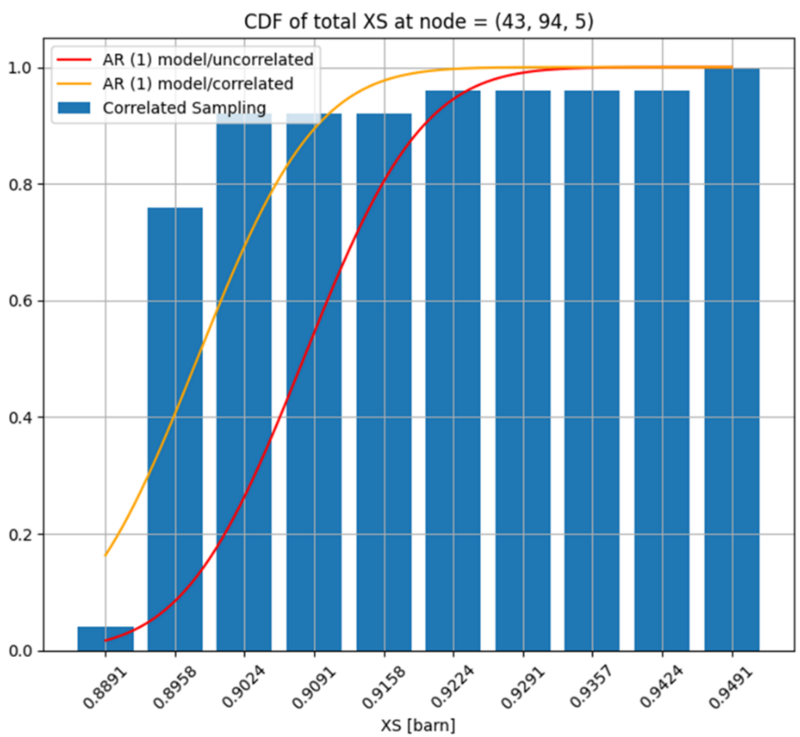


Figure 14. CDF of total cross-section at (43, 94, 5) compared with accumulated discrete CDF and AR (1) model estimation

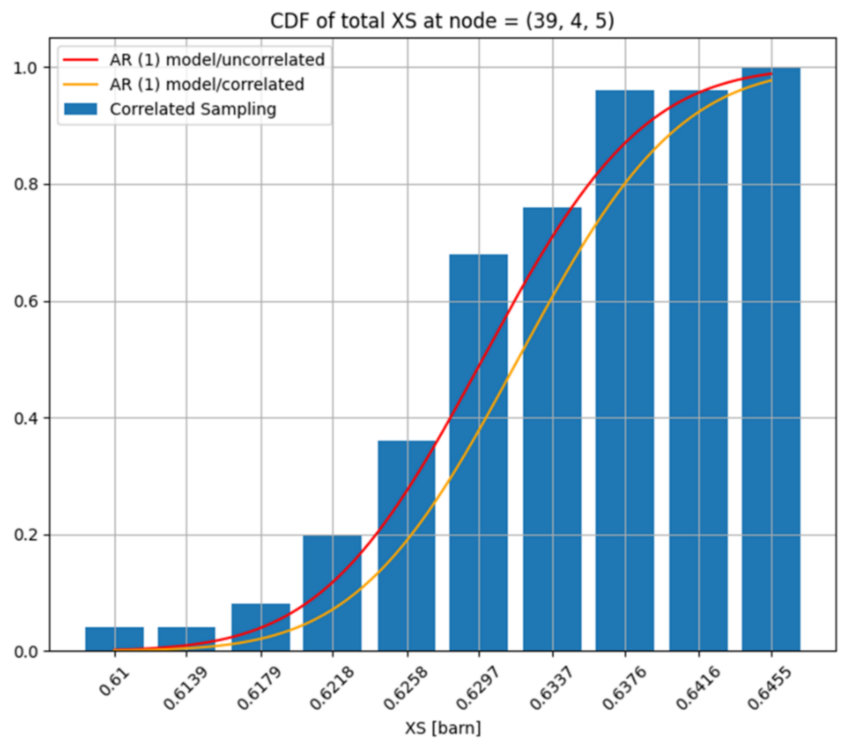


Figure 15. CDF of total cross-section at (39, 4, 5) compared with accumulated discrete CDF and AR (1) model estimation

- Real variance estimation using **correlated sampling** use accumulated CDF
- Real variance estimation using **AR (1) model** use uncorrelated AR (1) model estimated CDF

Real variance estimation using AR (1) model

Estimated standard deviation of eigenvalue using AR (1) model

– 5 MPI nodes (48 threads/node): Correlated Sampling – 82.20 min / AR (1) – 74.76 min

Cycle [#]	Correlated Sampling	**AR (1)**	Real
	s.d [pcm]	**s.d [pcm]**	s.d [pcm]
31	13.80	**19.06**	15.93
32	14.55	**18.17**	15.82
33	13.53	**16.78**	15.77
34	12.62	**16.65**	15.77
35	12.95	**17.38**	15.75
36	10.94	**17.68**	15.77
37	14.47	**16.76**	15.65
38	12.55	**16.89**	15.55
39	12.35	**15.94**	15.43
40	12.68	**17.13**	15.29

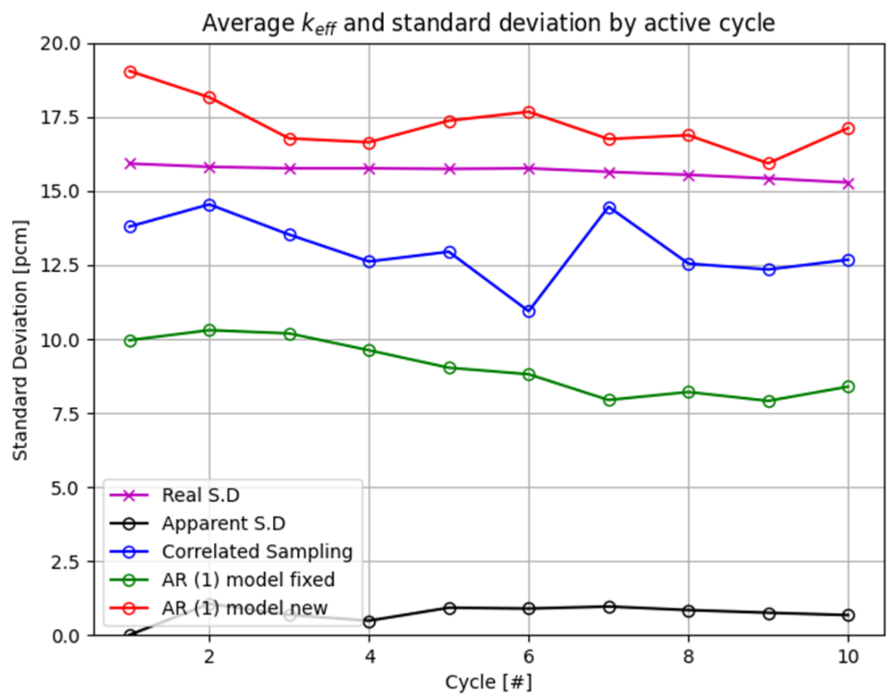


Figure 23. Standard deviation of apparent (black), correlated sampling (blue), AR (1) model (green), new AR (1) model (red) and real(magenta)

– 45 batch calculation for real variance

Problem description: SMR model

Solving Problem

- To observe the consistency of real variance estimation method with AR (1) model, more precise calculation has been conducted
- Same model with larger histories and cycles

- SMR model
  - FA1: 17-by-17 FA, Gd+U oxide
  - FA2: 17-by-17 FA, U oxide
  - 10 axial nodes
- 1.5e+6 → 2.0e+6 histories
- 30 → 60 inactive and 10 → 20 active cycles
- 15 → 30 cycles are skipped and accumulated

Cycle-wise Correlation Coefficient

– Correlation coefficients obtained from AR (1) model

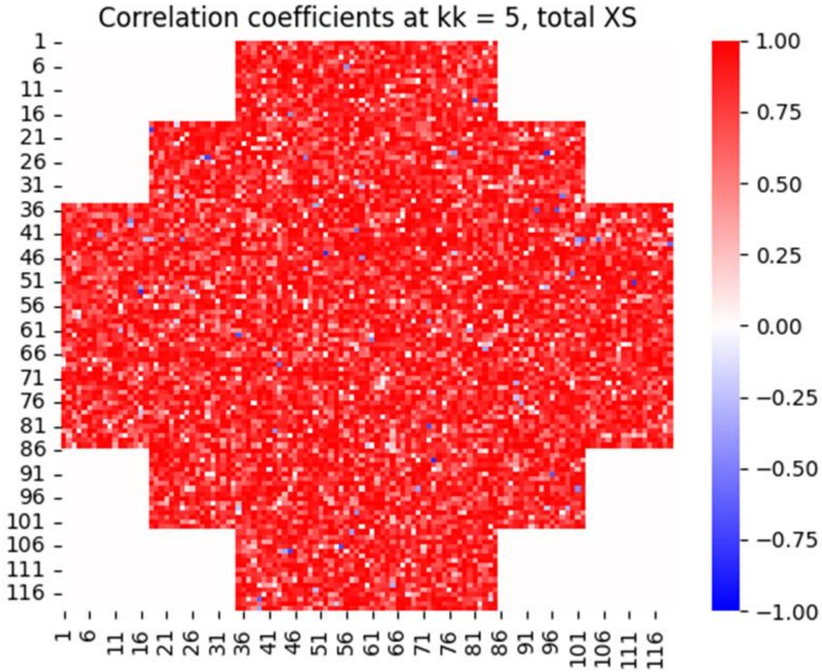


Figure 24. Correlation coefficient of total cross-section for each node at 5th axial plane

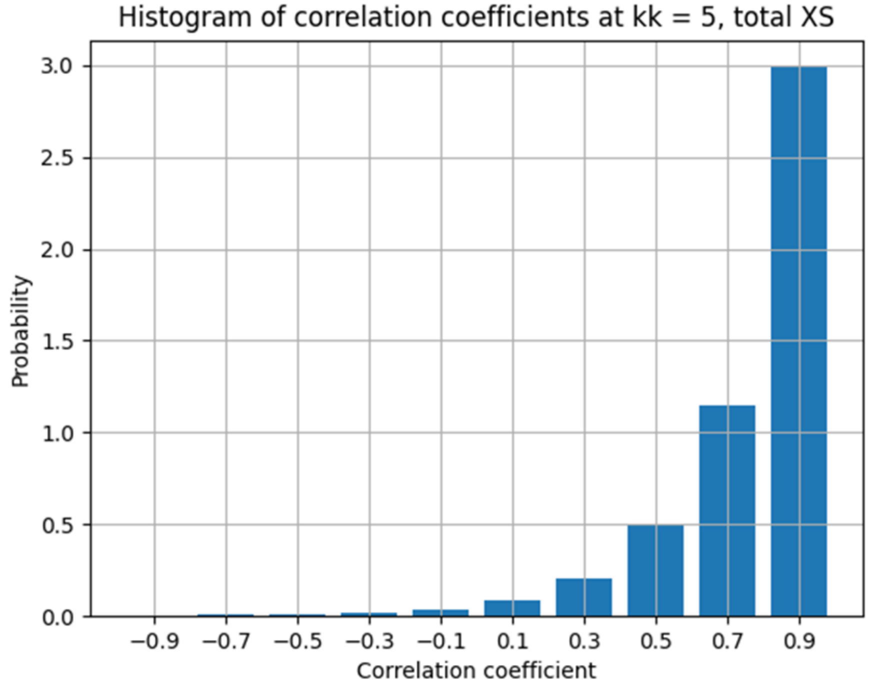


Figure 25. Histogram of correlation coefficient of total cross-section at 5th axial plane

→ Higher cycle-wise correlation estimated for increased cycles and histories

Real variance estimation using AR (1) model

Cross-section distribution by estimated AR (1) model

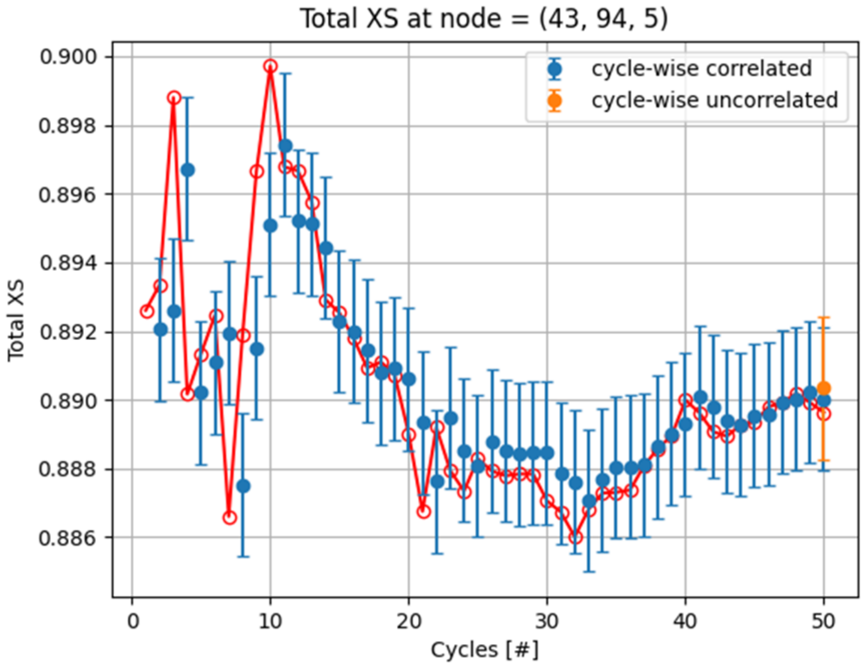


Figure 26. Accumulated total cross-section at (43, 94, 5) and AR (1) model estimation at 20th active cycle

[AR (1) parameters]
ϕ : 0.7548
μ : 0.8903
σ^2 : 4.3158e-5

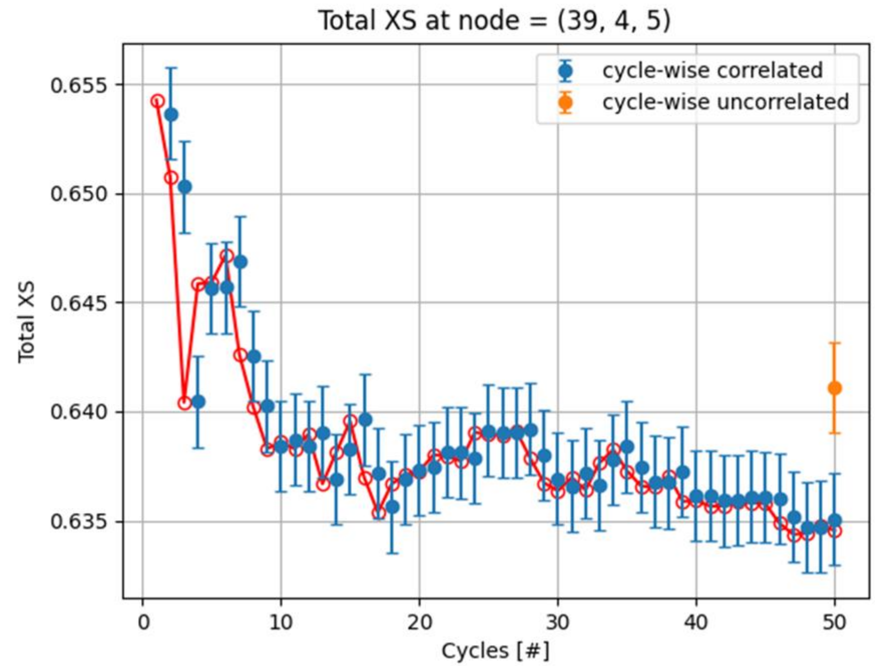


Figure 27. Accumulated total cross-section at (39, 4, 5) and AR (1) model estimation at 10th active cycle

[AR (1) parameters]
ϕ : 0.9532
μ : 0.6411
σ^2 : 4.3302e-5

– Overall estimations show higher correlation coefficient and lower variance

Estimated standard deviation of eigenvalue using AR (1) model

– 5 MPI nodes (40 threads/node): Correlated Sampling – 209.94 min / AR (1) – 208.88 min

Cycle [#]	Correlated Sampling	AR (1)	Real
	s.d [pcm]	s.d [pcm]	s.d [pcm]
61	11.29	12.64	8.53
62	10.47	12.91	8.33
63	10.71	10.75	8.35
…			
75	9.52	10.58	8.27
76	8.3	10.36	8.26
77	8.57	10.87	8.22
78	8.39	10.64	8.19
79	8.98	9.39	8.14
80	9.66	10.15	8.29

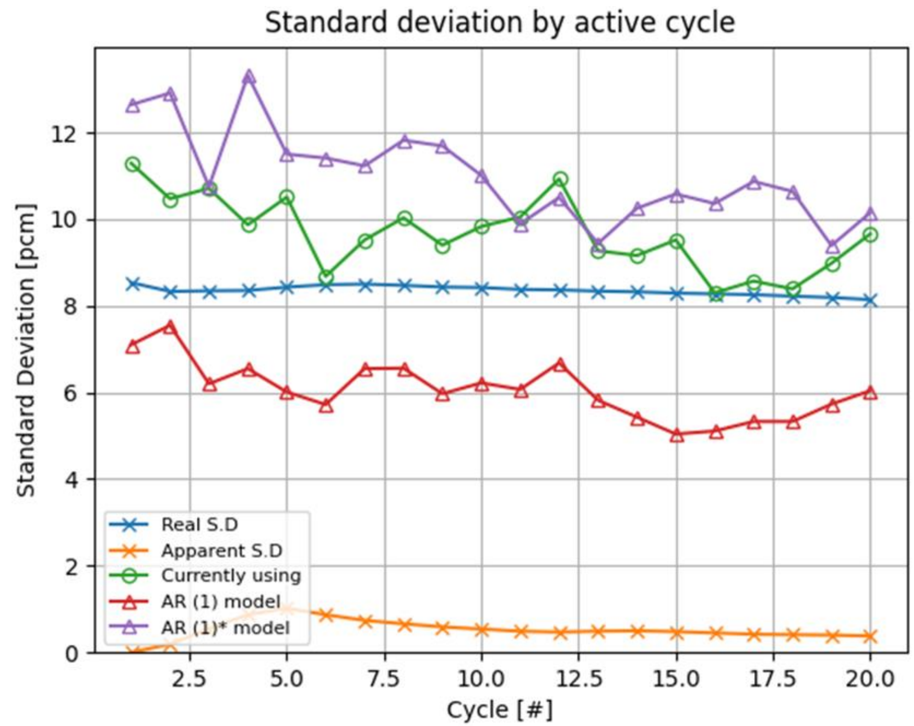


Figure 28. Standard deviation of real(blue), apparent(orange), correlated sampling(green), AR (1) model(red), and AR (1)* model(purple)

– Batch calculation result from 25 batch calculation

– Maximum iteration number for correlated sampling is 3

Real variance estimation using AR (1) model and SAM

Real variance estimation using SAM

– Accumulated inactive & active cycle's p-FMFD parameters → estimate AR(1) model's parameters

(1) Using AR(1) model, cycle-wise correlated parameters reproduced **without solving MC**

(2) Solve with p-FMFD or use 1st order perturbation theory for correlated parameters

(3) Use SAM for the eigenvalue of active and AR(1) estimated results to estimate real variance

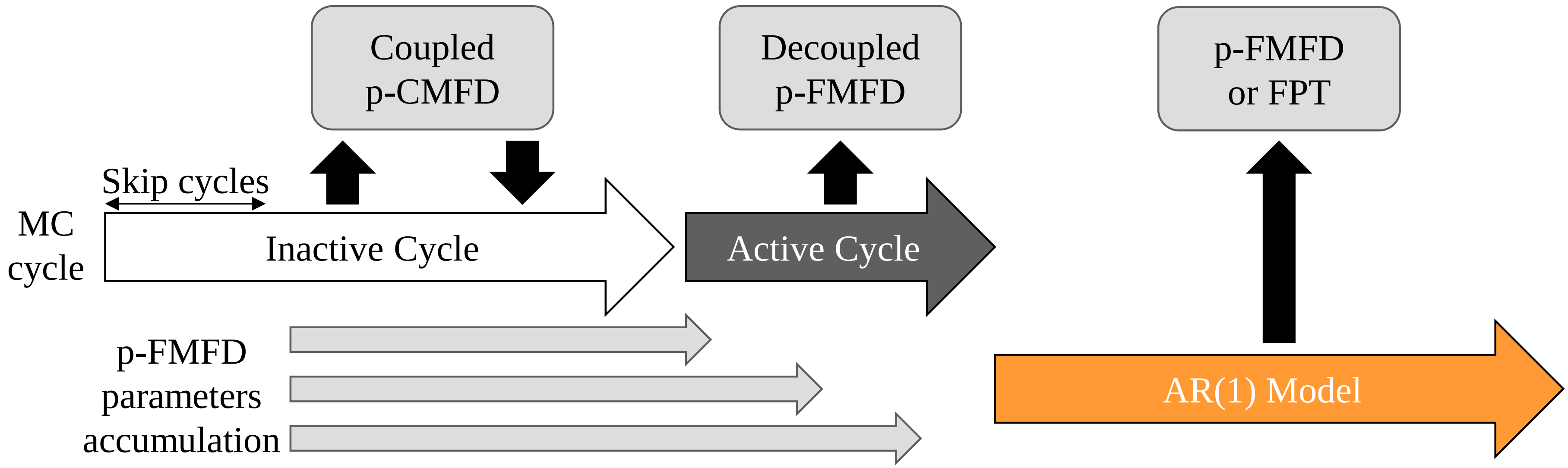


Figure 7. Schematic diagram of real variance estimation using SAM in iDTMC method

– Estimate real variance without model or estimate autocovariance functions

– Similar or shorter calculation time used to estimate real variance

Estimated standard deviation of eigenvalue using SAM

– 5 MPI nodes (48 threads/node): Correlated Sampling – 82.20 min / SAM – 78.41 min

Cycle [#]	Correlated Sampling	**SAM (M=1)**	**SAM (M=2)**	**SAM (M=3)**	Real
	s.d [pcm]	**s.d [pcm]**	**s.d [pcm]**	**s.d [pcm]**	s.d [pcm]
31	13.80	**18.75**	**13.76**	**11.36**	15.93
32	14.55	**17.91**	**15.12**	**12.41**	15.82
33	13.53	**15.94**	**12.12**	**10.63**	15.77
34	12.62	**5.207**	**5.124**	**6.843**	15.77
35	12.95	**9.479**	**7.398**	**6.892**	15.75
36	10.94	**12.81**	**10.87**	**14.22**	15.77
37	14.47	**5.617**	**7.033**	**6.203**	15.65
38	12.55	**9.817**	**7.431**	**6.142**	15.55
39	12.35	**19.65**	**14.57**	**12.35**	15.43
40	12.68	**9.811**	**9.731**	**8.080**	15.29

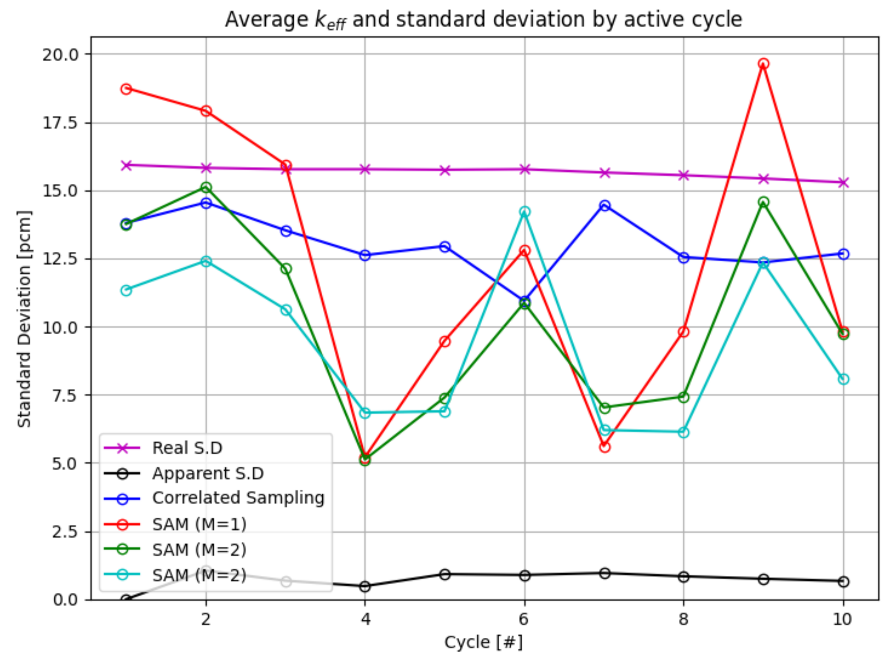


Figure 10. Standard deviation of apparent (black), correlated sampling (blue), SAM for M=1 (red), M=2 (green), M=3 (cyan) and real(magenta) for 100 propagated samples

– Real variance is calculated from 45 batch calculation

– Maximum iteration number for correlated sampling is 3

– 100 samples were propagated with AR (1) model and analysed with SAM

Real variance estimation using AR (1) model and SAM

Estimated standard deviation of eigenvalue using SAM

– 5 MPI nodes (48 threads/node): Correlated Sampling – 82.20 min / SAM – 172.53 min

Cycle [#]	Correlated Sampling	**SAM (M=1)**	**SAM (M=2)**	**SAM (M=3)**	Real
	s.d [pcm]	**s.d [pcm]**	**s.d [pcm]**	**s.d [pcm]**	s.d [pcm]
31	13.80	**5.204**	**4.010**	**4.977**	15.93
32	14.55	**5.641**	**6.596**	**5.676**	15.82
33	13.53	**3.964**	**2.976**	**3.078**	15.77
34	12.62	**9.637**	**7.212**	**5.989**	15.77
35	12.95	**4.785**	**5.275**	**6.618**	15.75
36	10.94	**2.771**	**4.818**	**4.238**	15.77
37	14.47	**1.221**	**2.132**	**1.836**	15.65
38	12.55	**4.383**	**7.182**	**6.340**	15.55
39	12.35	**4.306**	**5.236**	**4.426**	15.43
40	12.68	**1.312**	**3.042**	**3.040**	15.29

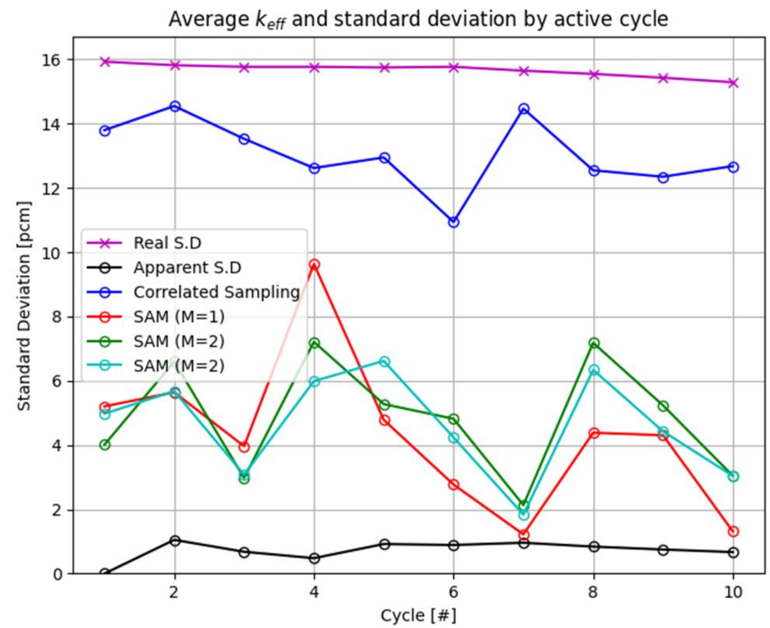


Figure 11. Standard deviation of apparent (black), correlated sampling (blue), SAM for M=1 (red), M=2 (green), M=3 (cyan) and real(magenta) for 1000 propagated samples

– Real variance is calculated from 45 batch calculation

– Maximum iteration number for correlated sampling is 3

– 1000 samples were propagated with AR (1) model and analysed with SAM

Real variance estimation using AR (1) model and SAM

Periodogram from SAM

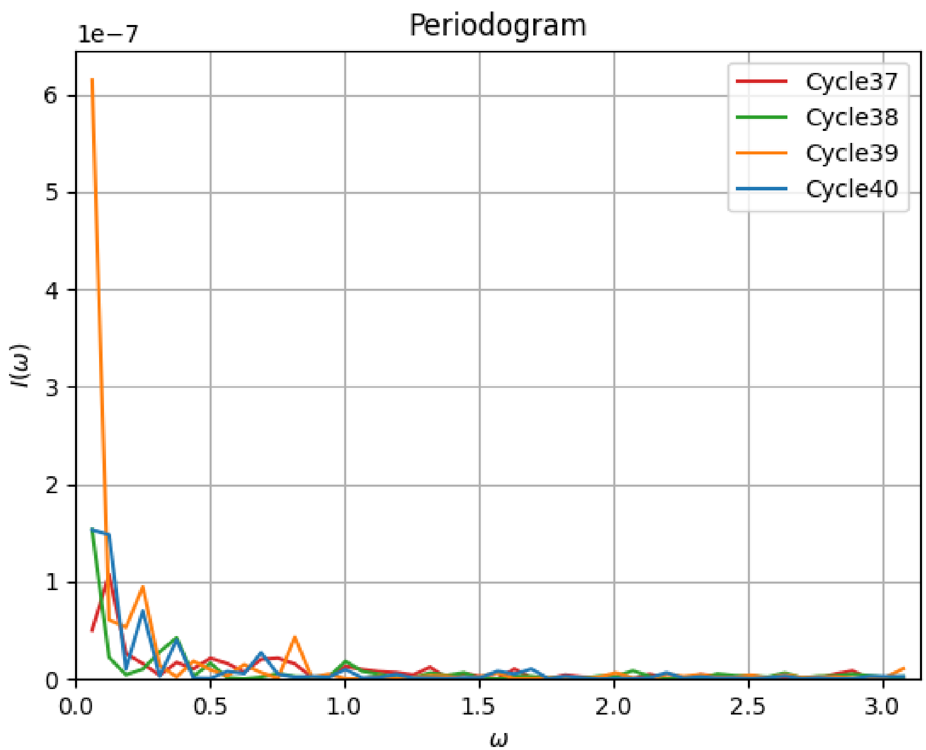


Figure 12. Periodogram for cycle 37, 38, 39, 40 when the propagated sample number is 100

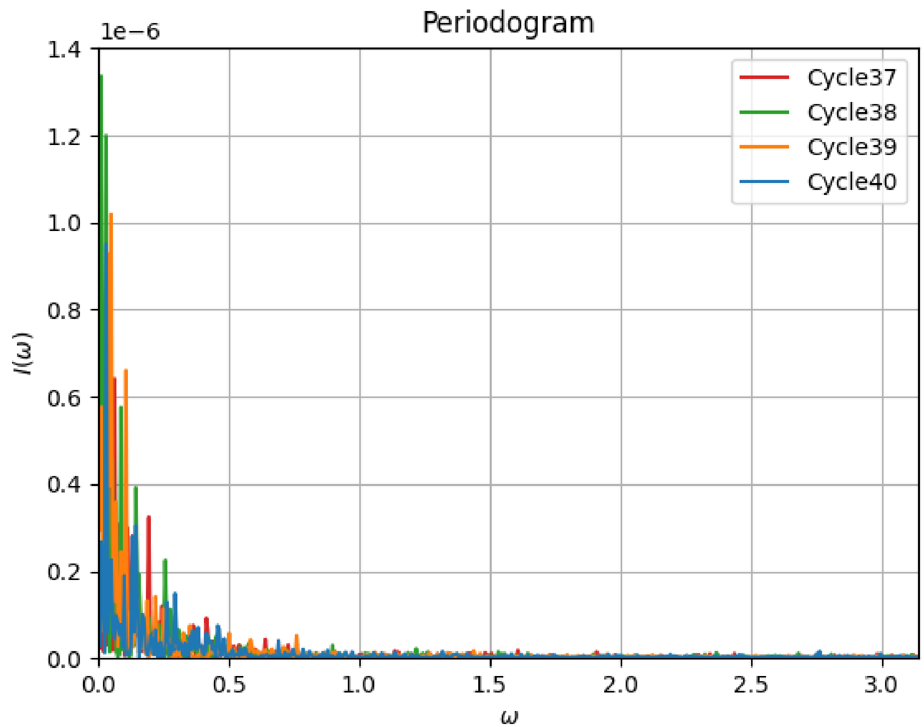


Figure 13. Periodogram for cycle 37, 38, 39, 40 when the propagated sample number is 1000

– As we expected from Taylor-series analysis:
  - **High variance** of estimation occurred when we use **100 propagated samples**
  - **High bias** of estimation occurred when we use **1000 propagated samples**

Real variance estimation using AR (1) model

- From the AR (1) model, t[th] parameter could be estimated as:

$$Y_t - \mu = \phi(Y_{t-1} - \mu) + Z_t(0, \sigma^2)$$

- When we replace ϕ to 0, we could sample cycle-wise uncorrelated parameters:

$$Y_t^{uncorr} = \mu + Z_t(0, \sigma^2)$$

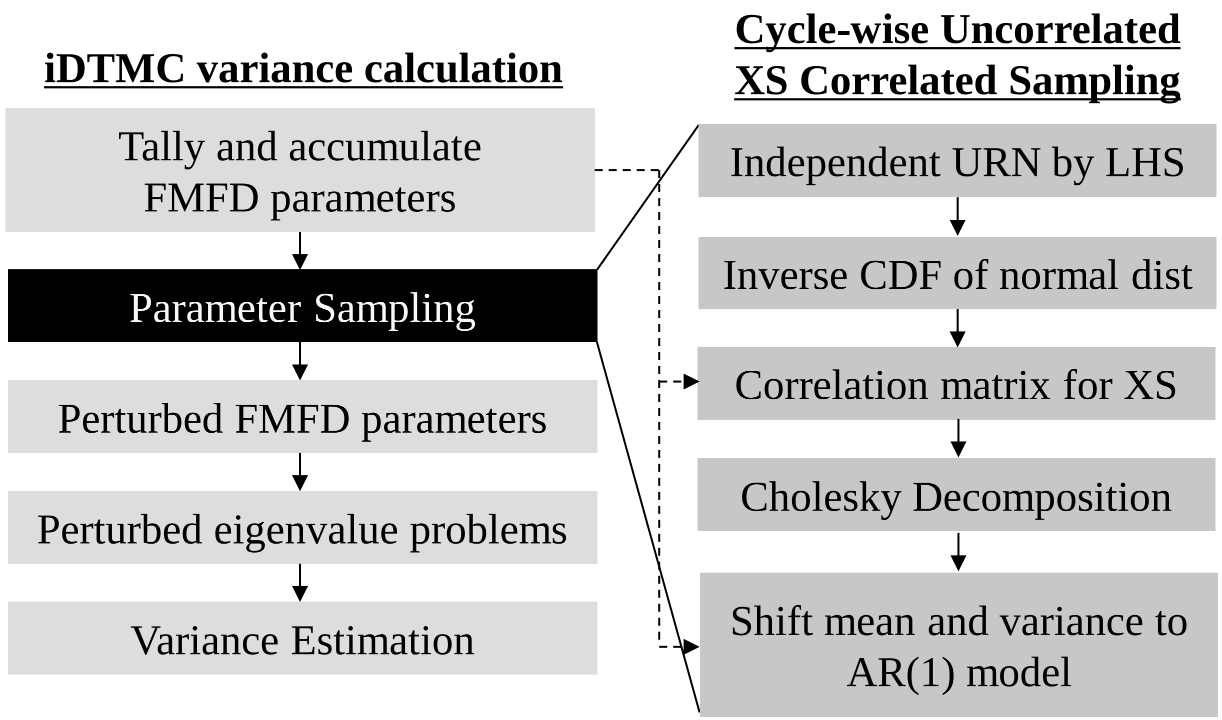


Figure 8. Schematic of real variance estimation using AR(1) model to produce cycle-wise uncorrelated parameters in IDTMC method

Real variance estimation using AR (1) model w/ parameter-wise correlation

Estimated standard deviation of eigenvalue using AR (1) model

– 5 MPI nodes (48 threads/node): Correlated Sampling – 82.20 min / AR (1) – 73.88 min

Cycle [#]	Correlated Sampling	**AR (1)**	Real
	s.d [pcm]	**s.d [pcm]**	s.d [pcm]
31	13.80	**9.96**	15.93
32	14.55	**10.30**	15.82
33	13.53	**10.19**	15.77
34	12.62	**9.62**	15.77
35	12.95	**9.03**	15.75
36	10.94	**8.81**	15.77
37	14.47	**7.94**	15.65
38	12.55	**8.21**	15.55
39	12.35	**7.91**	15.43
40	12.68	**8.39**	15.29

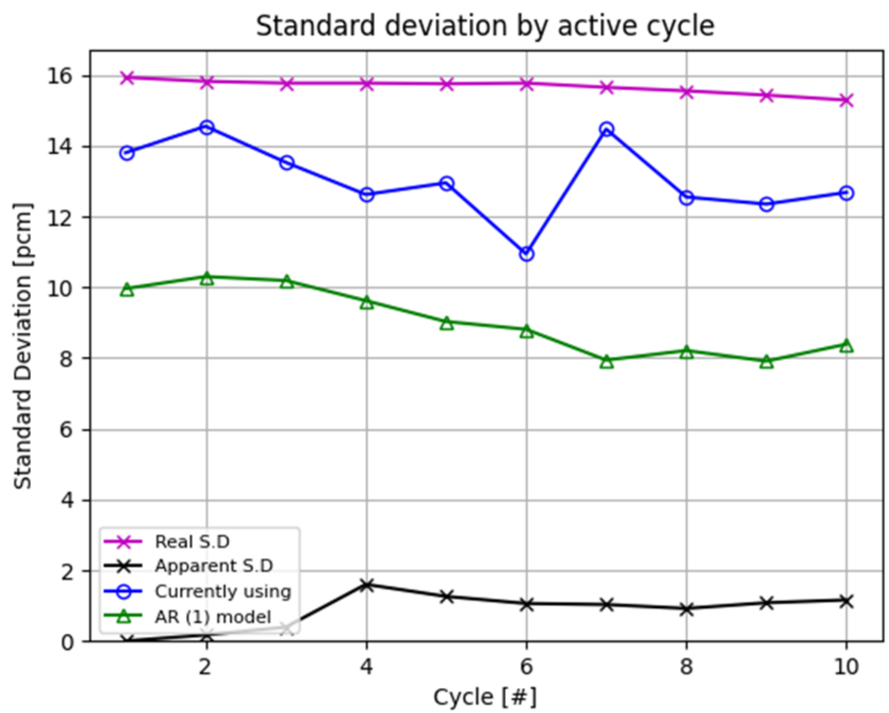


Figure 16. Standard deviation of apparent (black), correlated sampling (blue), AR (1) model (green) and real(magenta)

– Batch calculation result from 45 batch calculation

– Maximum iteration number for correlated sampling is 3

Summary and Conclusion

Limitations of the previous method for p-FMFD parameter sampling

- Cycle-wise correlation of the sampled parameters is observed, which is a well-established cause for various underestimation.

New parameter sampling scheme for accurate variance estimation

- A new sampling method based on the AR (1) model that explicitly removes cycle-wise correlation from the sampling process was developed and implemented.
- The variances estimated with this method were found to be quite similar to the real variance.

Future directions

- Estimation of the real variance of the power distribution using the AR (1) model is in progress.
- Application and verification of the AR (1) estimation for non-LWR problems.

Thank You

Any Questions?

Backup Slide

Correlation coefficient of correction factors, $\widehat{D}_p$

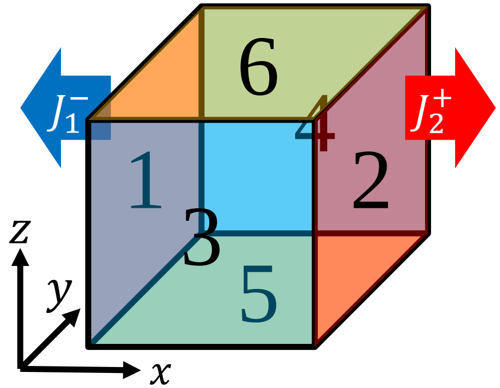
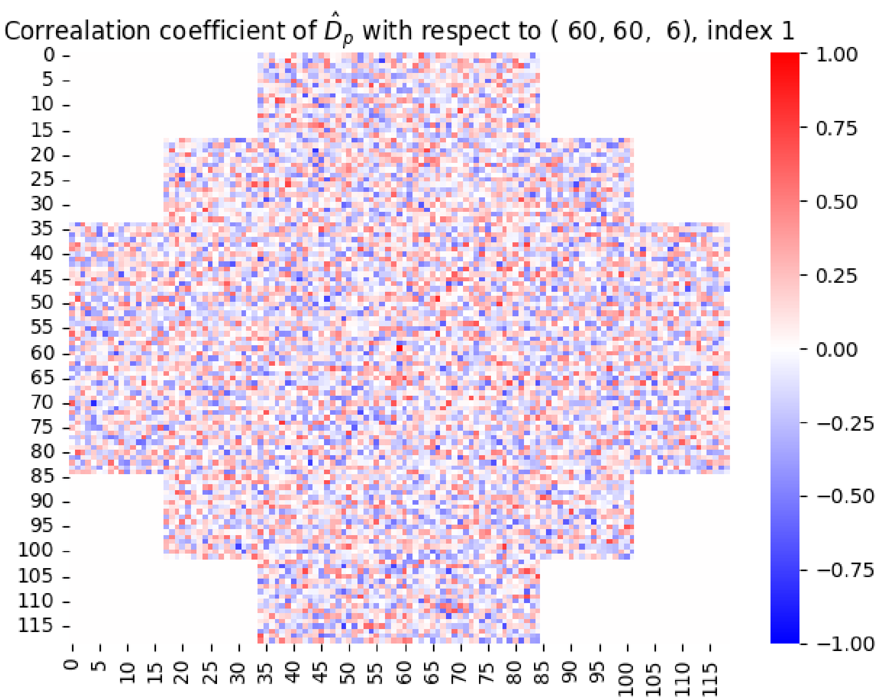


Figure 29. Schematic of surface numbering and current direction of

– Correlation coefficient, $\rho(X,Y)=\frac{Cov(X,Y)}{\sigma_X\sigma_Y}=\frac{E[XY]-E[X]E[Y]}{\sigma_X\sigma_Y}$

– All direction is outgoing direction of each node

Index	1	2	3	4	5	6
$\widehat{D}_s^{\pm}$	$\widehat{D}_1^-$	$\widehat{D}_2^+$	$\widehat{D}_3^-$	$\widehat{D}_4^+$	$\widehat{D}_5^-$	$\widehat{D}_6^+$



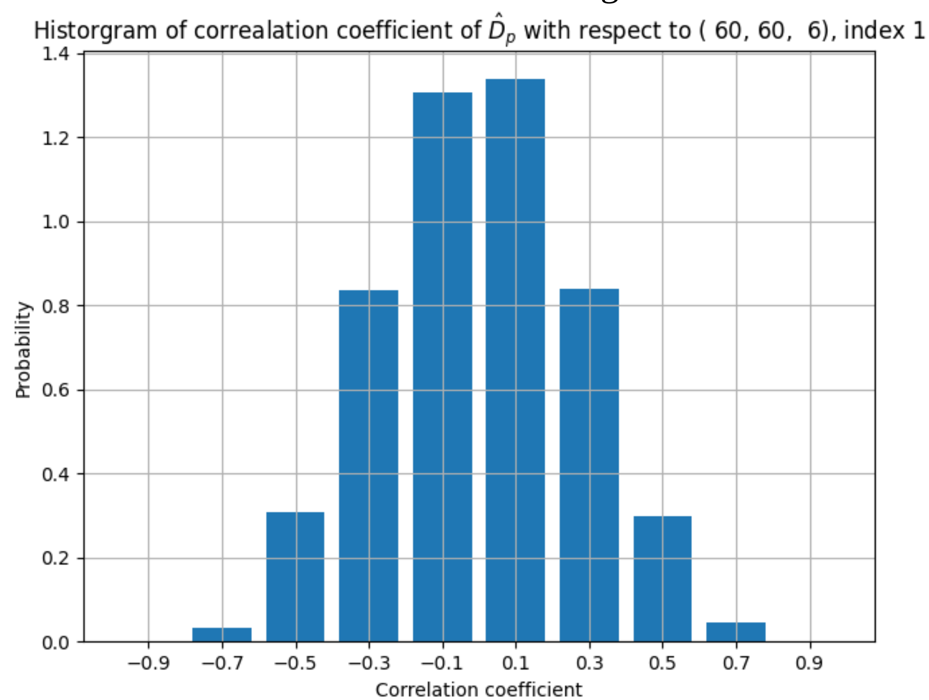


Figure 30. Heatmap and histogram of correlation coefficient with respect to node (60, 60, 6) and index 1

Correlation coefficient of correction factors, $\hat{D}_p$

Index	1	2	3	4	5	6
$\hat{D}_s^{\pm}$	$\hat{D}_1^{-}$	$\hat{D}_2^{+}$	$\hat{D}_3^{-}$	$\hat{D}_4^{+}$	$\hat{D}_5^{-}$	$\hat{D}_6^{+}$

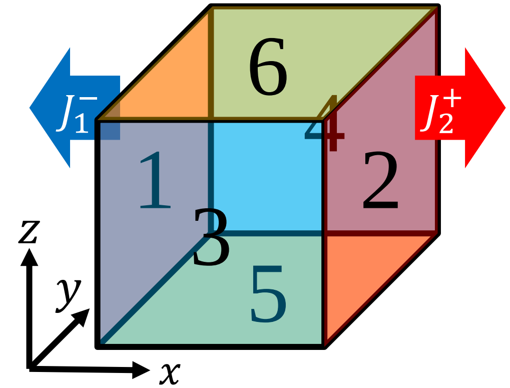


Figure 29. Schematic of surface numbering and current direction of specific node

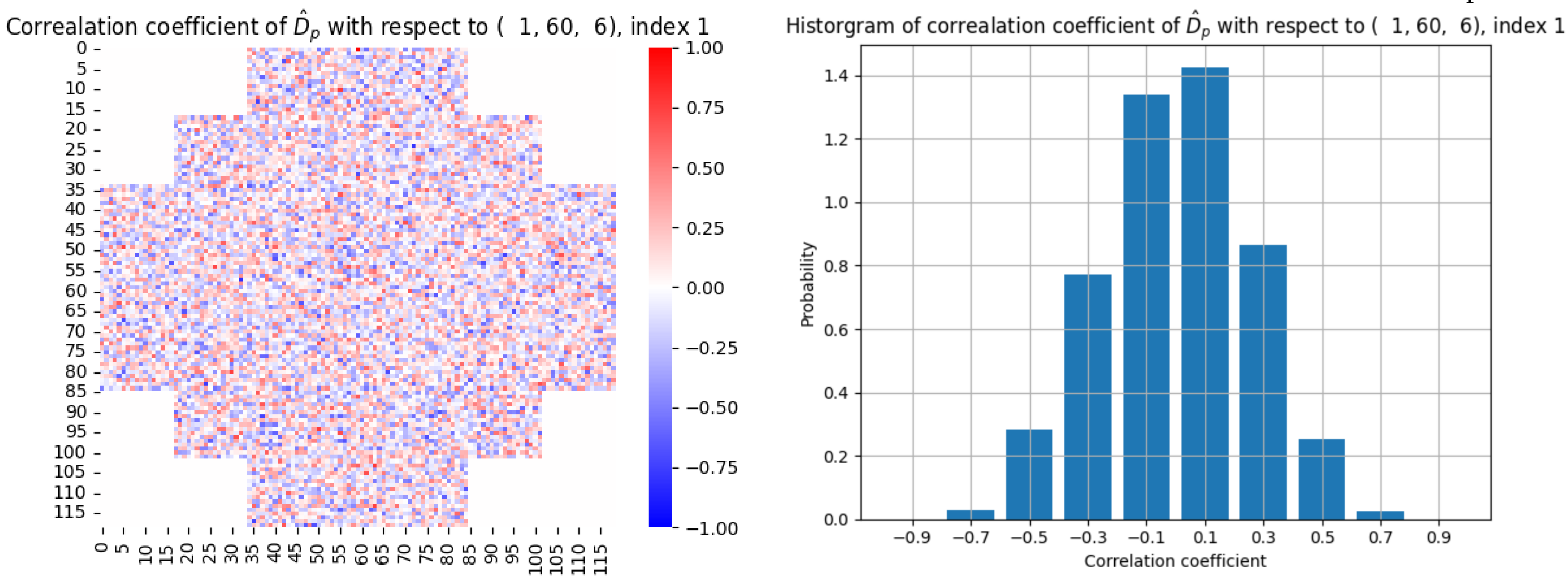


Figure 31. Heatmap and histogram of correlation coefficient with respect to node (1, 60, 6) and index 1

Correlation coefficient of correction factors, $\widehat{D}_p$

Index	1	2	3	4	5	6
$\widehat{D}_s^{\pm}$	$\widehat{D}_1^{-}$	$\widehat{D}_2^{+}$	$\widehat{D}_3^{-}$	$\widehat{D}_4^{+}$	$\widehat{D}_5^{-}$	$\widehat{D}_6^{+}$

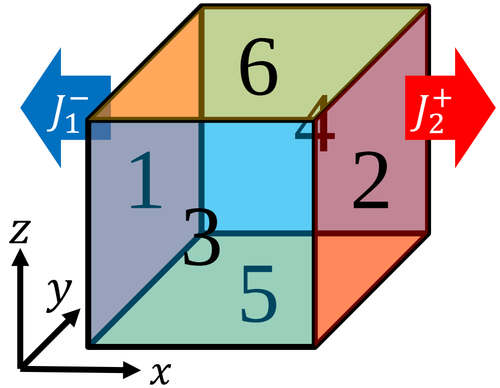


Figure 29. Schematic of surface numbering and current direction of specific node

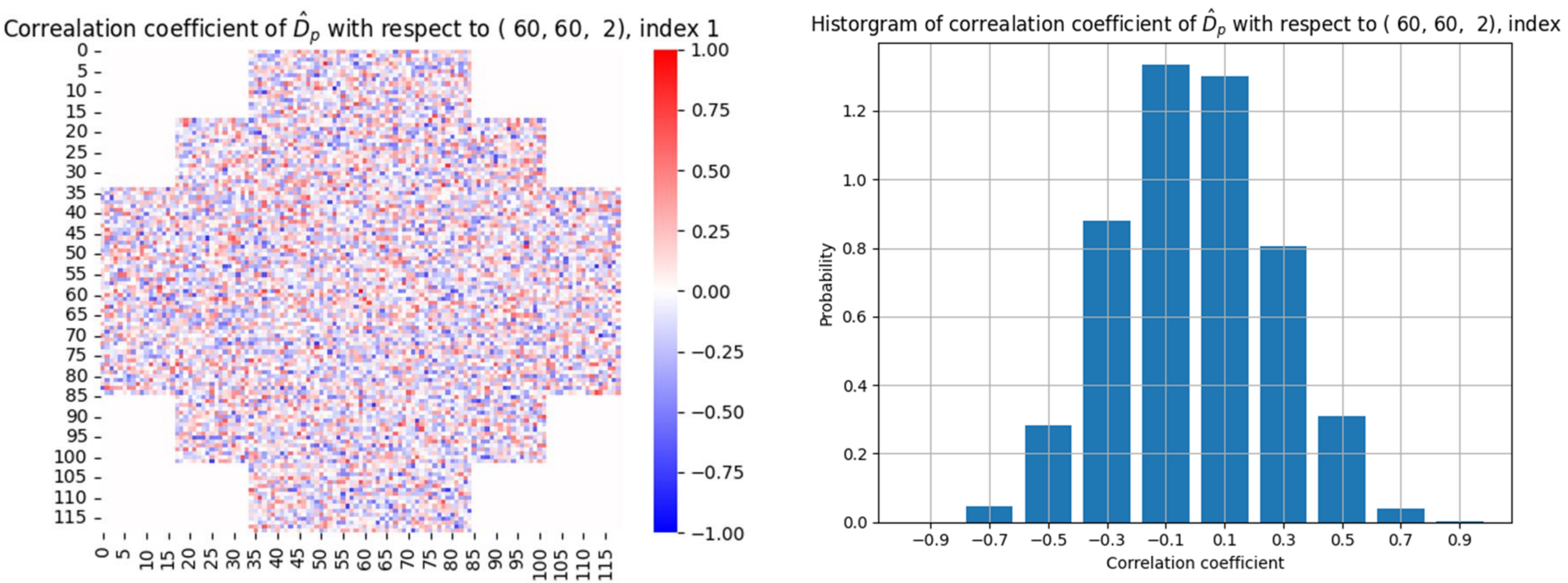


Figure 32. Heatmap and histogram of correlation coefficient with respect to node (60, 60, 2) and index 1

Correlation coefficient of correction factors, $\widehat{D}_p$

Index	1	2	3	4	5	6
$\widehat{D}_s^{\pm}$	$\widehat{D}_1^{-}$	$\widehat{D}_2^{+}$	$\widehat{D}_3^{-}$	$\widehat{D}_4^{+}$	$\widehat{D}_5^{-}$	$\widehat{D}_6^{+}$

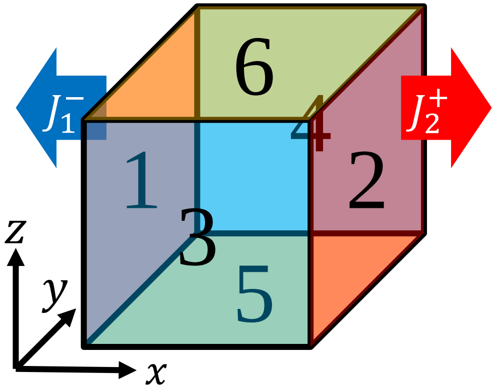
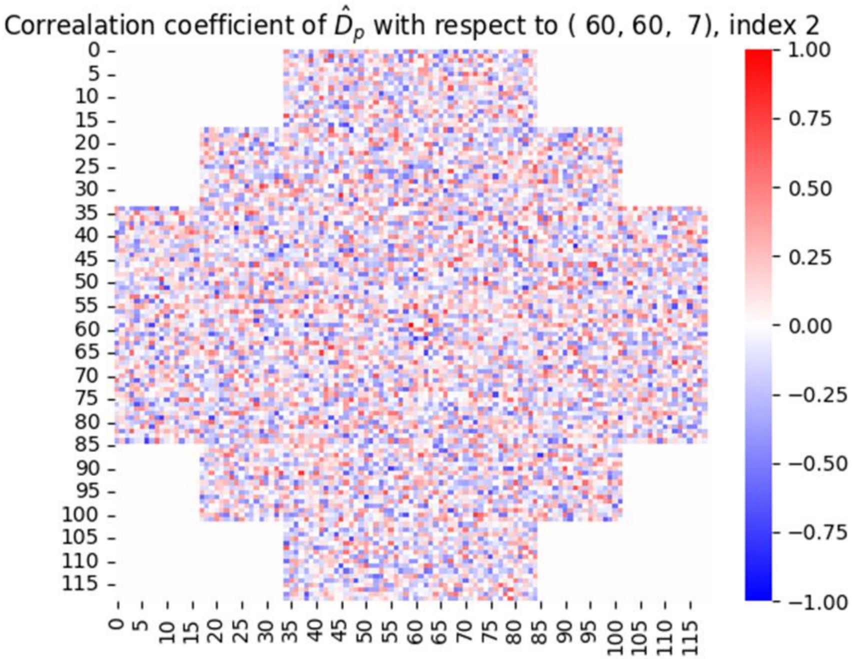


Figure 29. Schematic of surface numbering and current direction of specific node



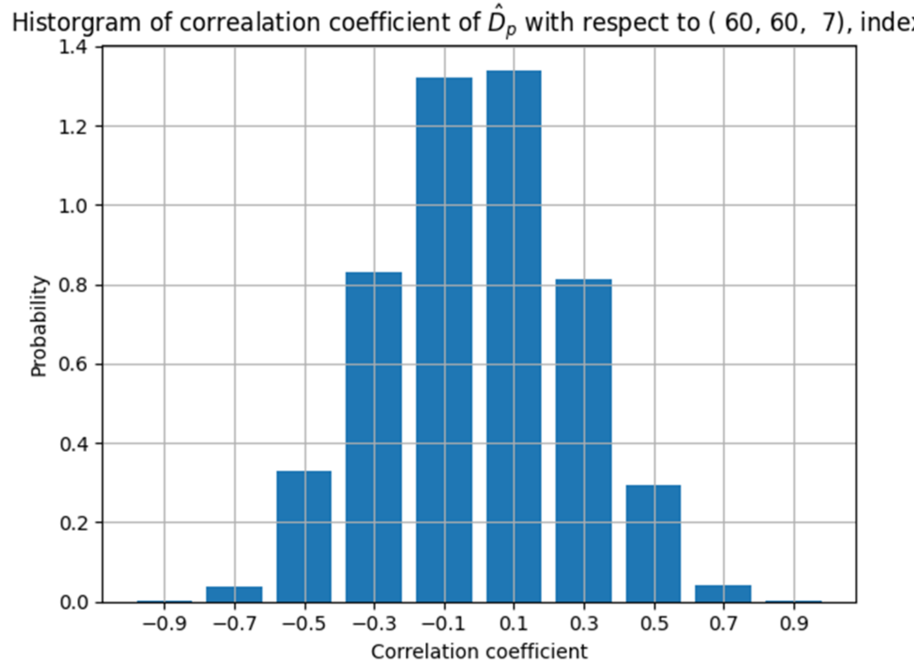


Figure 33. Heatmap and histogram of correlation coefficient with respect to node (60, 60, 7) and index 2

Correlation coefficient of correction factors, $\hat{D}_p$

Index	1	2	3	4	5	6
$\hat{D}_s^{\pm}$	$\hat{D}_1^{-}$	$\hat{D}_2^{+}$	$\hat{D}_3^{-}$	$\hat{D}_4^{+}$	$\hat{D}_5^{-}$	$\hat{D}_6^{+}$

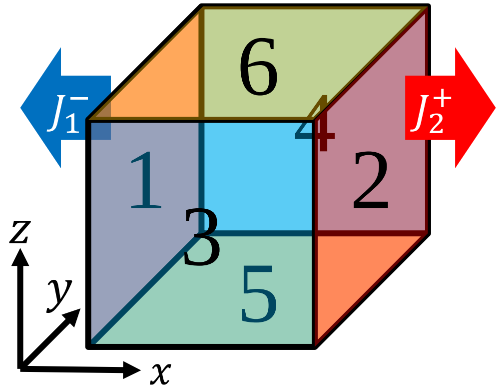
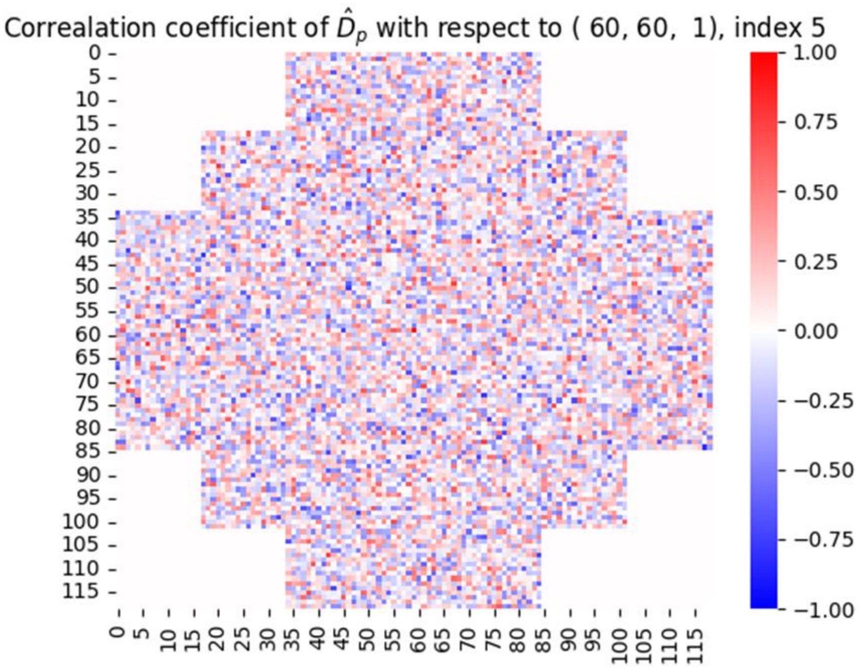


Figure 29. Schematic of surface numbering and current direction of specific node



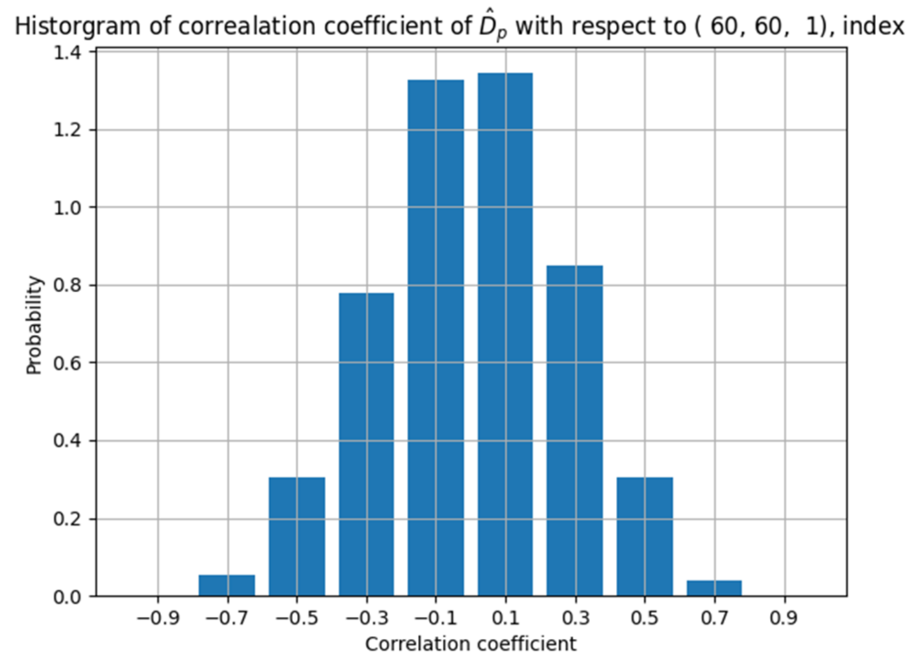


Figure 34. Heatmap and histogram of correlation coefficient with respect to node (60, 60, 0) and index 5

Real variance estimation using AR (1) model

Estimated standard deviation of eigenvalue using AR (1) model

– 5 MPI nodes (48 threads/node): Correlated Sampling – 82.20 min / AR (1) – 74.76 min

Cycle [#]	Correlated Sampling	AR (1)	**AR (1)***	Real
	s.d [pcm]	s.d [pcm]	**s.d [pcm]**	s.d [pcm]
31	13.80	9.96	**19.06**	15.93
32	14.55	10.30	**18.17**	15.82
33	13.53	10.19	**16.78**	15.77
34	12.62	9.62	**16.65**	15.77
35	12.95	9.03	**17.38**	15.75
36	10.94	8.81	**17.68**	15.77
37	14.47	7.94	**16.76**	15.65
38	12.55	8.21	**16.89**	15.55
39	12.35	7.91	**15.94**	15.43
40	12.68	8.39	**17.13**	15.29

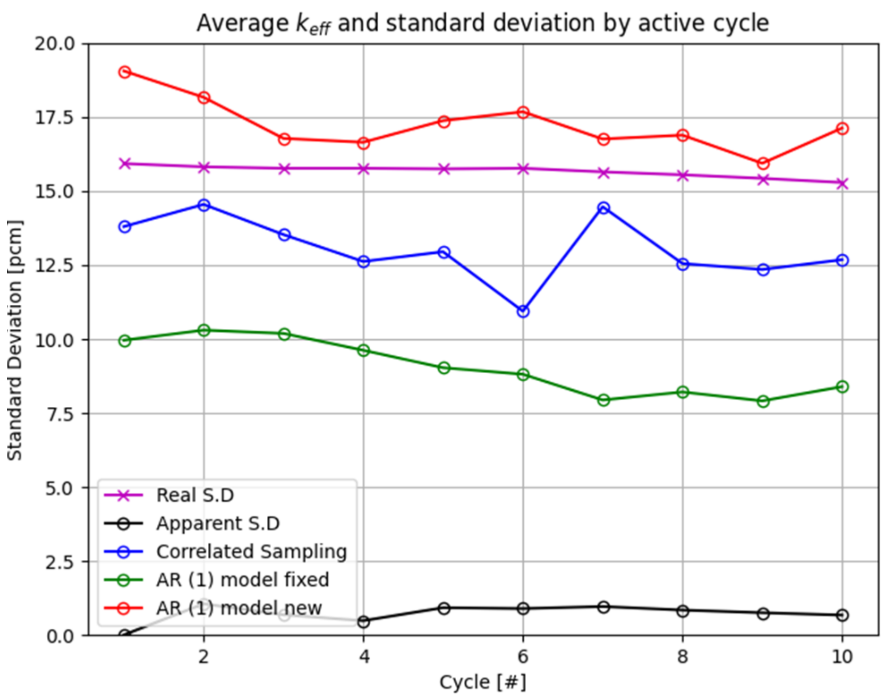


Figure 17. Standard deviation of apparent (black), correlated sampling (blue), AR (1) model (green), new AR (1) model (red) and real(magenta)

– New method(AR (1)*) **does not consider** correlation matrix of parameters

Real variance estimation using correlated sampling

Correlated Sampling

– p-FMFD parameters have strong correlation by reaction types, cycles, cells, etc

(1) Reproduce p-FMFD parameters with correlated sampling and probability density function

(2) Generate perturbed eigenvalue problems (iteration is needed to match the correlation matrix)

(3) Solve the problems with p-FMFD and estimate real variance or use 1st order perturbation theory

<Correlation Matrix>

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

$$\rho(\mathrm{X}, \mathrm{Y}) = \frac{Cov(X,Y)}{\sigma_X \sigma_Y} = \frac{E[XY] - E[X]E[Y]}{\sigma_X \sigma_Y}$$

<Cholesky Decomposition>

$$C = LL^T$$

For the uncorrelated normal sample X,

$$E[XX^T] = I$$

$$E[LXX^T L^T] = LE[XX^T]L^T = LL^T = C$$

So, we multiply L to X to form correlated URN.

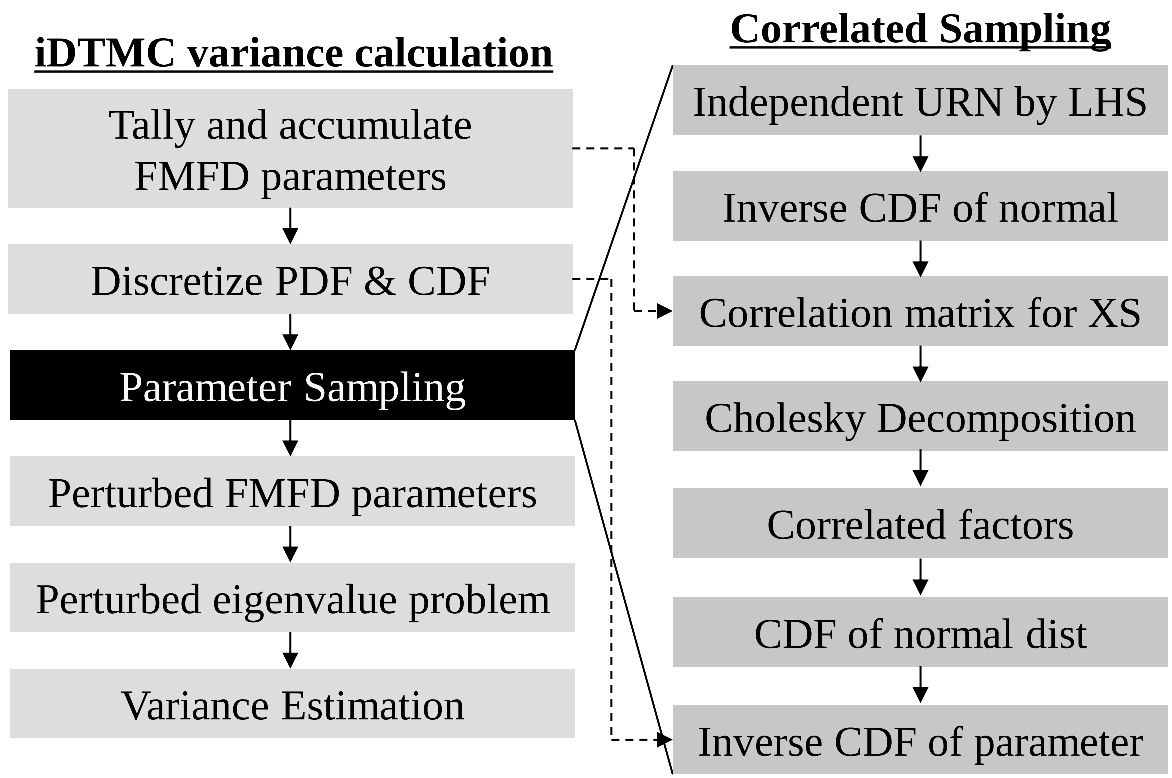


Figure 2. Schematic of real variance estimation in the iDTMC method

Spectral Analysis Method

- Spectral Analysis Method (SAM) used in noise signals and stationary time series analyses
- Let X_t be tallied value in the t^th active cycle, sample mean $\bar{X} = \sum_{t=1}^{T} X_t$, real mean μ
  - Autocovariance: $\gamma_h = Cov(X_t, X_{t+h}) = E[X_t X_{t+h}] - \mu^2$
  - Sample autocovariance: $\hat{\gamma}_h = \frac{1}{T-h}\sum_{t=1}^{T-h}(X_t - \bar{X})(X_{t+h} - \bar{X})$
  - Variance of sample mean: $V[\bar{X}] = \frac{1}{T^2} V[\sum_{t=1}^{T} X_t] = \frac{1}{T^2}\sum_{i=1}^{T}\sum_{j=1}^{T}\gamma_{(i-j)} = \frac{1}{T}\sum_{h=-T}^{T}\left(1 - \frac{|h|}{T}\right)\gamma_h$
- For $T \to \infty$, $V\left[\sqrt{T}\bar{X}\right] \to \sum_{h=-\infty}^{\infty}\gamma_h$ and sample deviation $\tilde{\sigma}^2 = \frac{1}{T(T-1)}\left\{\sum_{t=1}^{T} X_t^2 - \frac{\left(\sum_{t=1}^{T} X_t\right)^2}{T}\right\} = \frac{\hat{\gamma}_0}{T}$:

$$\frac{V[\bar{X}]}{\tilde{\sigma}^2} = \frac{V\left[\sqrt{T}\bar{X}\right]}{\hat{\gamma}_0} \to \frac{\sum_{h=-\infty}^{\infty}\gamma_h}{\gamma_0}$$

- Autocovariance structure of random process is equivalent to certain frequency pattern:

$$f(\omega) = \frac{1}{2\pi}\sum_{h=-\infty}^{\infty}\gamma_h e^{i\omega h}, \ \omega \in (-\pi, \pi)$$

- Then, with the spectral density $f(\omega)$, $\boldsymbol{V[\bar{X}] \approx \frac{2\pi f(0)}{T}}$

Autoregressive (1) model and Spectral Analysis method (3/3)

Spectral Analysis Method

- With periodogram $I(\omega_k) = \frac{1}{2\pi T}\left|\sum_{t=1}^{T} X_t e^{-it\omega_k}\right|$ where $\omega_k = \frac{2\pi k}{T}$, estimate $\hat{f}(0) = \frac{1}{M}\sum_{m=1}^{M} I(\omega_m)$
- So, we could estimate real variance $\boldsymbol{V[\bar{X}] = \frac{2\pi}{MT}\sum_{k=1}^{M} I(\omega_k)}$

- From the definition we could derive $E[I(\omega_k)] \to f(\omega_k)$ for $\omega_k \neq 0$
- With the Taylor series analysis, bias and variance of $\hat{f}(0)$ could be approximated:

$$E\left[\hat{f}(0)\right] - f(0) \approx \frac{\pi f'(0)(M+1)}{T}$$

$$V\left[\hat{f}(0)\right] \approx \frac{1}{M^2}\sum_{m=1}^{M} \hat{f}\,(\omega_m)$$

- Trade-off between the bias and variance depending on M
- For accurate approximation, large number of active cycles(T) are needed

Real variance estimation using AR (1) model and SAM (1/4)

Previous Research of Real Variance Estimation of MC/p-CMFD with SAM

– (HyeonTae Kim, 2020) Real Variance Estimation in Monte Carlo Criticality Calculation Accelerated by p-CMFD Feedback Using Spectral Analysis Method

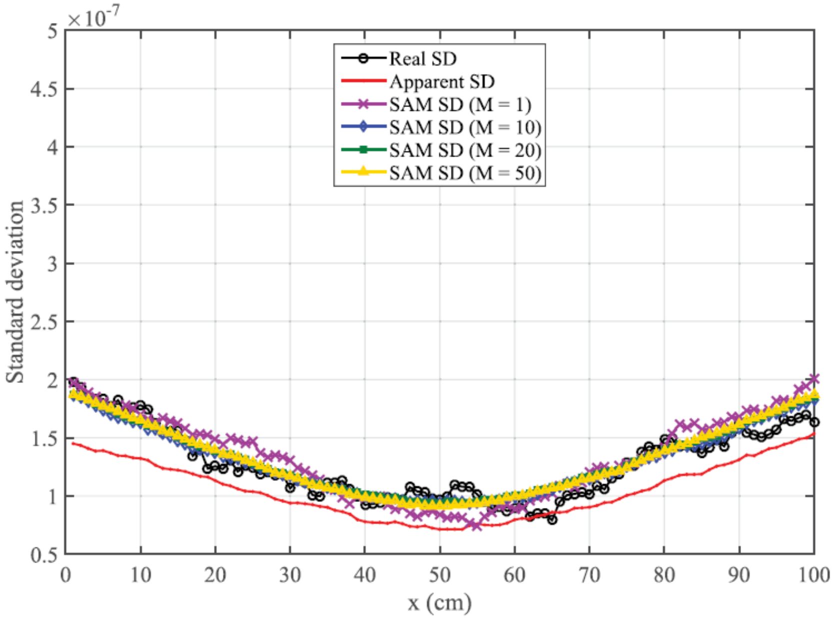


Figure 3. Comparisons of flux real SD, apparent SD, and SAM SDs (M=1, 5, 10, 20) from MC/p-CMFD

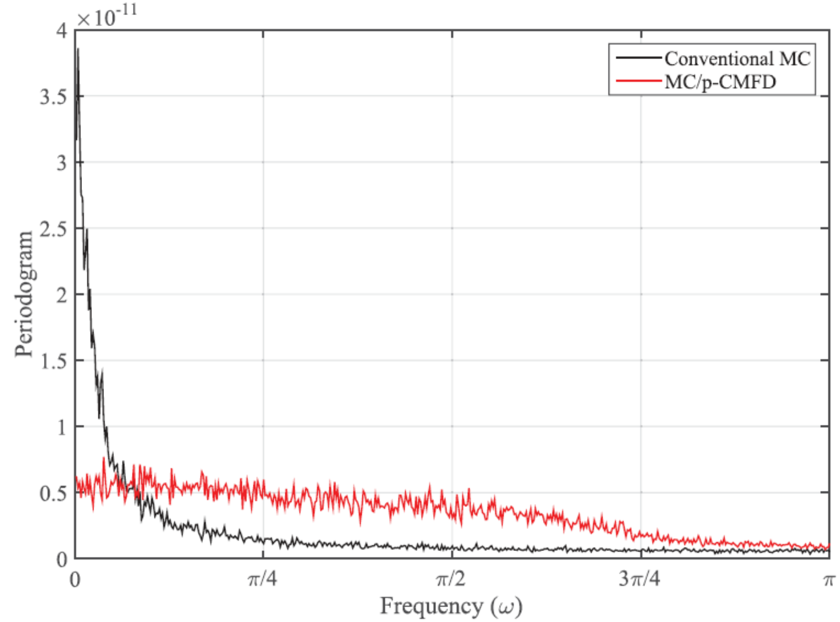


Figure 4. Periodogram plot over discretized frequency from MC and MC/p-CMFD at *x*=0cm

– SAM accurately estimate real variance for simple one-dimensional and BEAVRS problem

– To reduce bias and variance for $\hat{f}(0)$, sufficient number of active cycles are required