An Improved Deterministic Truncation of Monte Carlo Solutions for Nuclear Reactor Analysis

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Introduction

Monte Carlo (MC) calculation for high-fidelity reactor criticality analysis

– **A stochastic method** to solve **a statistical problem** finding out the **average behavior of the unknown parameters based on probabilistic inference**

- Simulation of individual particle based on stochastic random sampling
- Calculation of reactor parameters based on statistical treatment (i.e. average and variance)

$$S^{i+1} = \frac{1}{k_{eff}^{i}} HS^{i} \quad \Leftrightarrow \quad (L+T-S)\psi^{i+1} = \frac{1}{k_{eff}^{i}} F\psi^{i} \qquad (1)$$

where $k_{eff}^{i} = \dfrac{\text{fission rate at iteration } i}{\text{fission rate at iteration } i-1} = \dfrac{\text{fission rate at iteration } i}{\text{loss rate at iteration } i}$

ψ : neutron angular flux $\qquad \vec{r} = (x, y, z)$: position vector

S : neutron source $\qquad H$: transport operator $\qquad \hat{\Omega} = (u, v, w)$: direction vector

$L\psi = \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, E)$ (leakage loss term)

$T\psi = \sigma_t(\vec{r}, \hat{\Omega}, E)\psi(\vec{r}, \hat{\Omega}, E)$ (collision loss term)

$S\psi = \int d\hat{\Omega}' \int dE' \sigma_s(\vec{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E)\psi(\vec{r}, \hat{\Omega}', E')$ (scattering production term)

$F\psi = \int d\hat{\Omega}' \int dE' \nu\sigma_f(\vec{r}, \hat{\Omega}', E')\psi(\vec{r}, \hat{\Omega}', E')$ (fission production term)

Introduction

Monte Carlo (MC) calculation for high-fidelity reactor criticality analysis

Pros	Cons
▪ **High accuracy** - Direct simulation of particles' whole behavior - No discretization of variables (energy, angle, space) - No constraints on geometry construction ▪ **High parallelization** - Parallel calculation of individual particles	▪ **Computationally expensive** - Large memory to describe explicit geometry and to utilize cross section data - Long time to obtain the converged source distribution and to get quantities of interest ▪ **Uncertainties and inconsistency** - Stochastic uncertainties - Underestimation of variance ▪ **Fundamental dilemma** - The main calculation is activated when the FSD converges

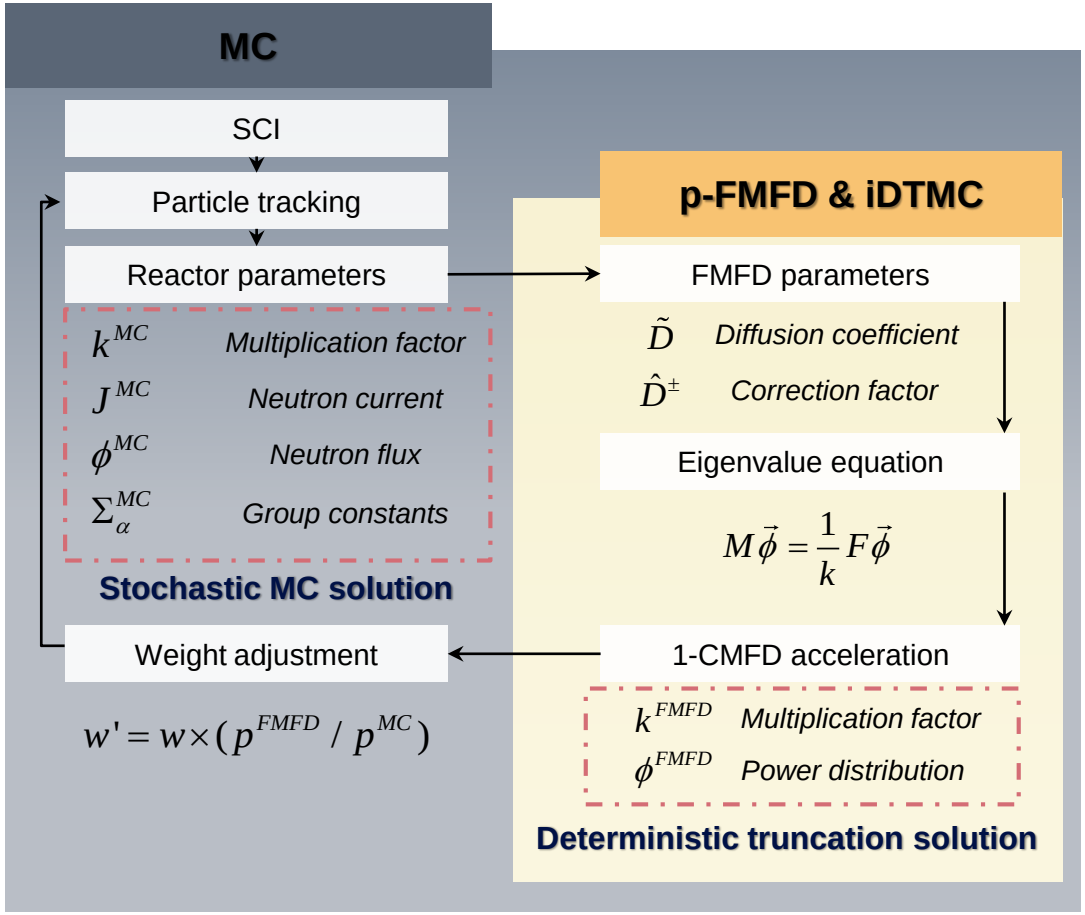
– Several studies have been conducted to accelerate the calculation speed and to reduce stochastic uncertainties more efficiently

- Coarse mesh finite difference (CMFD) method
- Modified power method
- ...

Overview

– **A statistic treatment of deterministic solutions determined by FMFD-assisted MC**

- To accelerate the convergence of the fission source distribution by adjusting particles' weight
- To provide a subset of solutions to the original MC approach



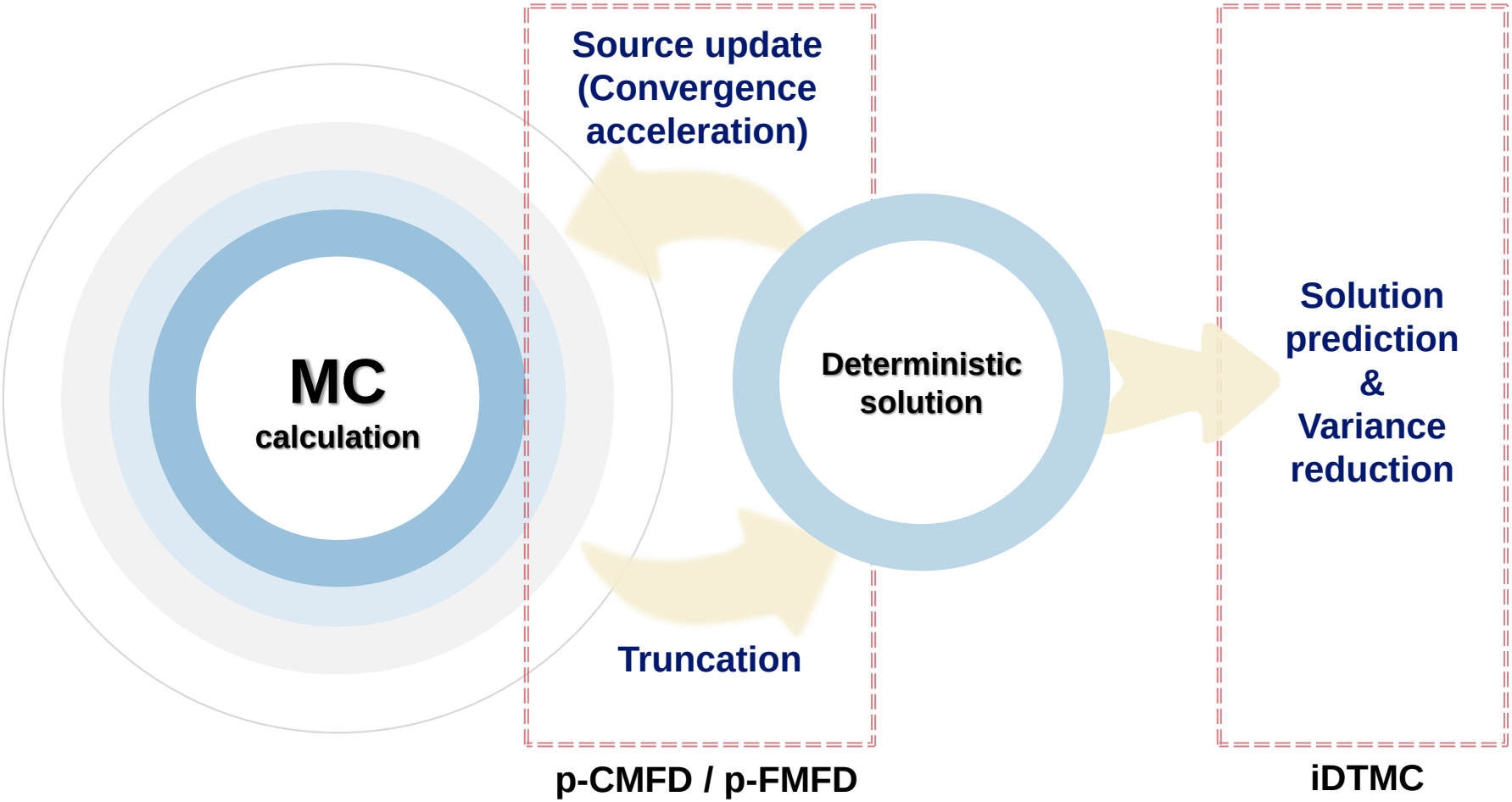
Deterministic solutions
truncated by MC simulation

- ✓ *Short computing time*
- ✓ *Fast convergence of FSD*
- ✓ *Low uncertainty*
- ✓ *MC-equivalent solution (High fidelity solution)*

**FMFD : Fine mesh difference method*

Introduction

Improved DTMC in a MC simulation

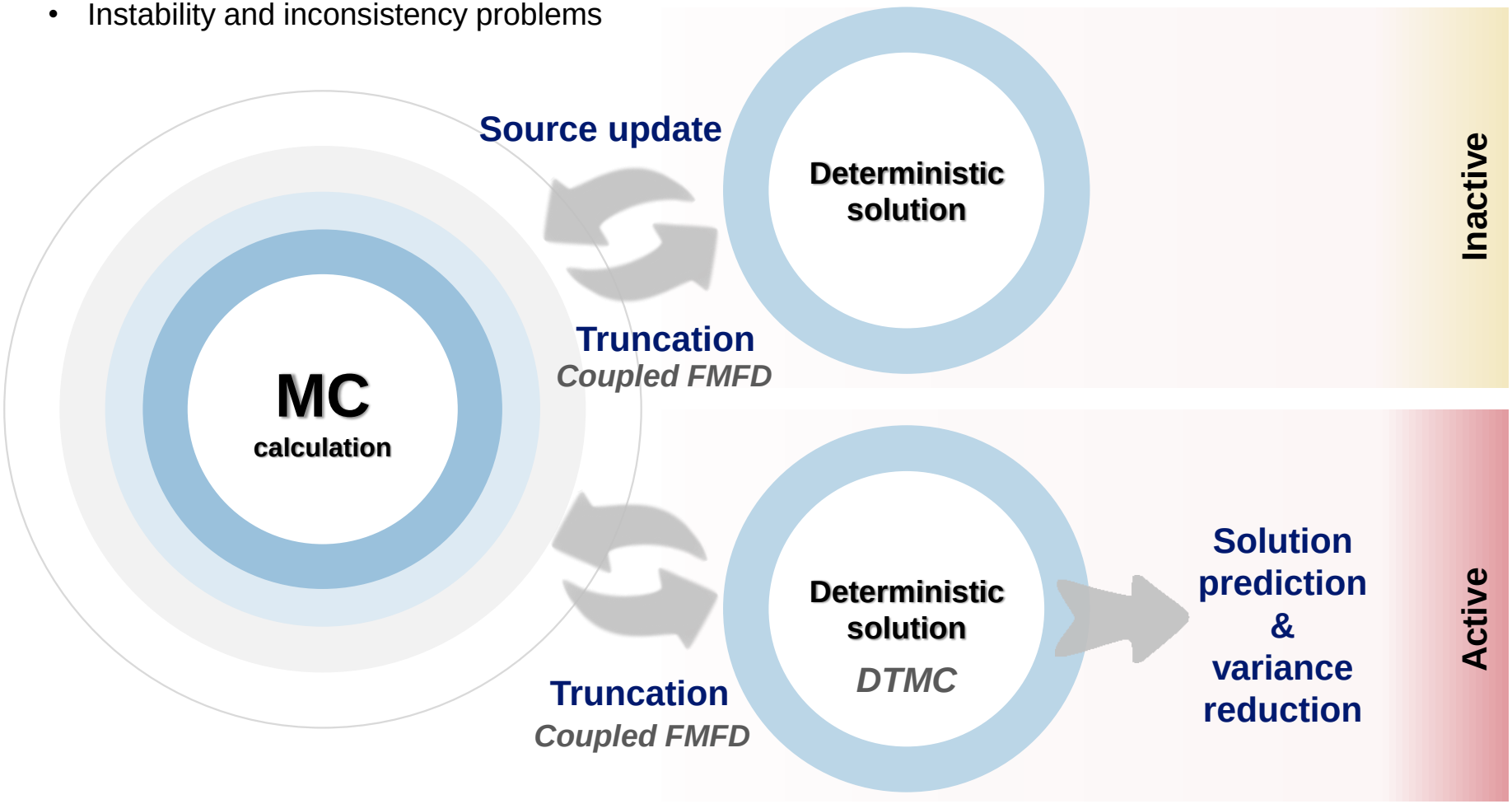


- ✓ p-CMFD (partial current based coarse mesh finite difference)
- ✓ p-FMFD (partial current based fine mesh finite difference)
- ✓ iDTMC (improved deterministic truncation of MC solution)

Deterministic truncation of MC solution method

– **A conventional numerical scheme of the DTMC method**

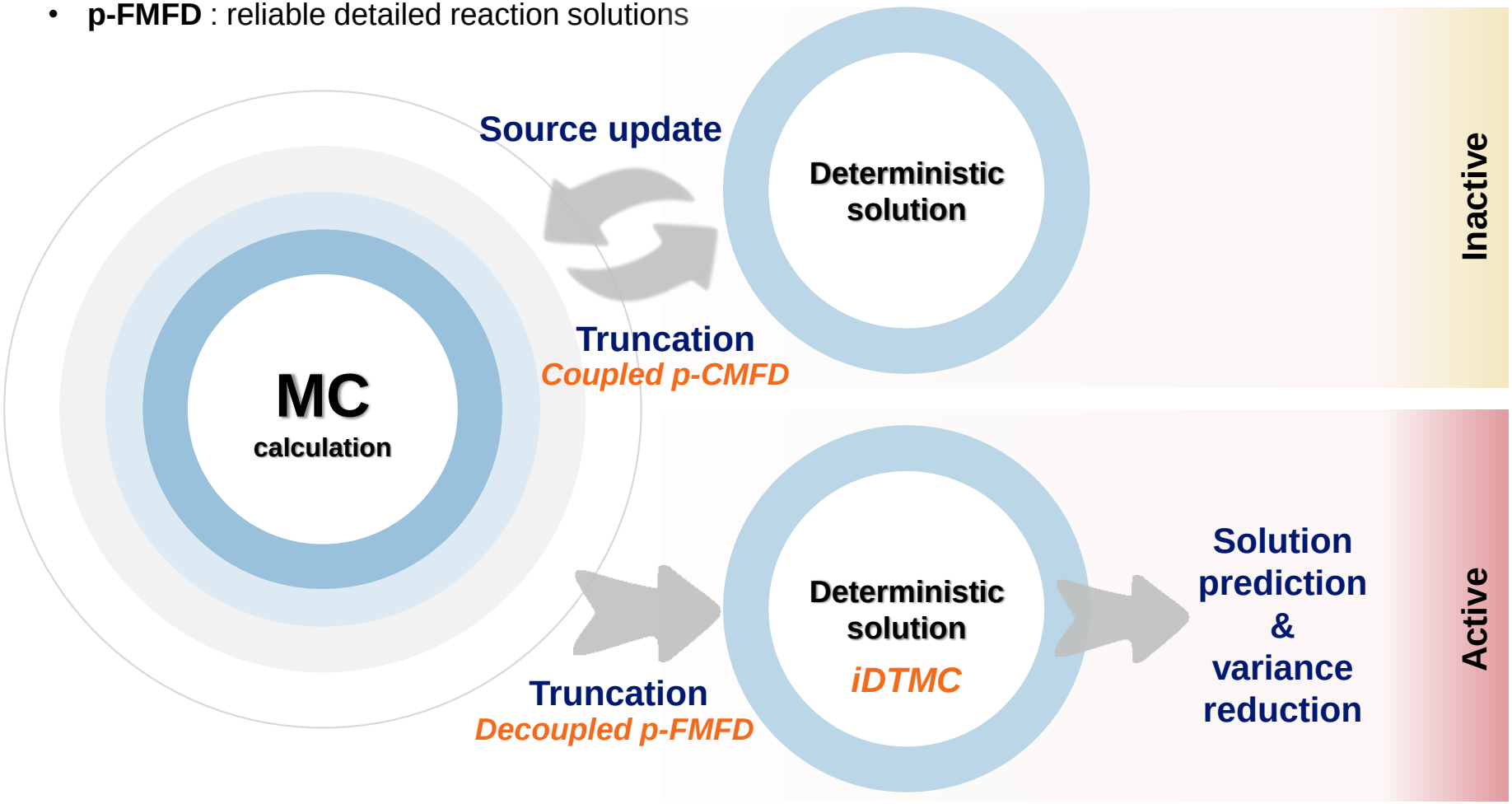
- FMFD has been applied throughout the simulation for both acceleration and variance reduction
- Instability and inconsistency problems



Improved deterministic truncation of MC solution method

– **A numerical strategy has been applied by the p-CMFD and p-FMFD in a combined way**

- **p-CMFD** : stable and consistent deterministic calculation, and more efficient than the p-FMFD
- **p-FMFD** : reliable detailed reaction solutions



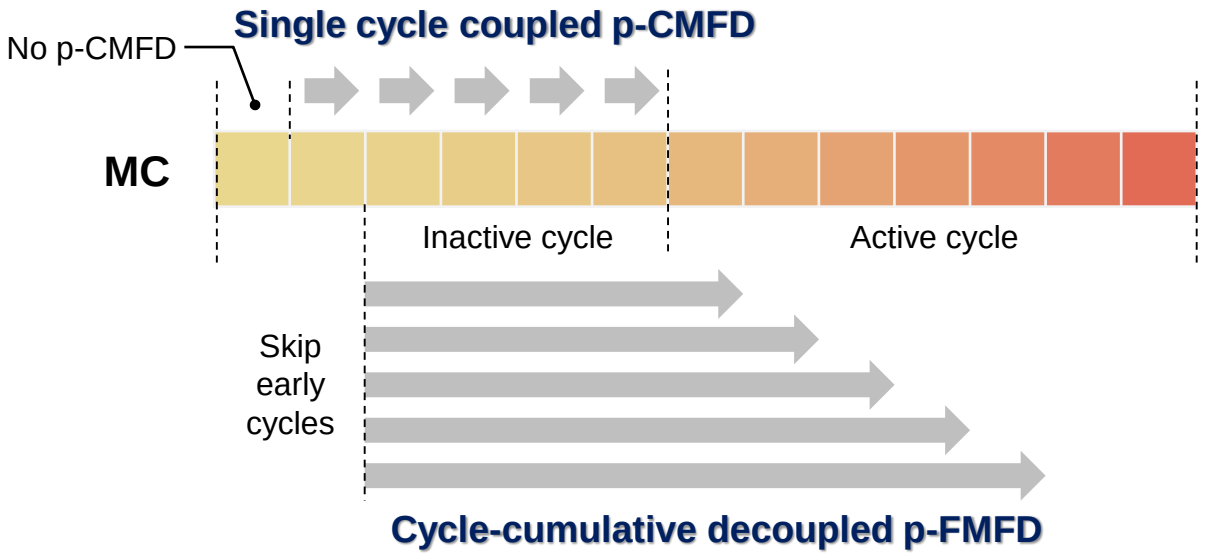
Improved deterministic truncation of MC solution method

– **Single cycle coupled p-CMFD**

- A stable and consistent deterministic calculation is available even without the cycle accumulation
- The p-CMFD enables the fast convergence of the FSD

– **Cycle-cumulative decoupled p-FMFD**

- A stable and reliable deterministic solutions can be obtained with long cycle accumulation
- The only reliable deterministic solutions are obtained from the p-FMFD method
- Coupling is not necessary because the FSD already converged



CMFD & FMFD

Coarse mesh finite difference (CMFD) method

– Solving the lower-order diffusion-like equation with the surface current correction

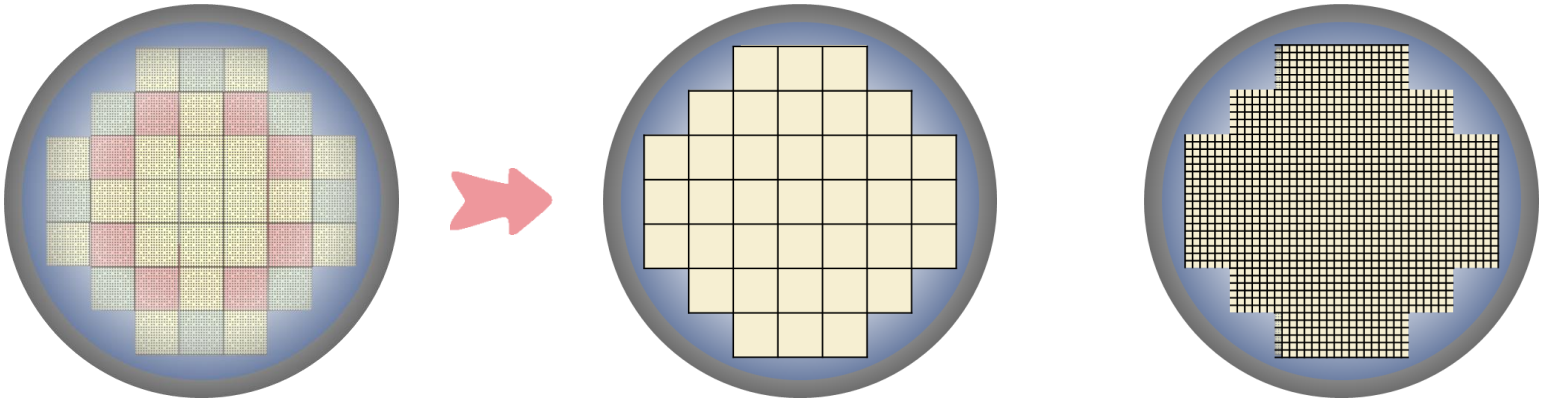
- Fast and efficient deterministic calculation
- MC-equivalent accuracy based on the generalized equivalent theory (GET)

– Unavailable to produce the detailed power distribution → radial direction : assembly size (~ 20 cm)

Fine mesh finite difference (FMFD) method

– **Fine mesh grid to generate the detailed pin-wise power distribution**

- Radial direction : pin size (~ 1 cm)
- Axial direction : 10 – 15 cm



MC **CMFD grid** **FMFD grid**

Partial current based fine mesh finite difference (p-FMFD) method

– **Neutron balance equation (diffusion-like one-group deterministic equation)**

$$\sum_{s=x,y,z} \frac{a_s}{v_i}\left(\left(j_{s_1}^{+}-j_{s_1}^{+}\right)-\left(j_{s_0}^{+}-j_{s_0}^{-}\right)\right)+\sigma_a^i\phi_i=\bar{s}_i \qquad (2)$$

where $j^{\pm}$: partial current

σ_a : absorption cross section

$\nu\sigma_f$: no. of fission neutrons $\times$ fission XS

ϕ : neutron flux

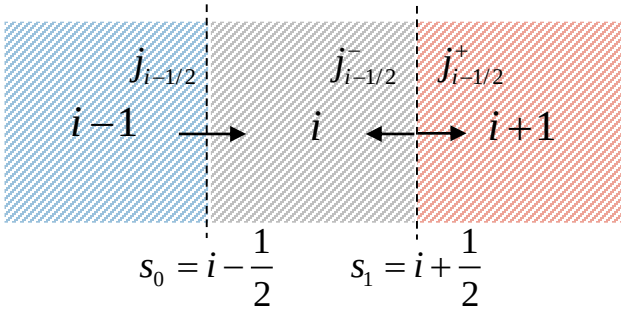
a : surface area

v : node volume

s : surface index (s_1=i+1/2 and s_0=i-1/2)

i : node index

$\bar{s}_i=\frac{1}{k}\nu\sigma_f^i\phi_i$: fission source (3)



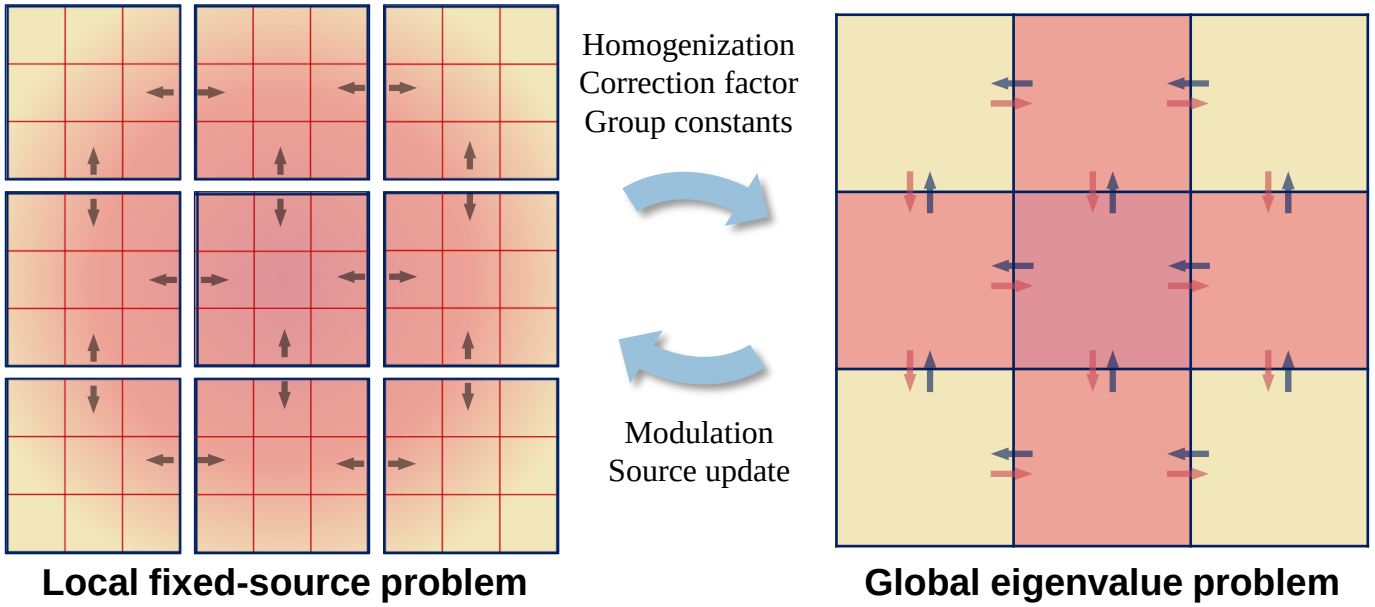
One node p-CMFD

One-node CMFD acceleration

– **1-CMFD scheme** is applied to accelerate the FMFD deterministic calculation

– **Coarse mesh grid**

- Radial direction : assembly size (~ 20 cm)
- Axial direction : 20 – 30 cm



– **Fast and efficient calculation**

– **High parallelism**

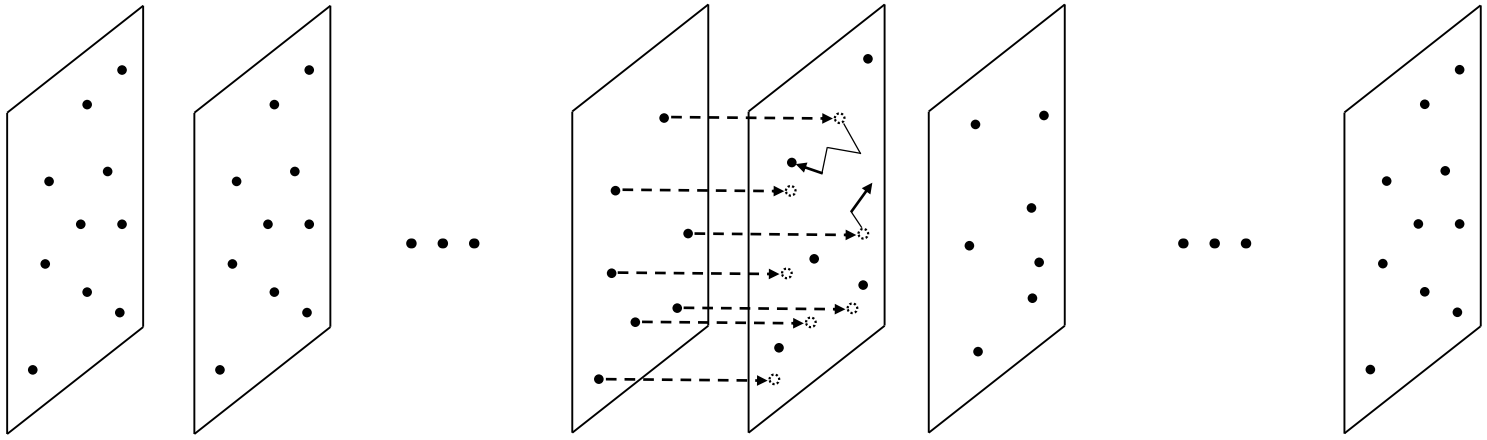
Methods :

Stochastic error in MC calculation

– **Stochastic error cannot be exactly estimated with a single MC run**

- Apparent standard deviation (SD) is underestimated due to a cycle correlation
- Variance underestimation is more critical issue in iDTMC method
  because of correlation of the cycles and parameters

- Fission reaction



Fission reaction in current generation ➔ Neutron source in next generation

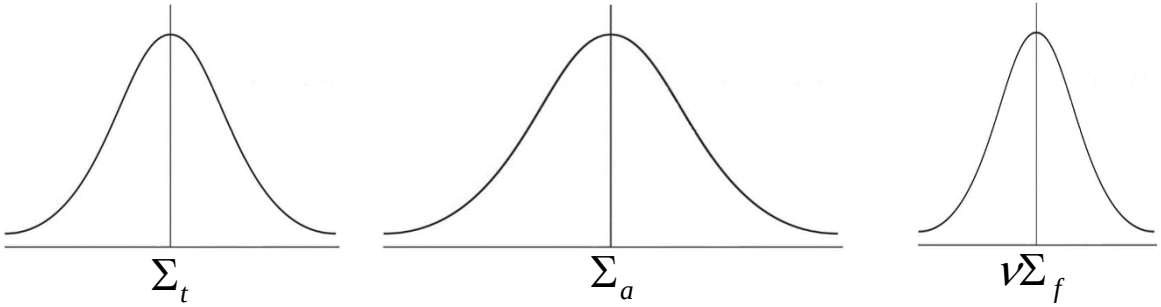
Variance Estimation by Parameter Sampling

Error quantification of iDTMC method

– **Overview**

MC simulation

PDFs of FMFD parameters



Re-sampling FMFD parameters

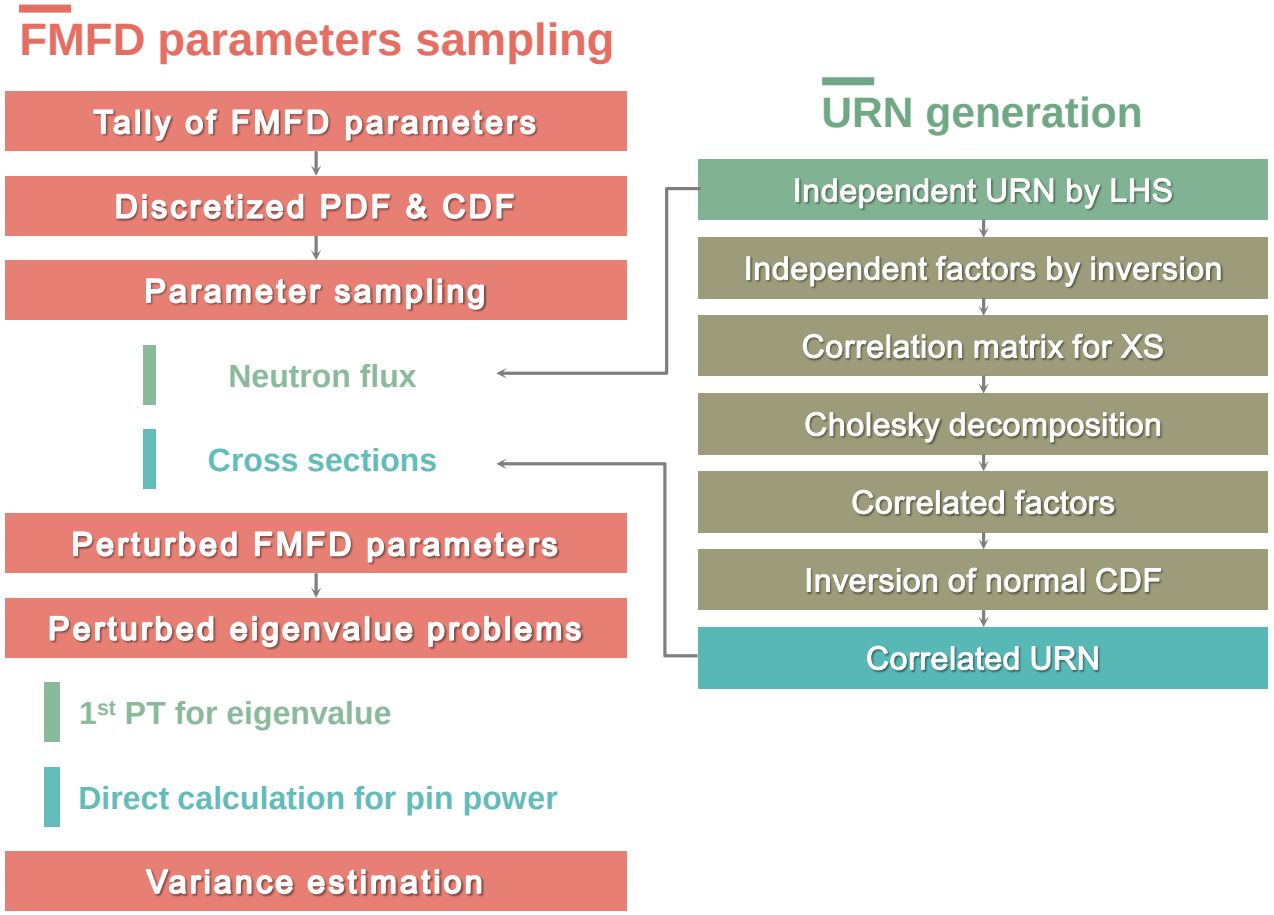
Perturbed eigenvalue calculation

Variance estimation

Variance Estimation by Parameter Sampling

Error quantification of iDTMC method

– **Flow chart**

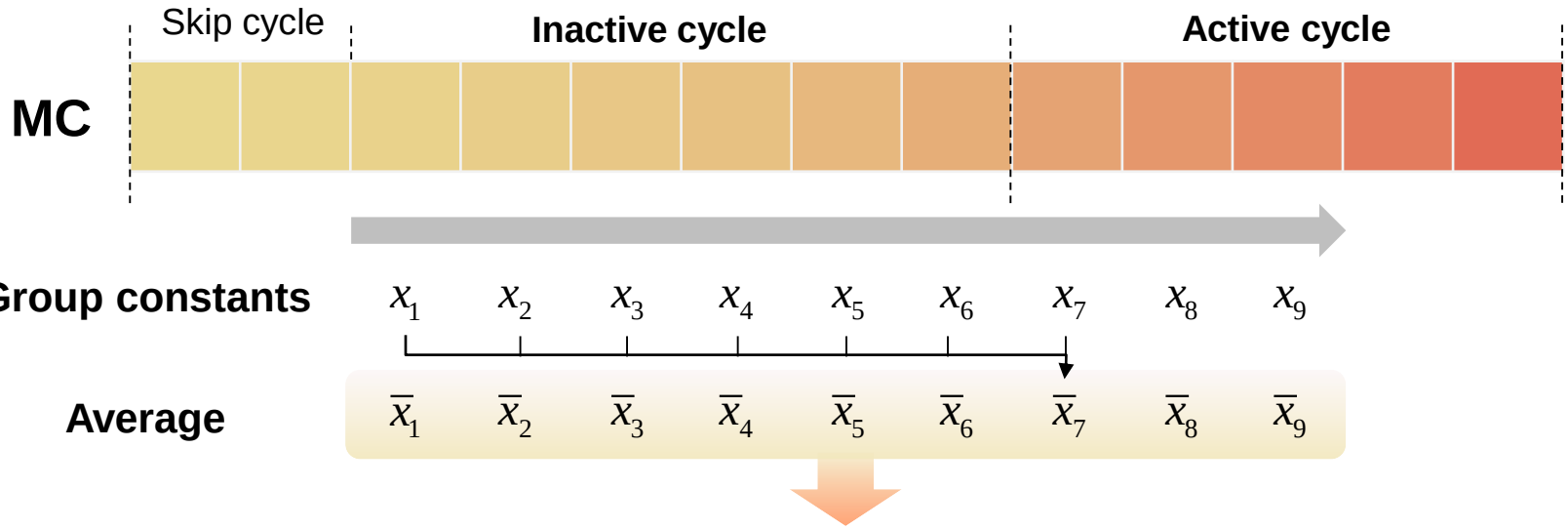


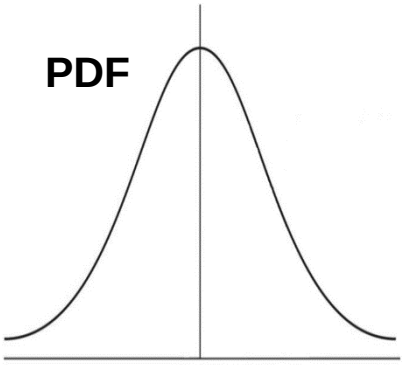
Variance Estimation by Parameter Sampling

Error quantification of iDTMC method

– **FMFD parameters to calculate k_{eff}**

- Group constants (cross sections) are calculated from MC simulation every cycle





Resampling of cross sections

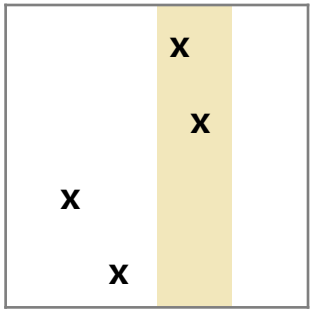
- Resampling parameters include cross sections and flux (i.e. total, absorption, and fission cross sections)
- Current are just taken from the MC simulation as a solution to preserve the nodal balance by a reference

Variance Estimation by Parameter Sampling

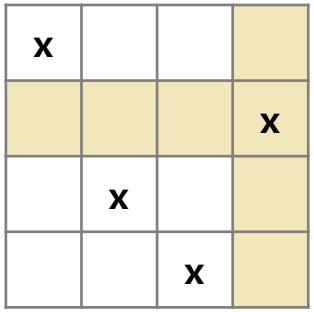
Random number generation

– **Latin hypercube sampling (LHS)**

- A statistical method for generating a near random sample of parameter values from a multidimensional distribution
- An efficient random sampling by analyzing variable space
  - how many sample points to use
  - in which row and column the sample point was taken
- More evenly and fairly distributed for the limited sample size



Random sampling



LHS sampling

Variance Estimation by Parameter Sampling

Correlation sampling

– Correlation matrix

- Correlation between total, absorption and nu X fission cross section
- Correlation coefficient can be calculated by

$$\rho_{X,Y} = \frac{\mathrm{cov}(X,Y)}{\sigma_X \sigma_Y}$$

- Correlation matrix can be composed as the follows

$$\mathbf{C} = \begin{array}{c|ccc} & \Sigma_t & \Sigma_a & \nu\Sigma_f \\ \hline \Sigma_t & \rho_{t,t} & \rho_{t,a} & \rho_{t,f} \\ \Sigma_a & \rho_{a,t} & \rho_{a,a} & \rho_{a,t} \\ \nu\Sigma_f & \rho_{f,t} & \rho_{f,a} & \rho_{f,f} \end{array}$$

– Cholesky decomposition

- Correlation matrix **C** (positive-definite) is decomposed to be a form of

$$\mathbf{C} = \mathbf{L}\mathbf{L}^T$$

- Positive definiteness should be improved for pseudo non-positive definite due to stochastic uncertainty

$$\mathbf{C}' = \mathbf{C} + 0.1 \times I$$

Variance Estimation by Parameter Sampling

Correlation sampling

– Conversion by inverse cumulative density function (CDF)

- Underlying function is assumed to be a normal distribution
- Random parameters can be obtained by the uniform random number (URN) calculated from LHS

$$p = \sqrt{2} erf^{-1}(\gamma) \in P^{3 \times N_s}$$

where erf : error function

γ : URN $\in [0,1)$

– Correlated parameters generation

- Correlated parameters can be generated by multiplying the Cholesky-decomposed lower triangular matrix and the matrix for random parameters calculated by LHS

$$\mathbf{G} = \mathbf{L} \times \mathbf{P}$$
$$(3 \times N_s) = (3 \times 3) \times (3 \times N_s)$$

– Correlated URN

- Correlated parameters are again converted to be URNs
- Correlated URNs can be obtained by the CDF conversion

$$\gamma' = \frac{1}{2}\left(1 + erf\left(\frac{g}{\sqrt{2}}\right)\right)$$

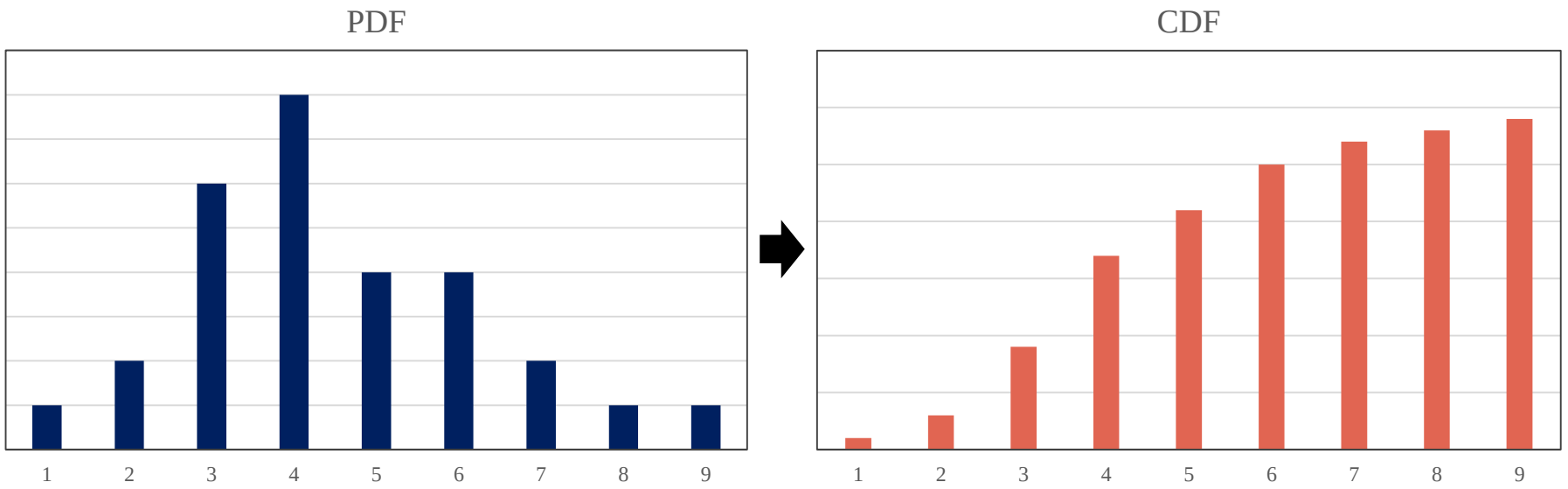
where g : element of matrix $\mathbf{G}$

Variance Estimation by Parameter Sampling

Correlation sampling

– **Correlated cross section sampling**

- Using the correlated URNs, the correlated cross sections can be sampled
- In the sampling of the cross section, the probability function is created by the FMFD parameters
  ➔ PDF made from the FMFD parameters does not follow the normal distribution
- The cross sections are directly sampled from the **actual given PDF**



Variance Estimation by Parameter Sampling

Eigenvalue calculation by 1st order perturbation theory

– **1st order perturbation theory**

- Multiplication factor can be easily calculated with the perturbed parameters

$$\Delta\rho = \frac{1}{k'} - \frac{1}{k} = \frac{(\phi^*, [\lambda\Delta\mathbf{F} - \Delta\mathbf{M}]\phi)}{(\phi^*, \mathbf{F}\phi)} \tag{36}$$

where $\lambda = \frac{1}{k}$

$\mathbf{M}, \mathbf{F}$: unperturbed matrices

k : unperturbed reference eigenvalue

ϕ : unperturbed flux (forward flux)

ϕ^* : adjoint flux

$\Delta\mathbf{M}, \Delta\mathbf{F}$: perturbed $\mathbf{M}$ and $\mathbf{F}$

– Forward and adjoint fluxes are different in the p-FMFD method due to the correction factors

– But they are comparable each other with some reasons

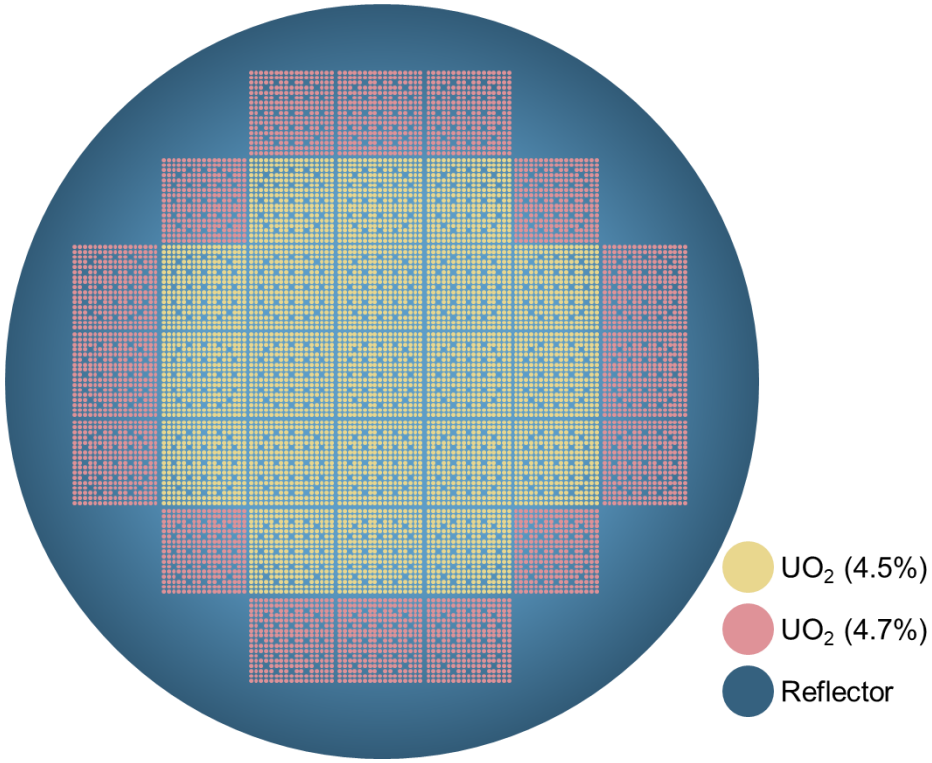
– Therefore, the self-adjointness is assumed in 1st PT error quantification

Numerical Results

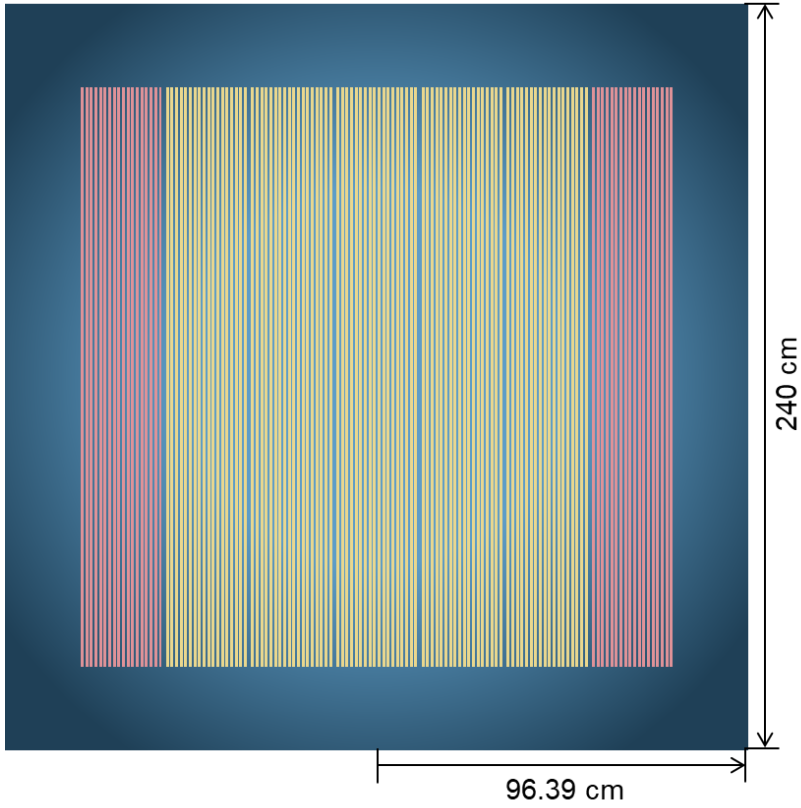
Core configuration

– A small modular reactor problem

– 7 X 7 fuel assemblies surrounded by a water reflector



Radial configuration



Axial configuration

Numerical Results

Calculation condition

- Total **112 cores** of Xeon E5-2697 with clock speed of **2.60 GHz**
- Skip p-CMFD : 1
- Skip early cycles : 5
- According to SCI
  - Minimum generation size = 6,000,000 histories per cycle

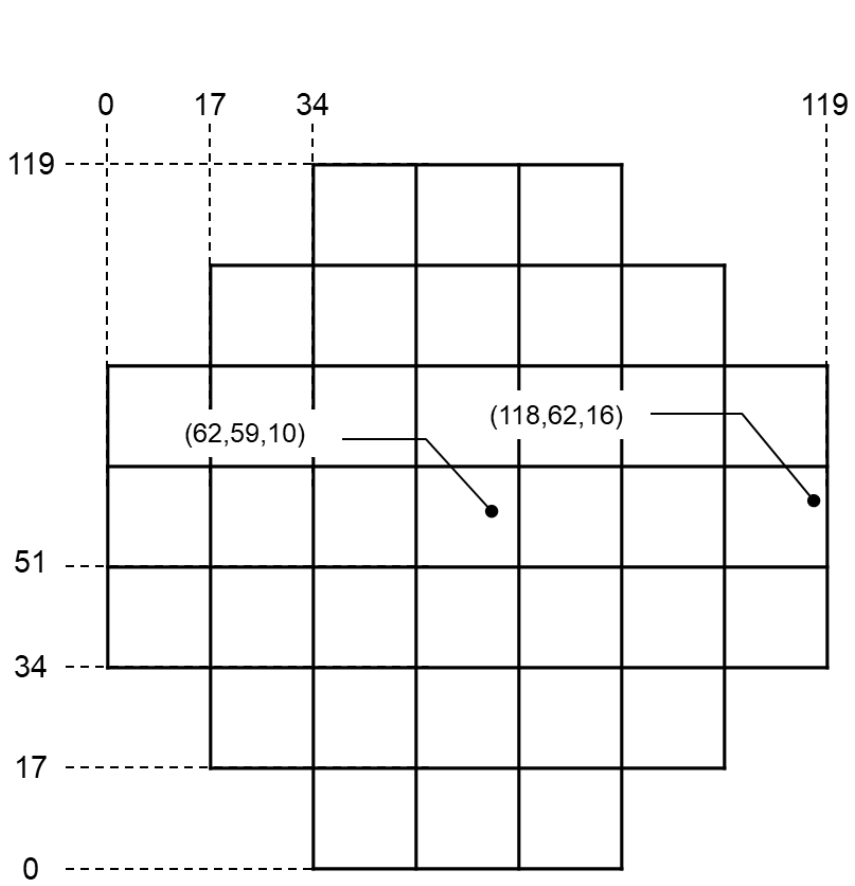
Total number of fine nodes		*No. of neutrons*		*Off-peaking*			*Optimum generation size*
213,860	×	5.86	/	0.2	=	6,266,098	≅ 6,000,000

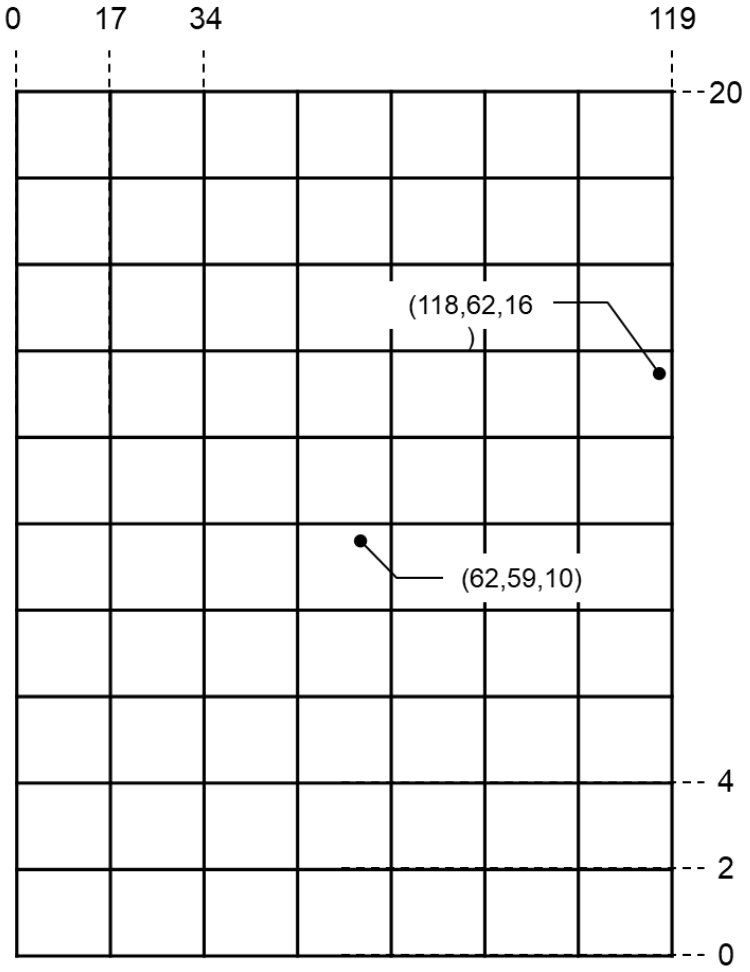
  - The number of inactive cycles were automatically determined
- 10 active cycles were used
- For real standard deviation, 20 independent runs simulated with different random seeds
- **Reference solution** : 1.27774 ± 1.2 pcm
  - No. of histories : 6,000,000
  - No. of inactive cycles 120
  - No. of active cycles : 500
  - No. of batches : 2

Numerical Results

FMFD parameters

– **Three pin positions are arbitrarily selected to characterize the FMFD parameters**

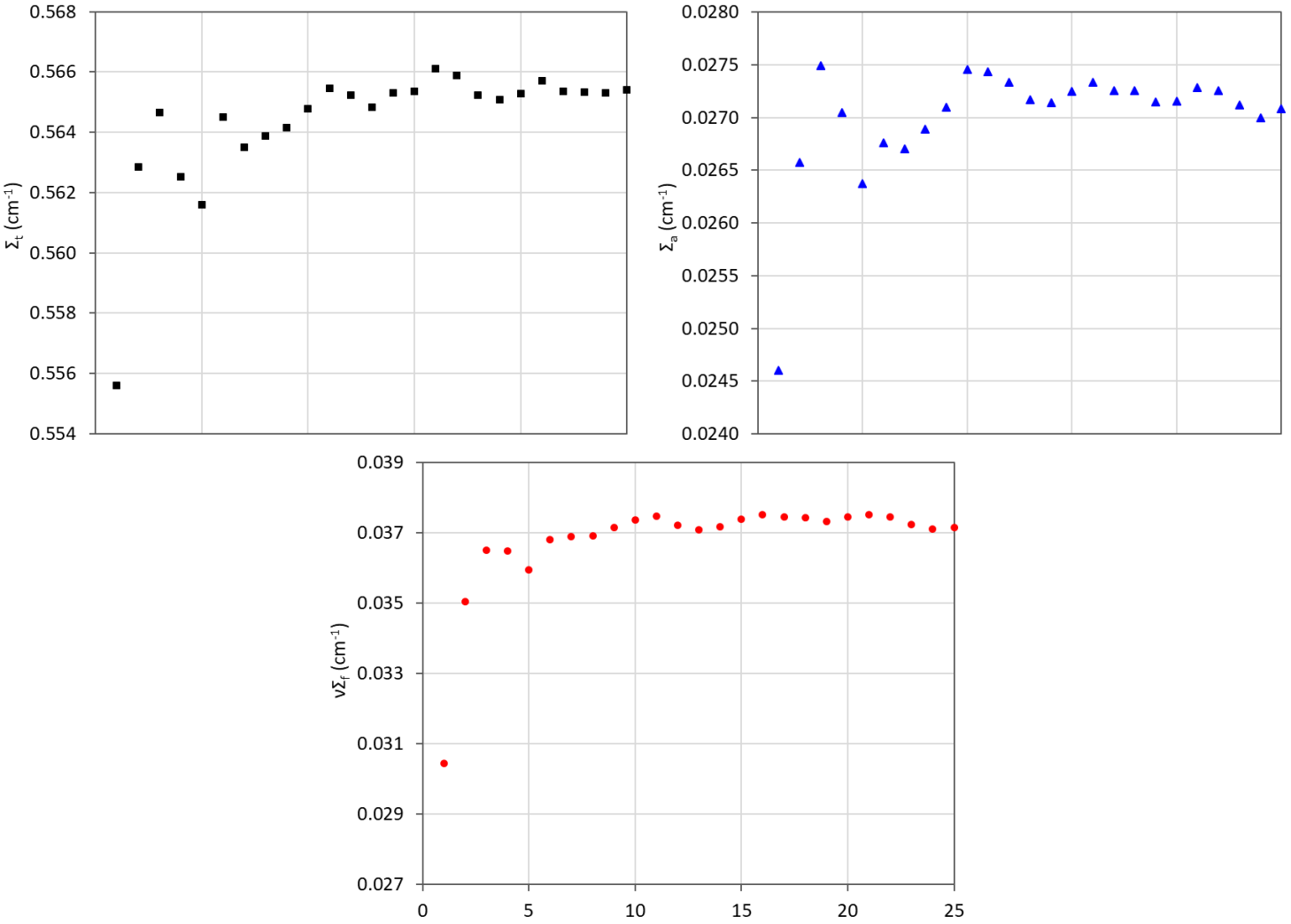




Numerical Results

FMFD parameters

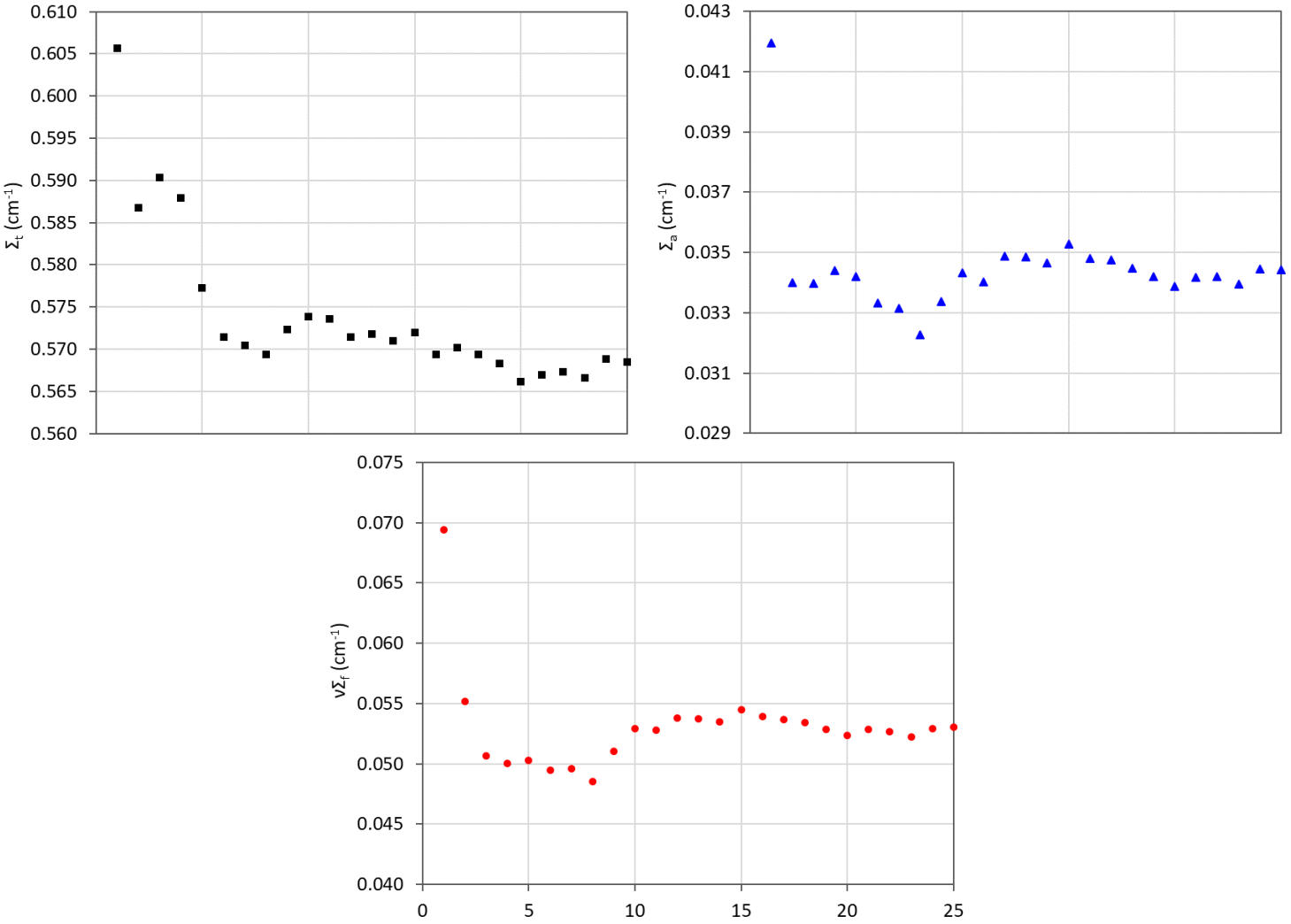
– **Convergence behavior; central region (62,59,10)**



Numerical Results

FMFD parameters

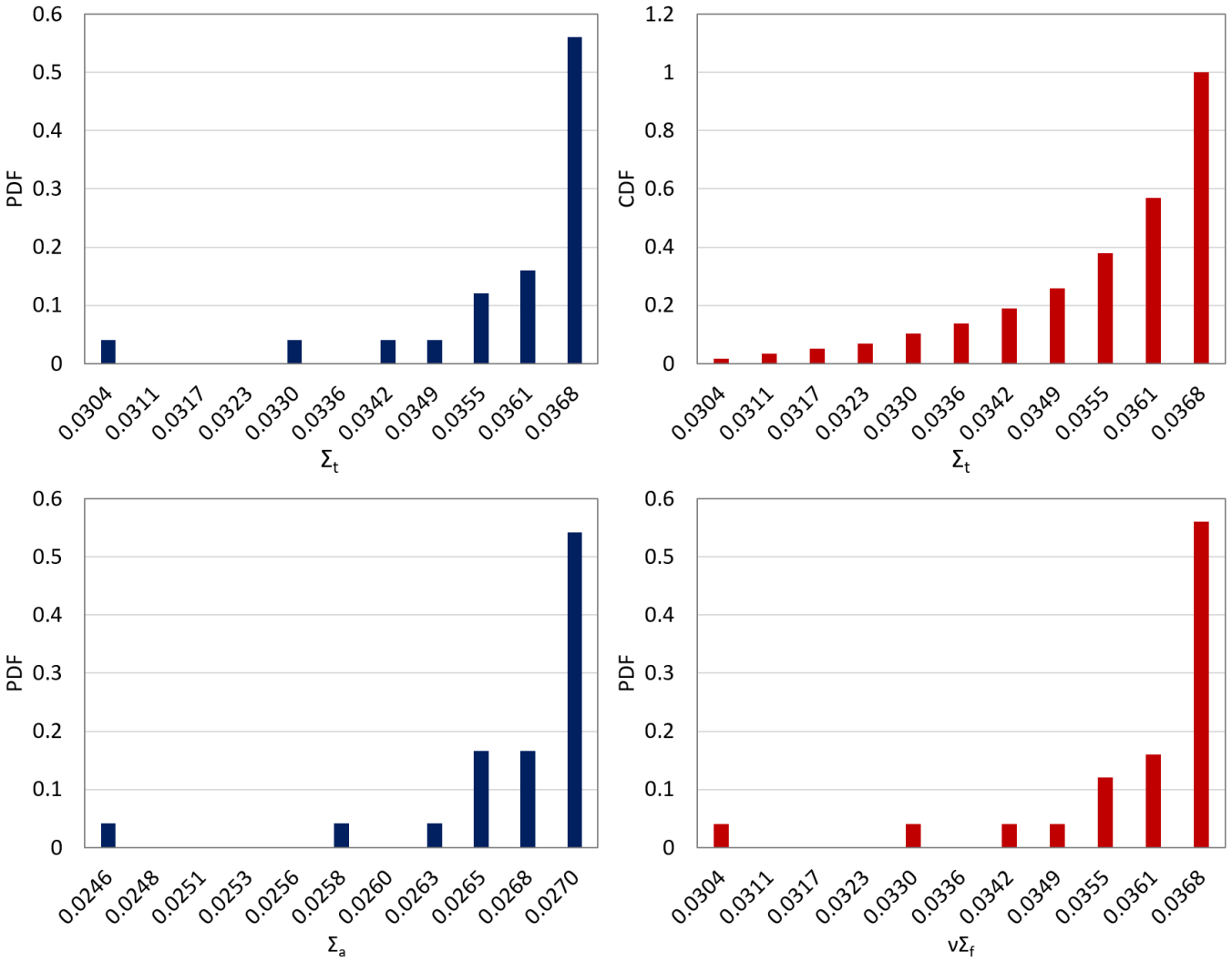
– **Convergence behavior; peripheral region (52,24,10)**



Numerical Results

FMFD parameters

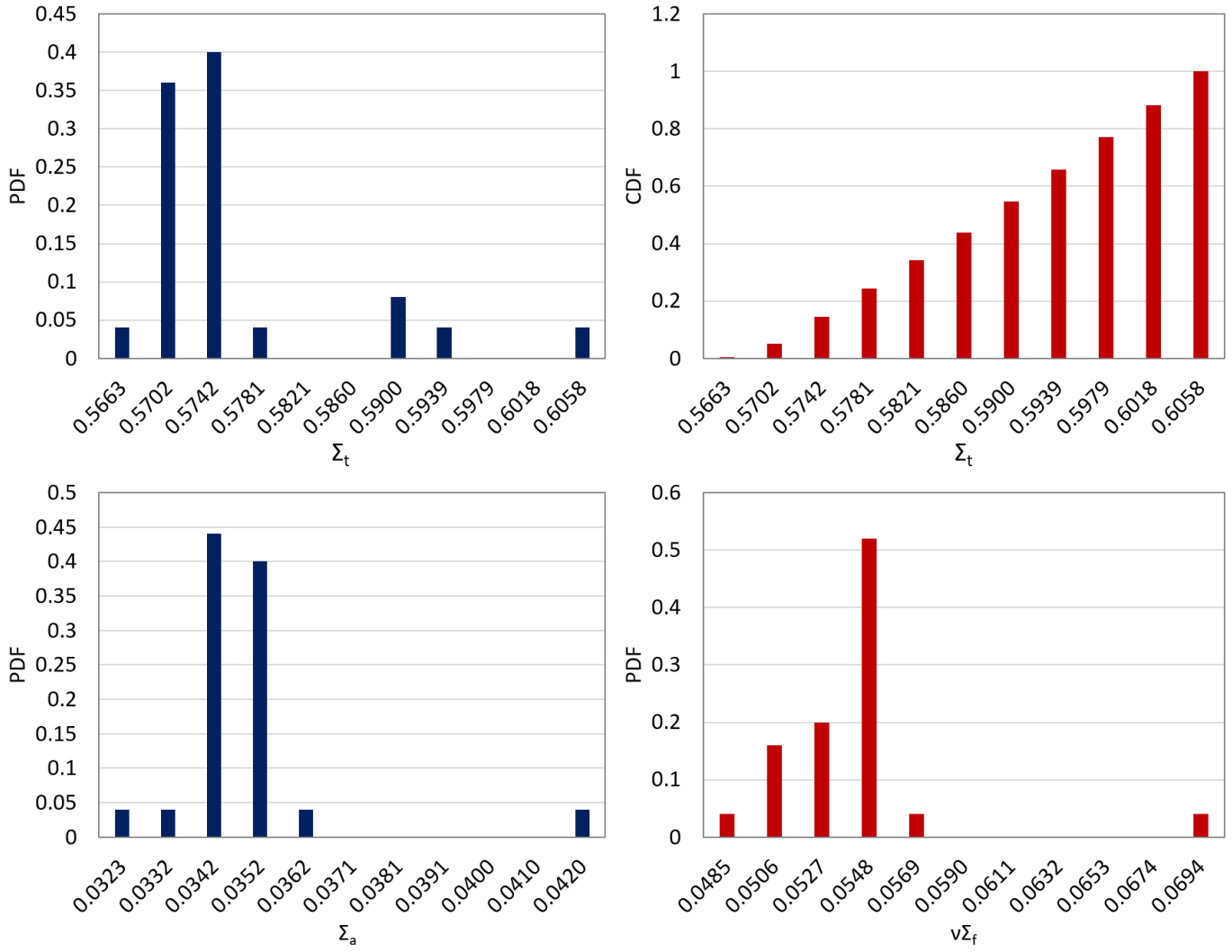
– **PDF and CDF; non-central region (62,59,10)**



Numerical Results

FMFD parameters

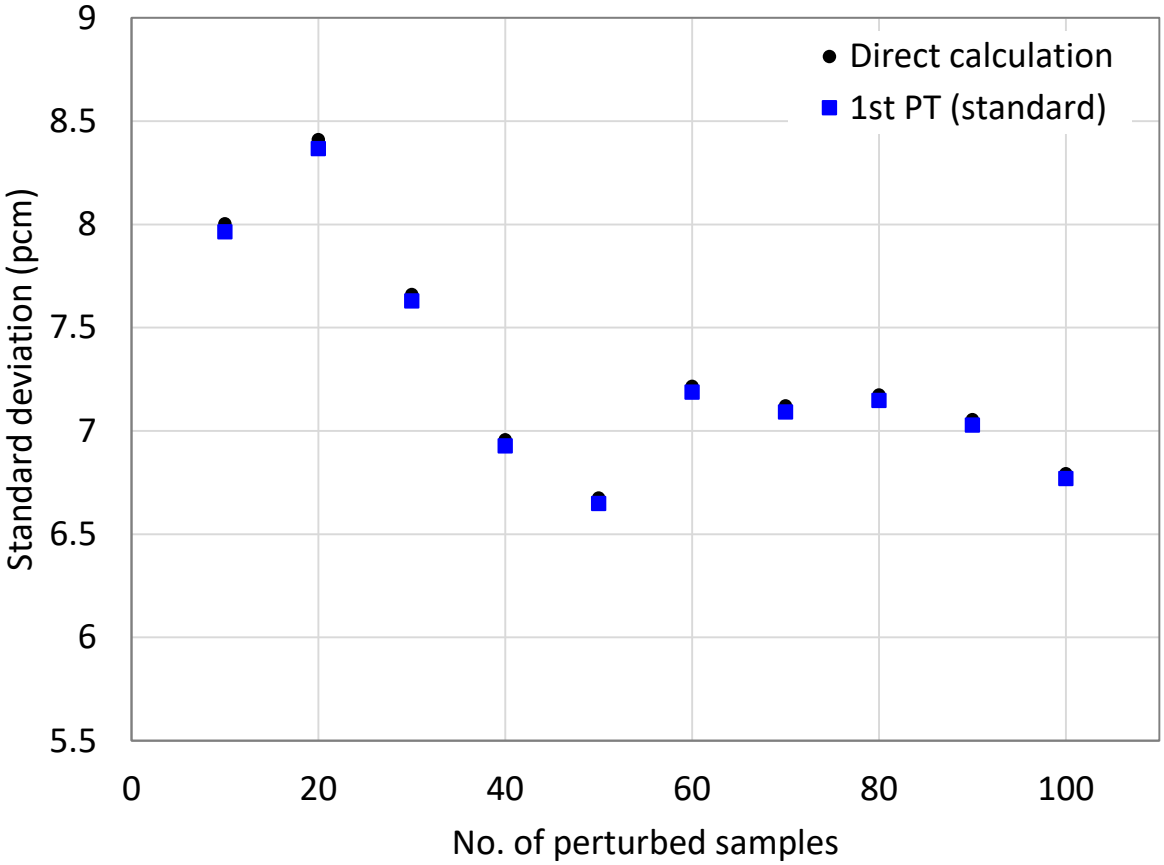
– **PDF and CDF; peripheral region (118,62,16)**



Numerical Results

1st PT vs. direct calculation

– **The number of samples**



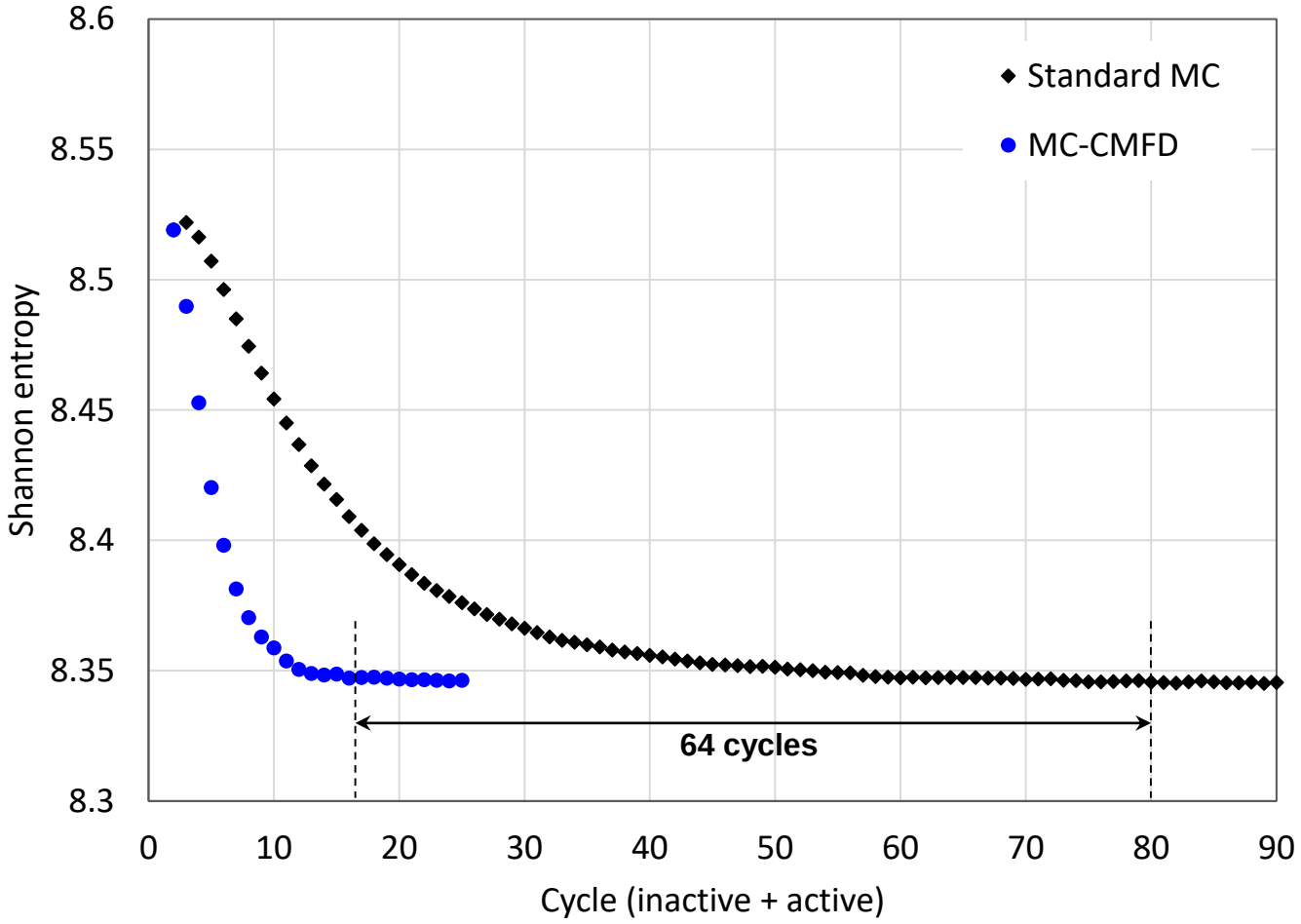
▪ **Computing time of 1st PT vs. direct calculation for 100 samples**

	1st PT	Direct
Time (sec.)	4.7	158.8

Numerical Results

FSD convergence

– **By the Shannon entropy**



Numerical Results

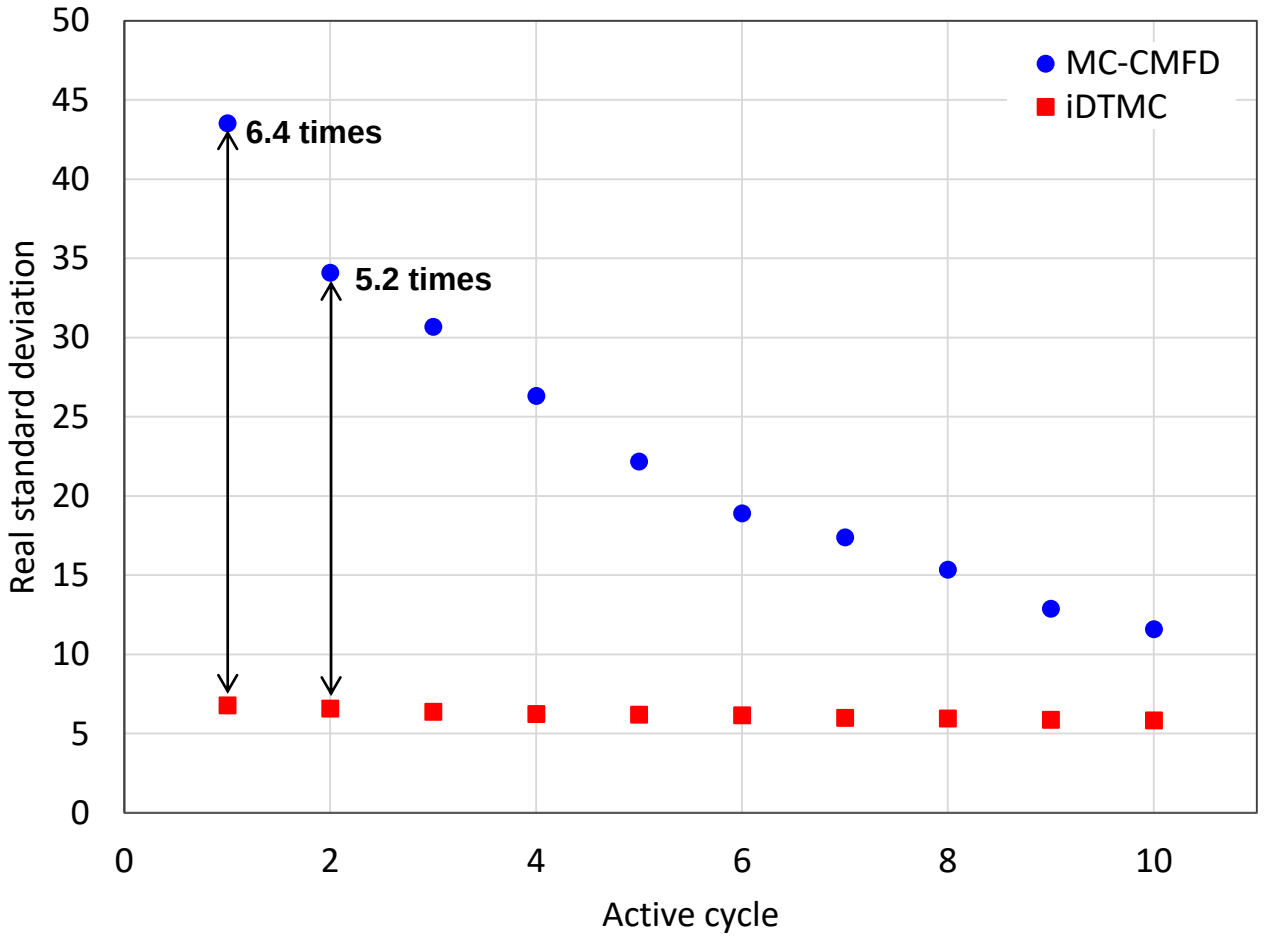
Multiplication factor & stochastic errors

Parameter		Cycle				
		1	3	10	15	20
MC-CMFD	k_{eff}	1.27706	1.27763	1.27781	1.27782	1.27778
	σ_a	-	18.3	13.0	9.9	8.9
	σ_r	46.4	24.2	13.7	13.4	11.3
iDTMC	k_{eff}	1.27777	1.27776	1.27776	1.27775	1.27775
	σ_a	-	0.6	0.5	0.5	0.5
	σ_r	5.7	5.7	5.2	4.9	4.8
	1^{st} PT	6.4	6.6	6.0	5.5	5.2

* $k_{eff}^{ref} = 1.27774 \pm 1.2$ pcm

Numerical Results

Real standard deviation of the multiplication factor

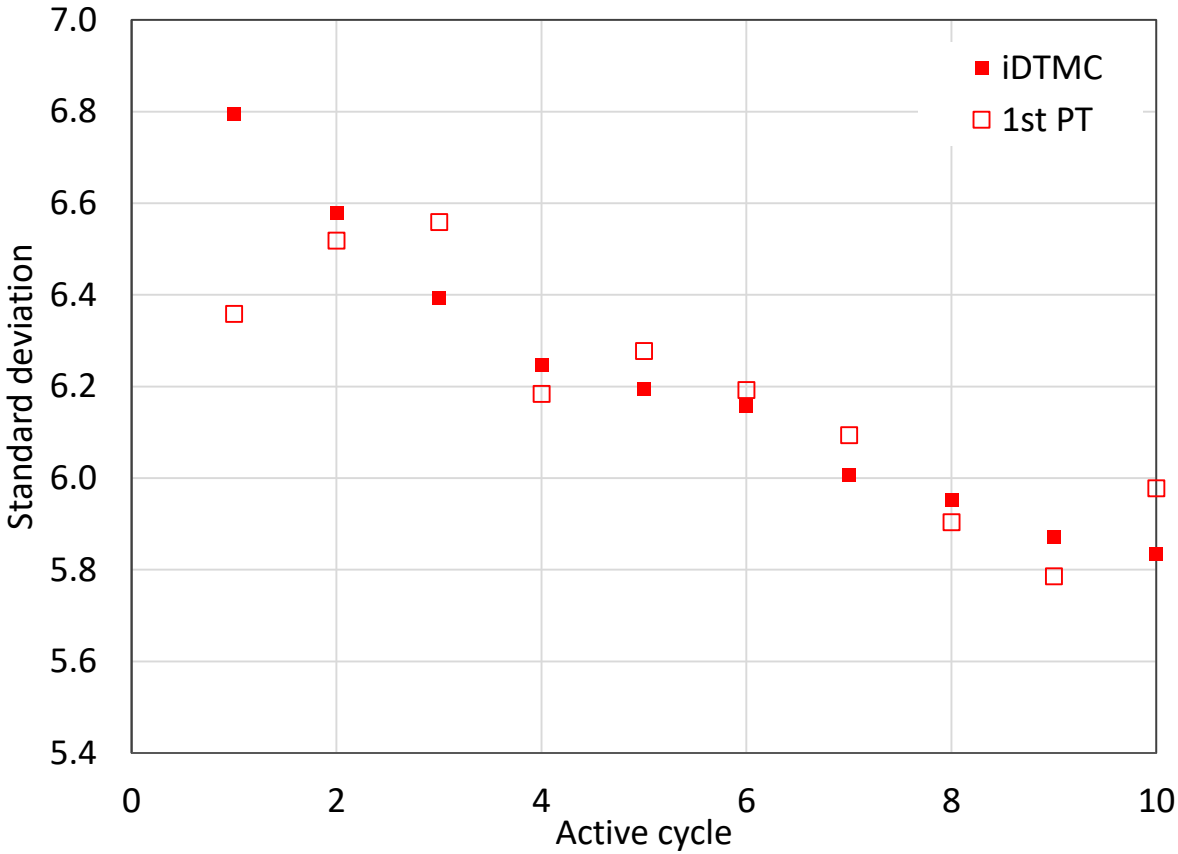


Much more reliable solutions can be obtained with the iDTMC method
Remind that the iDTMC method is designed to pursue the early truncation

Numerical Results

Comparison of standard deviation

– **iDTMC vs. 1st PT**



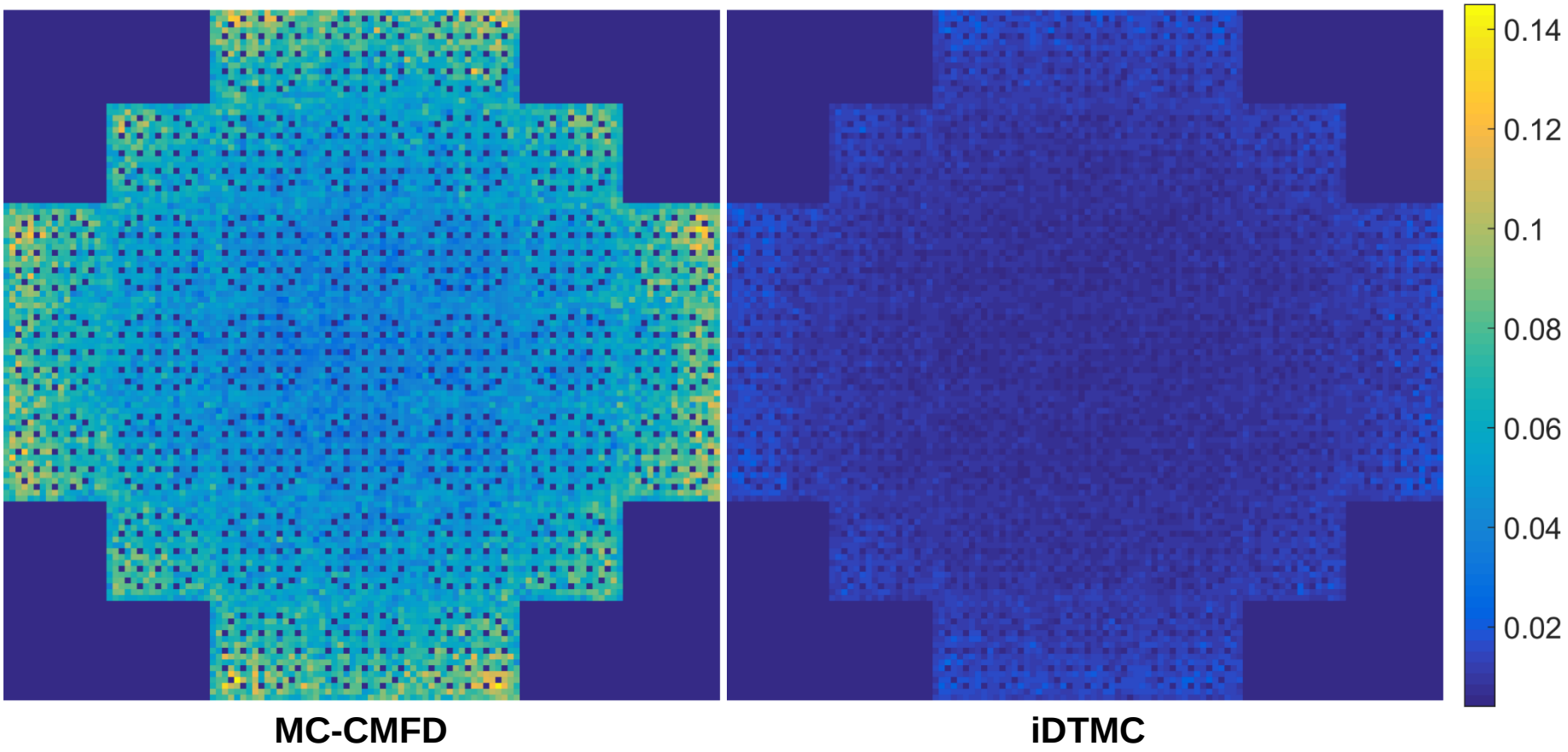
They show great agreement each other throughout the simulation
The reliable stochastic error can be calculated with a single batch calculation

Numerical Results

Real standard deviation of the 2D pin power

– **At cycle 1**

Cycle 1	MC-CMFD	iDTMC
Avg.	0.058	0.011



MC-CMFD **iDTMC**

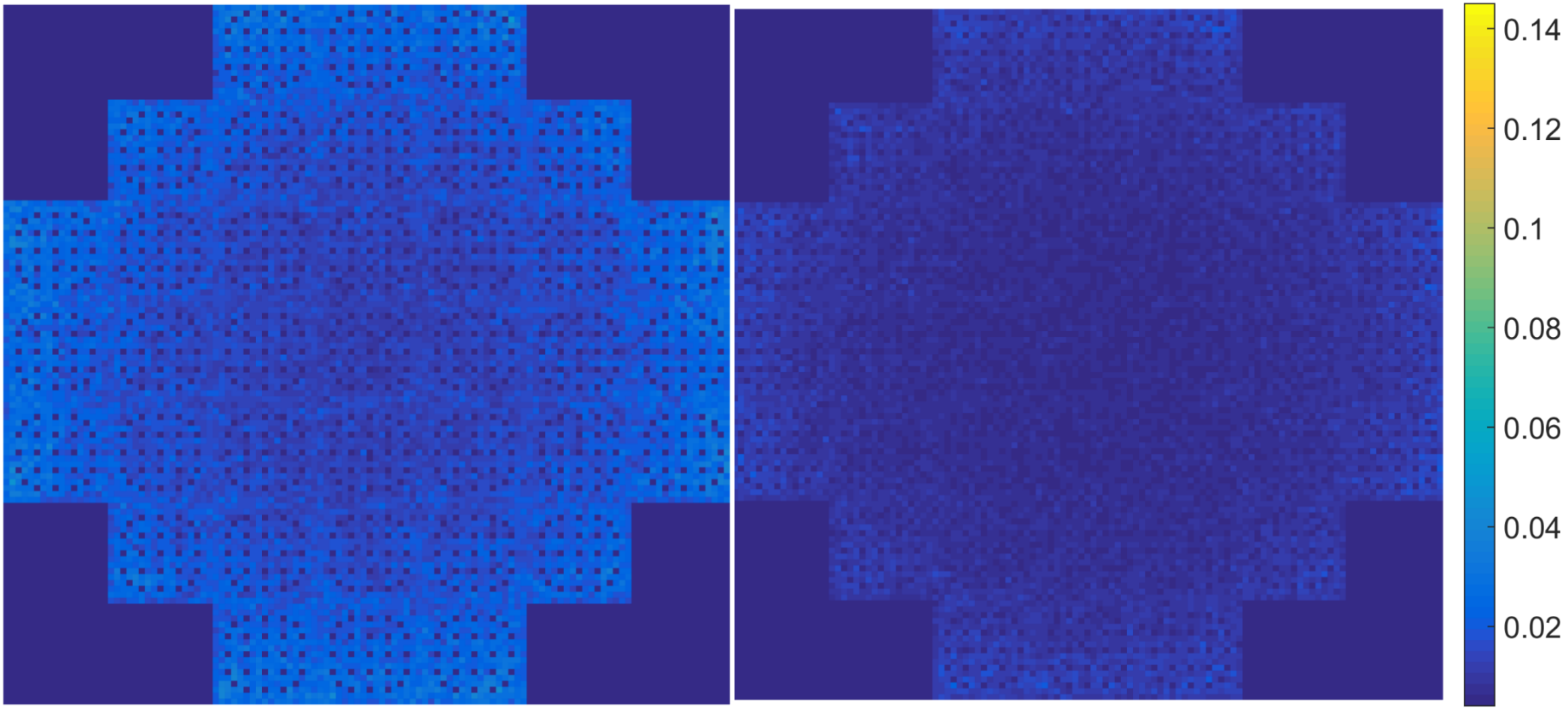
$$\sigma_{i,j} = \frac{1}{N_b}\sum_{b}^{N_b}(p_{i,j}^{b} - \bar{p}_{i,j})^2 \quad \text{where } b: \text{batch number}, N_b: \text{No. of batches} \qquad (39)$$

Numerical Results

Real standard deviation of the 2D pin power

– **At cycle 10**

Cycle 10	MC-CMFD	iDTMC
Avg.	0.019	0.009



MC-CMFD **iDTMC**

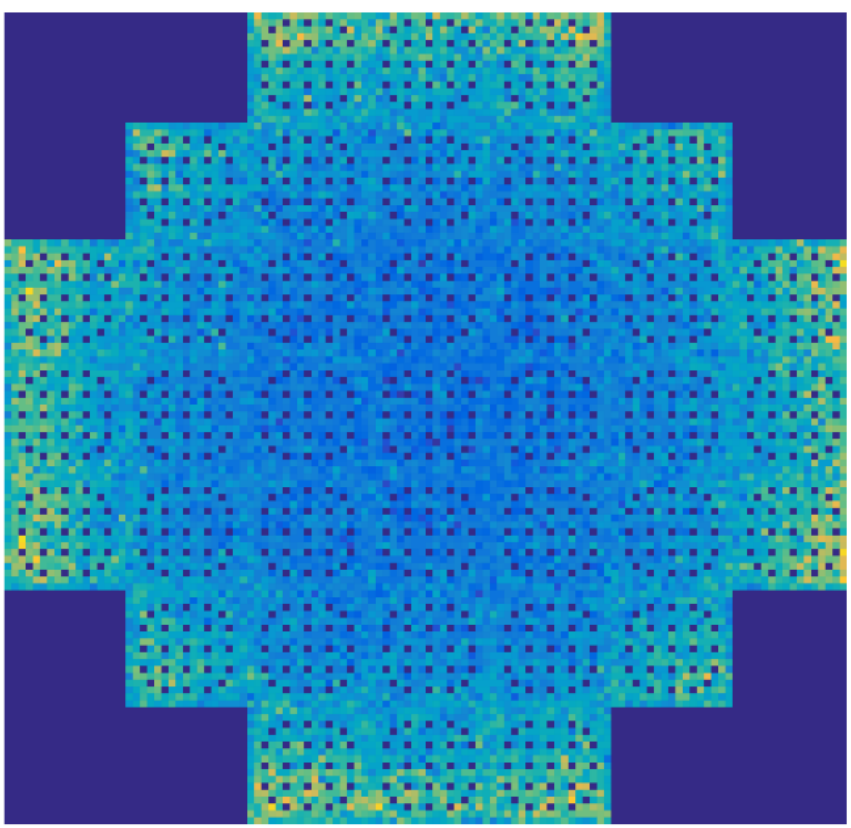
$$\sigma_{i,j} = \frac{1}{N_b}\sum_{b}^{N_b}(p_{i,j}^{b} - \bar{p}_{i,j})^2 \quad \text{where } b: \text{batch number, } N_b: \text{No. of batches} \qquad (40)$$

Numerical Results

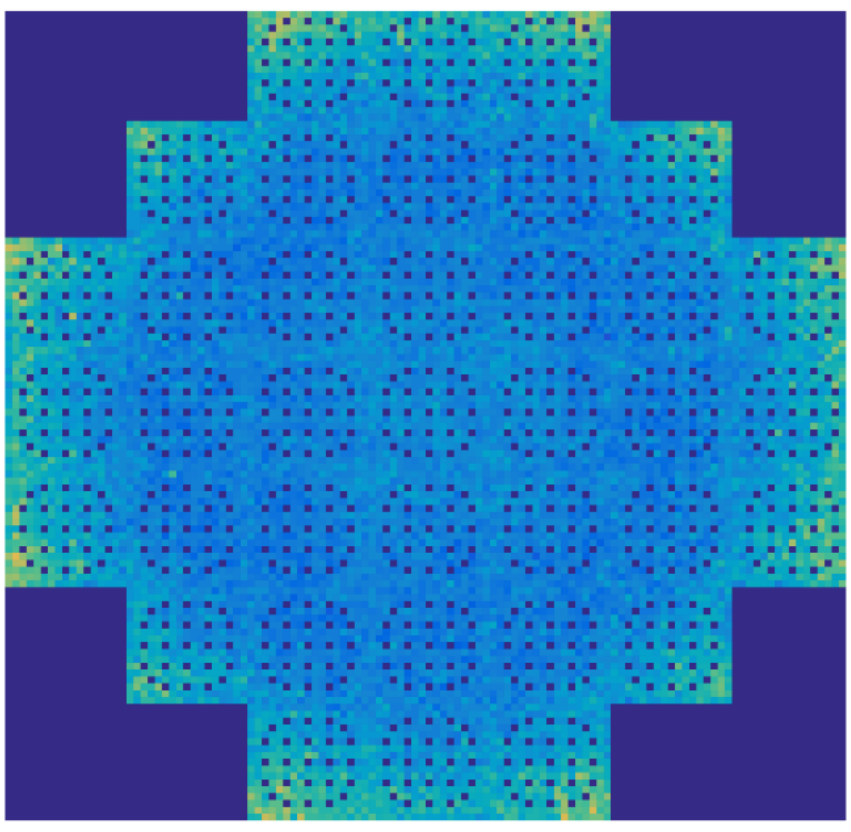
Real standard deviation of the 2D pin power

– **At cycle 10**

Cycle 10	iDTMC	Direct
Avg.	0.009	0.009



iDTMC



Parameter sampling

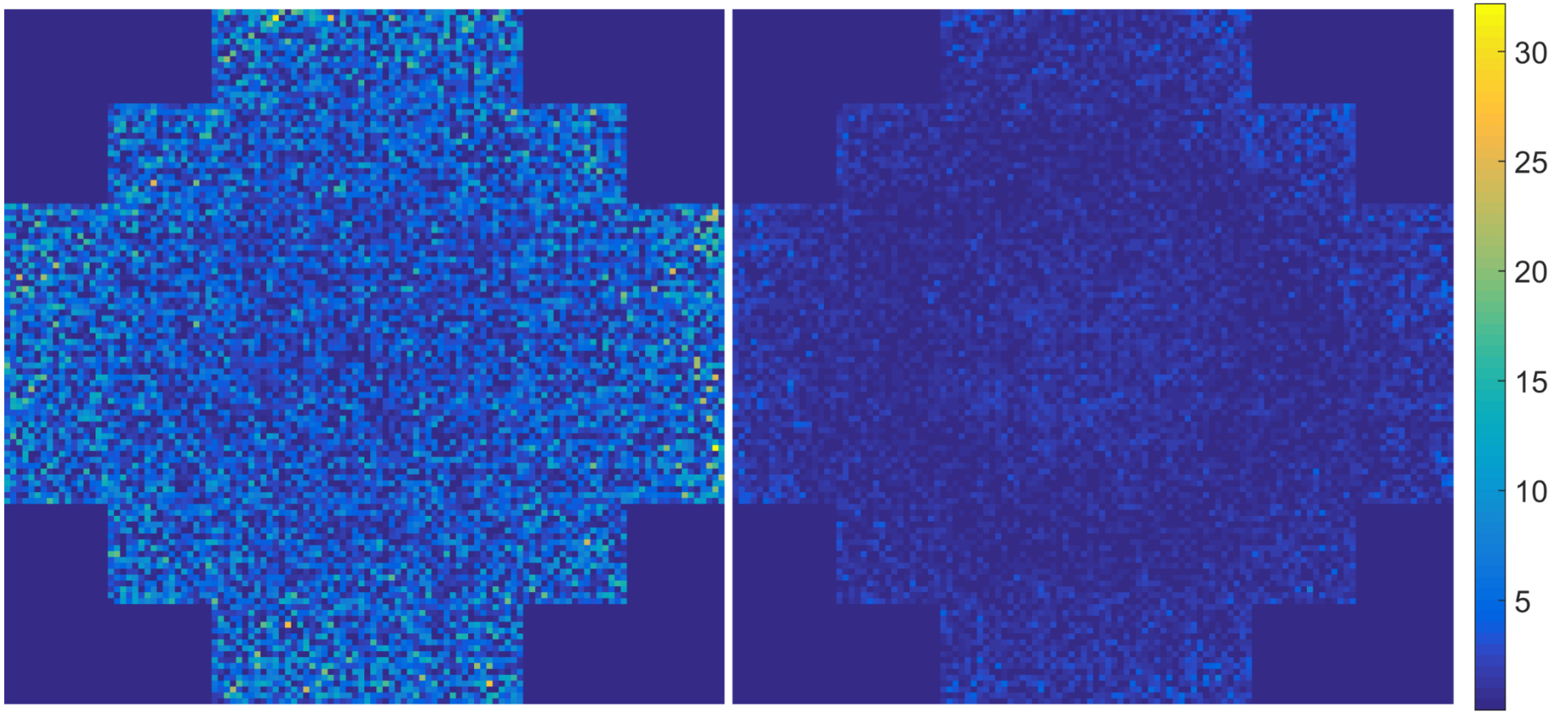
$$\sigma_{i,j} = \frac{1}{N_b}\sum_{b}^{N_b}(p_{i,j}^{b} - \bar{p}_{i,j})^2 \quad \text{where } b: \text{batch number}, N_b: \text{No. of batches} \qquad (40)$$

Numerical Results

Relative error distribution for the 2D pin power

– **At cycle 1**

Error (%)	MC-CMFD	iDTMC
Avg.	3.2	0.8
Max.	32.2	7.5



MC-CMFD **iDTMC**

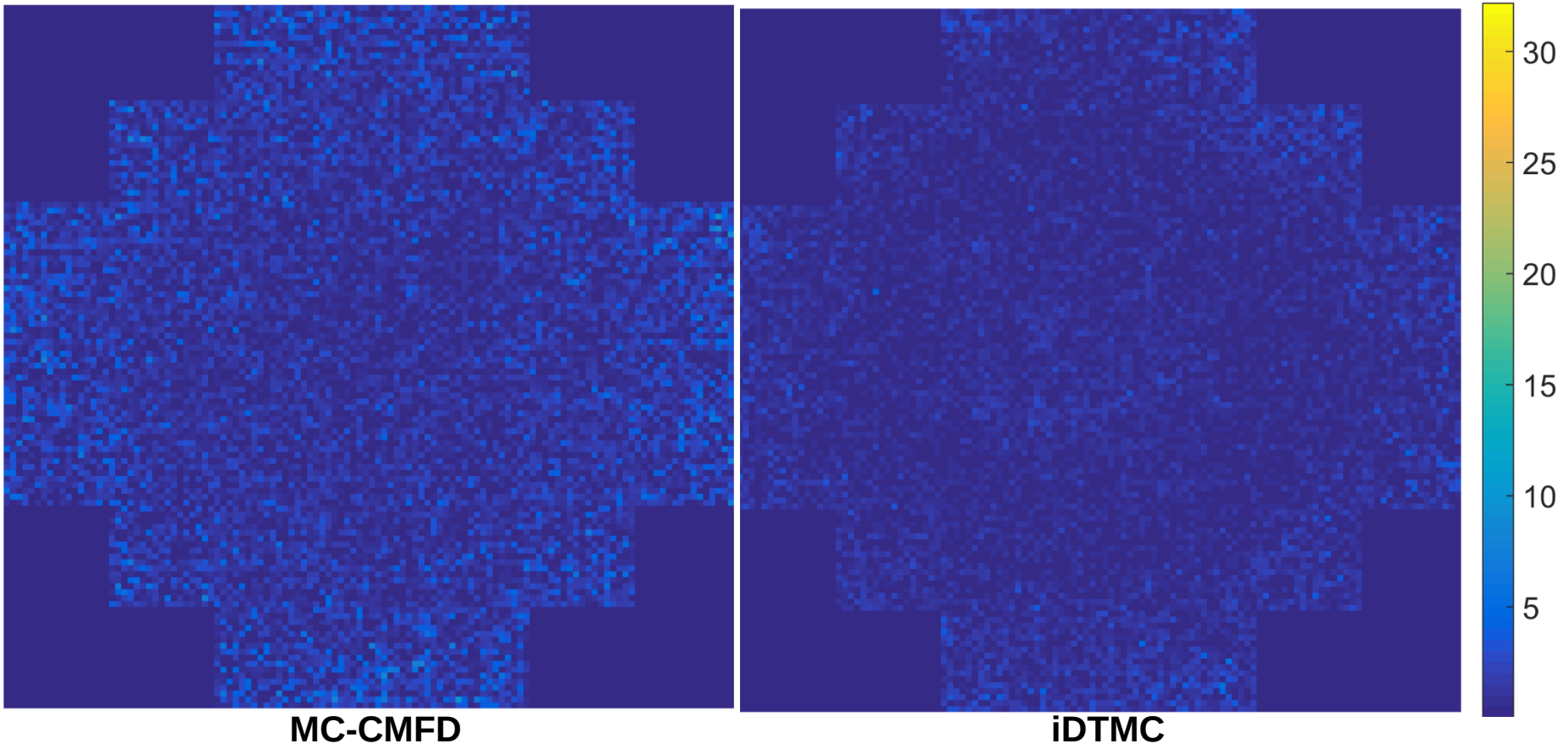
$$\varepsilon_{i,j} = \left| \frac{p_{i,j} - p^*_{i,j}}{p^*_{i,j}} \right| \times 100\ (\%) \qquad \text{where } p^* \text{ : reference pin power} \qquad (41)$$

Numerical Results

Relative error distribution for the 2D pin power

– **At cycle 10**

Error (%)	MC-CMFD	iDTMC
Avg.	1.0	0.6
Max.	9.6	5.6



$$\varepsilon_{i,j} = \left| \frac{p_{i,j} - p^*_{i,j}}{p^*_{i,j}} \right| \times 100\ (\%) \qquad \text{where } p^* \text{ : reference pin power} \qquad (42)$$

Numerical Results

Computing time

– **Deterministic calculation**

Methods	p-CMFD	p-FMFD	
		w/o one-node p-CMFD	w/ one-node p-CMFD
Time (sec.)	0.03	97.9	1.4

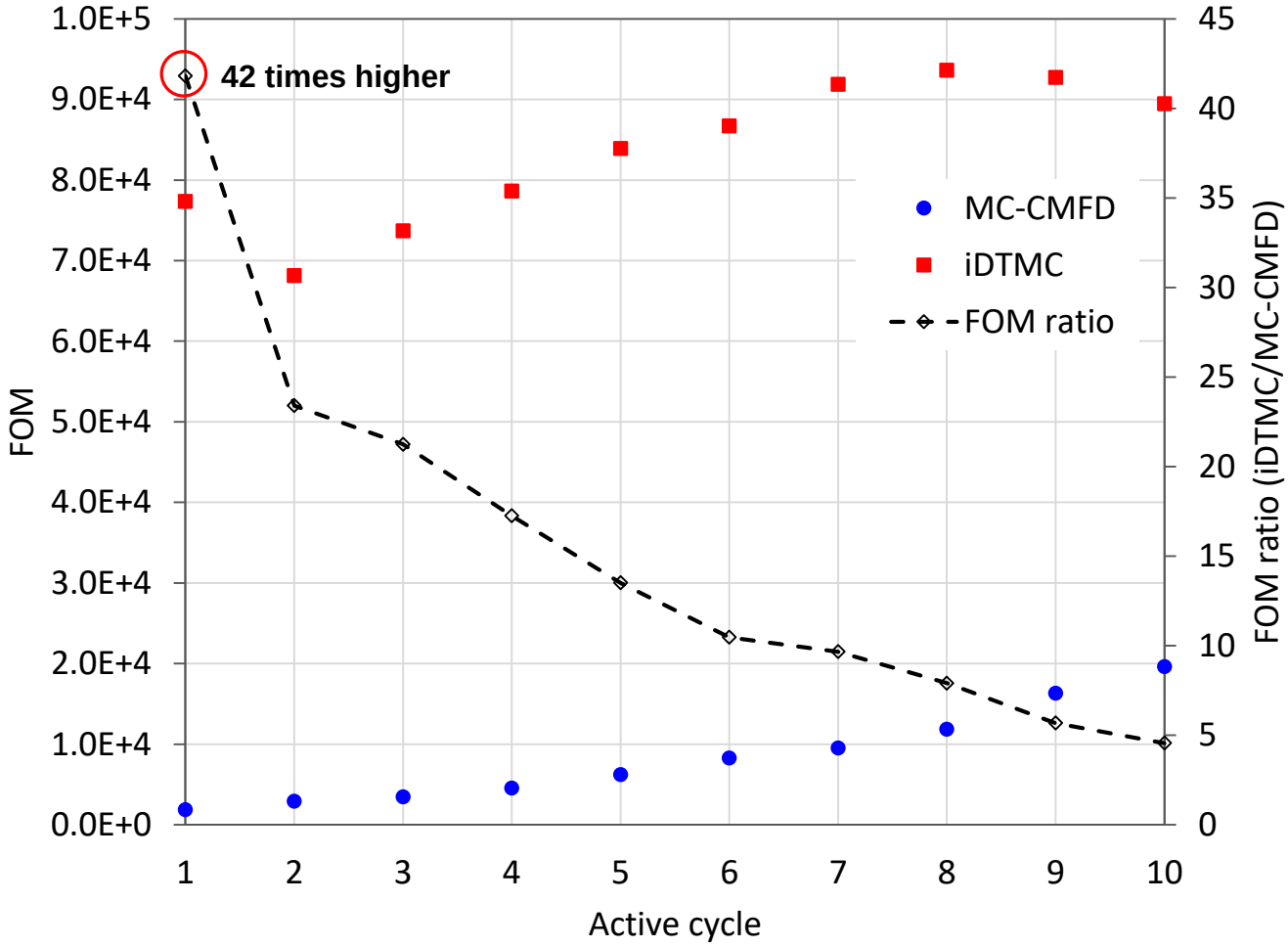
– **MC calculation**

	Standard MC	MC-CMFD	iDTMC
No. of inactive cycles	81	23.1	23.1
No. of active cycles	10	10	10
Inactive time (hr.)	1.2	0.7	0.8
Active time (hr.)	0.29	0.29	0.51
Total time (hr.)	1.47	0.95	1.29

+ p-FMFD for solution prediction
Variance estimation

Numerical Results

FOM for the multiplication factor

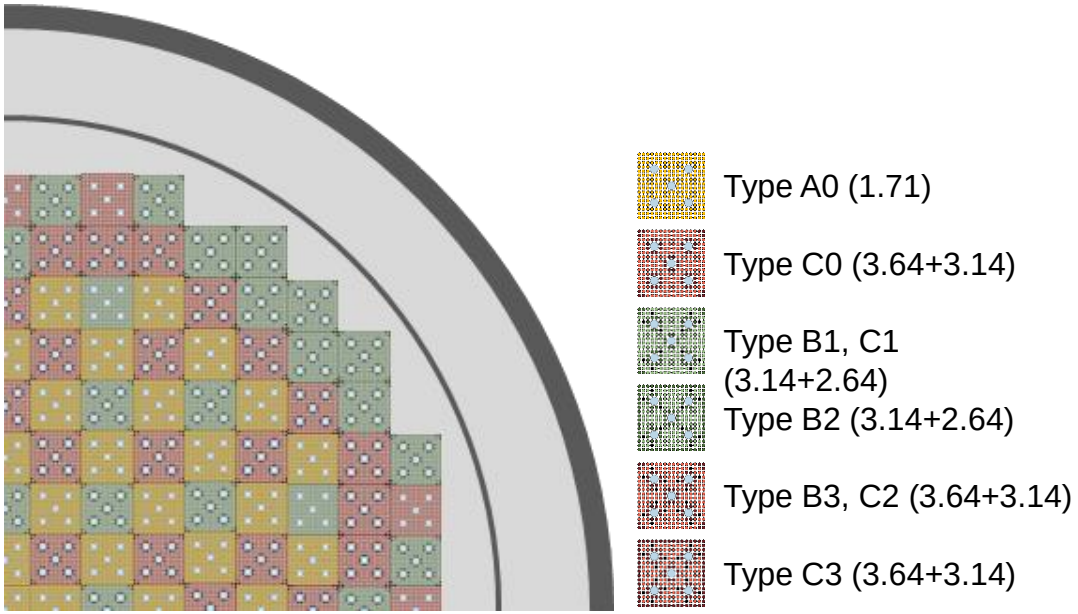


$$FOM = \frac{1}{\sigma^2 T} \quad \text{where } T \text{ : time (sec), } \sigma^2 \text{ : variance}$$

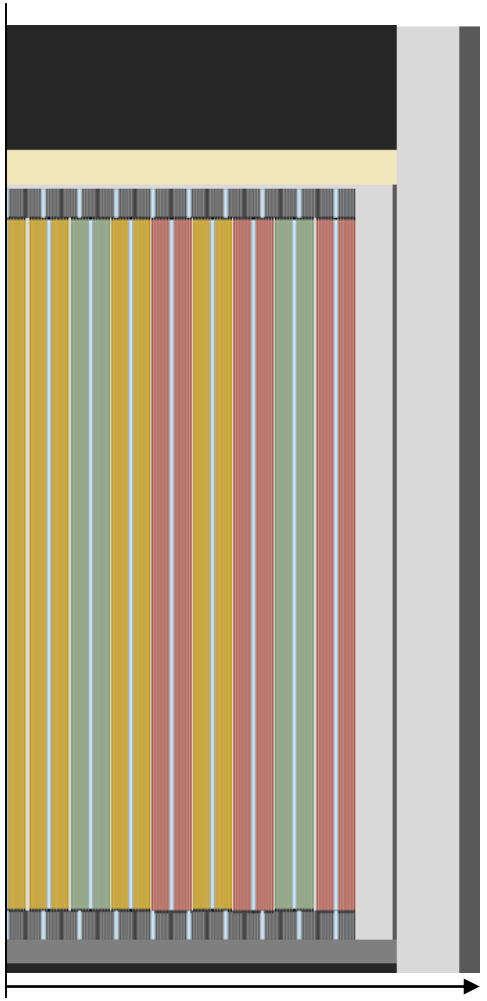
Numerical Results

APR1400 quarter core problem

- 1st cycle fuel loading pattern
- 241 fuel assemblies
- Fuel zoning & Bas are modelled



Radial configuration



Axial configuration

Numerical Results

Calculation condition

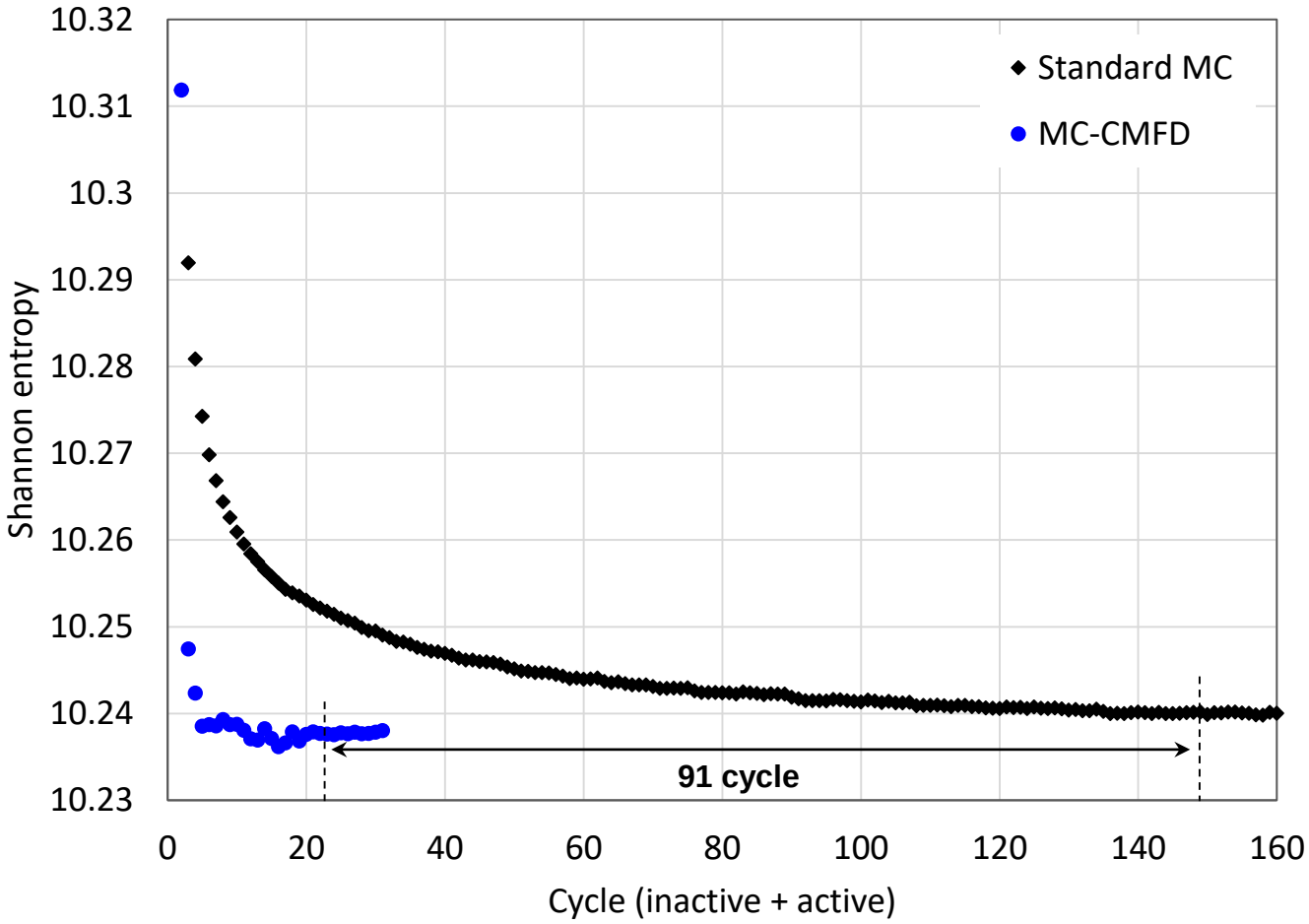
- Total **112 cores** of Xeon E5-2697 with clock speed of **2.60 GHz**
- Skip p-CMFD : 1
- Skip early cycles : 5
- According to the SCI
  - Minimum generation size = 6,000,000 histories per cycle

Total number of fine nodes		*No. of neutrons*		*Off-peaking*				*Optimum generation size*
586,112	×	5.86	/	0.2	=	17,173,081	≅	20,000,000

  - The number of inactive cycles were automatically determined
- 10 active cycles were used
- For real standard deviation, 30 independent runs simulated with different random seeds
- **Reference solution** : 1.20392 ± 0.82 pcm
  - No. of histories : 10,000,000
  - No. of inactive cycles 60
  - No. of active cycles : 300
  - No. of batches : 4

Numerical Results

FSD convergence behavior



Much faster source convergence is achieved in the big size reactor problem which has a higher dominance ratio compared to the standard MC

Numerical Results

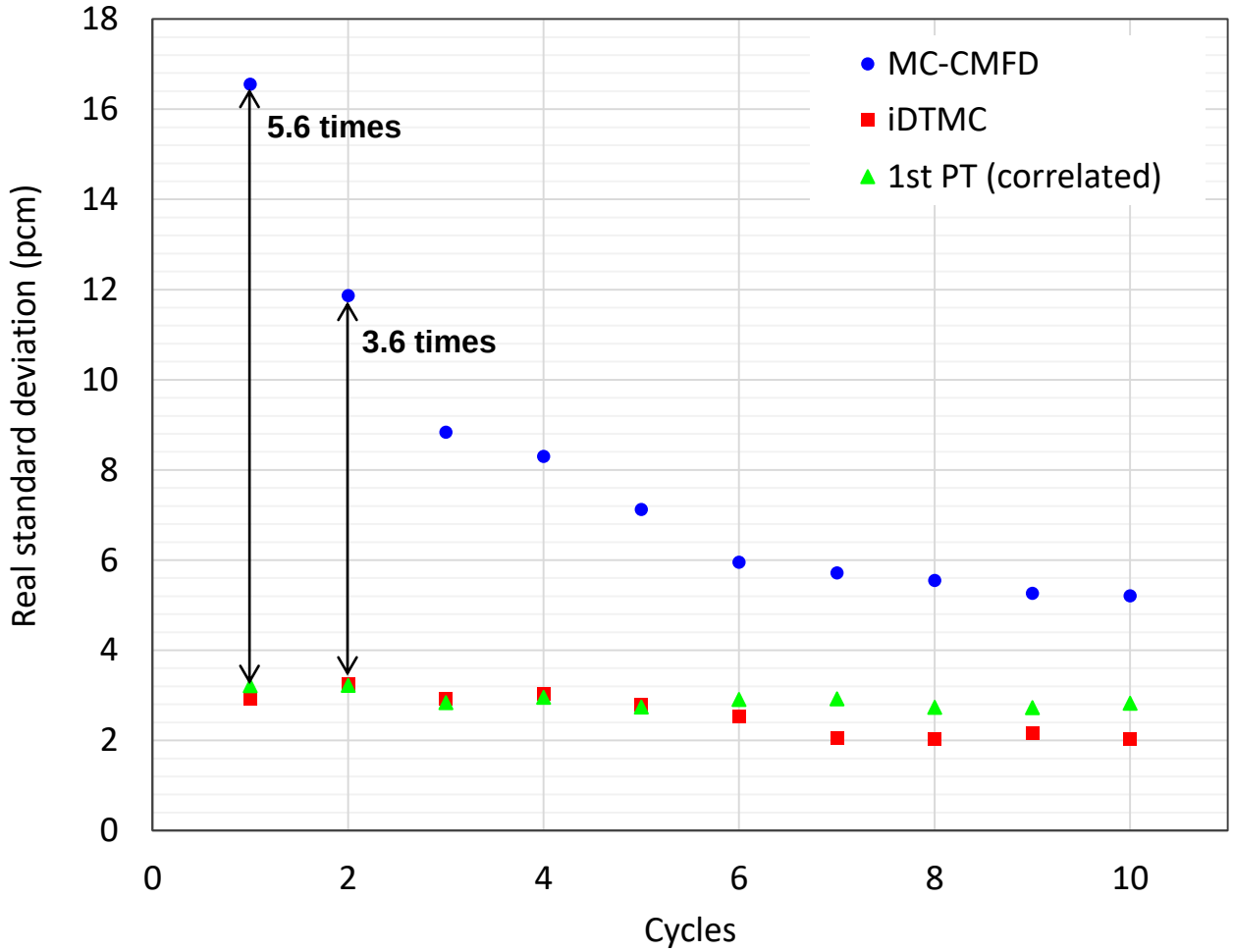
Multiplication factor & stochastic errors

Parameter		Cycle				
		1	3	10	15	20
MC-CMFD	k_{eff}	1.20390	1.20392	1.20391	1.20394	1.20390
	σ_a	-	10.8	10.0	6.5	-
	σ_r	16.6	8.8	7.1	5.2	16.6
iDTMC	k_{eff}	1.20392	1.20392	1.20389	1.20391	1.20392
	σ_a	-	0.4	0.4	0.4	-
	σ_r	2.9	2.9	2.8	2.0	2.9
	1^{st} PT	3.2	2.8	2.7	2.8	3.2

* $k_{eff}^{ref} = 1.20392 \pm 0.82$ pcm

Numerical Results

Real standard deviation of the multiplication factor



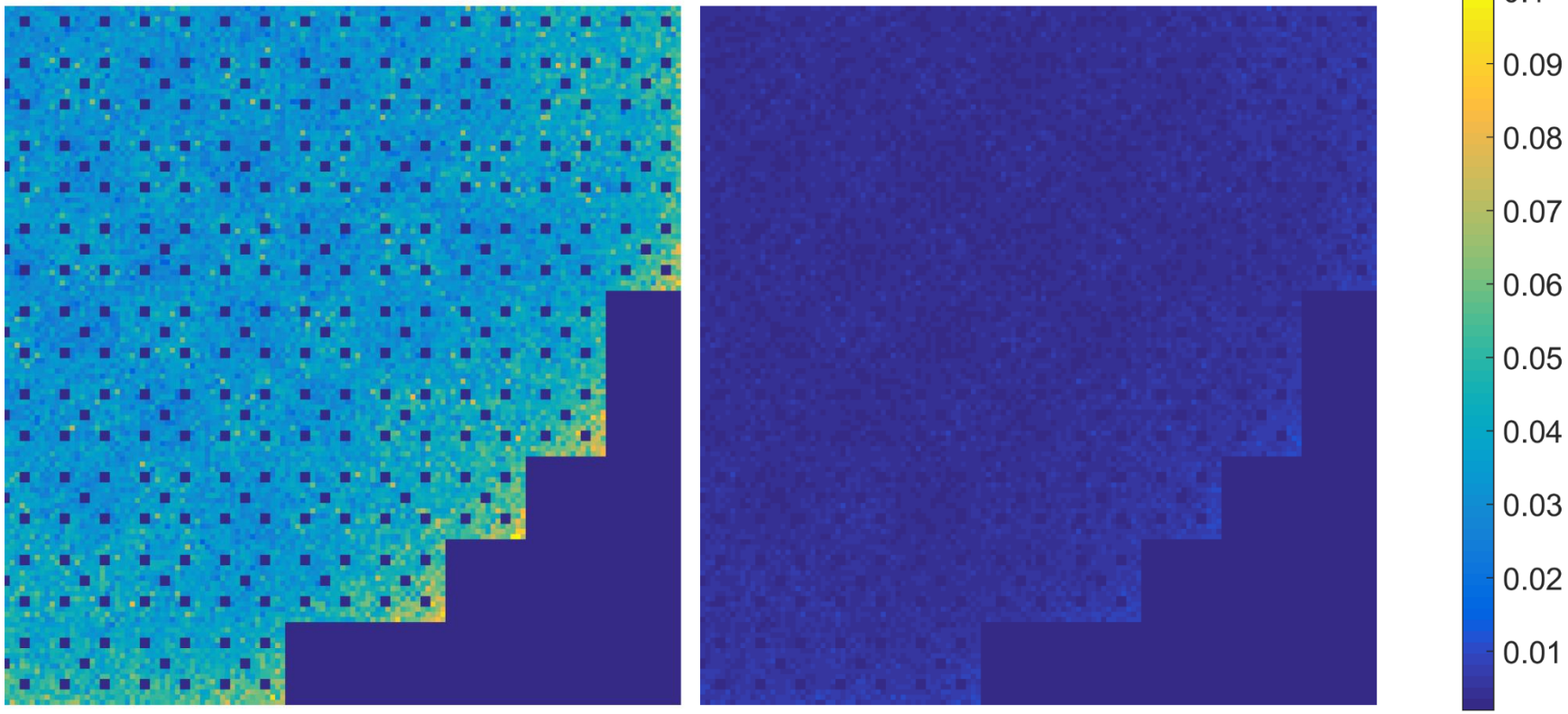
Much more reliable solutions are obtained with the iDTMC method compared to the CMFD
Consistent results are shown in the different types of the problem

Numerical Results

Real standard deviation of the 2D pin power

– **At cycle 1**

Cycle 1	MC-CMFD	iDTMC
Avg.	0.037	0.0048



MC-CMFD **iDTMC**

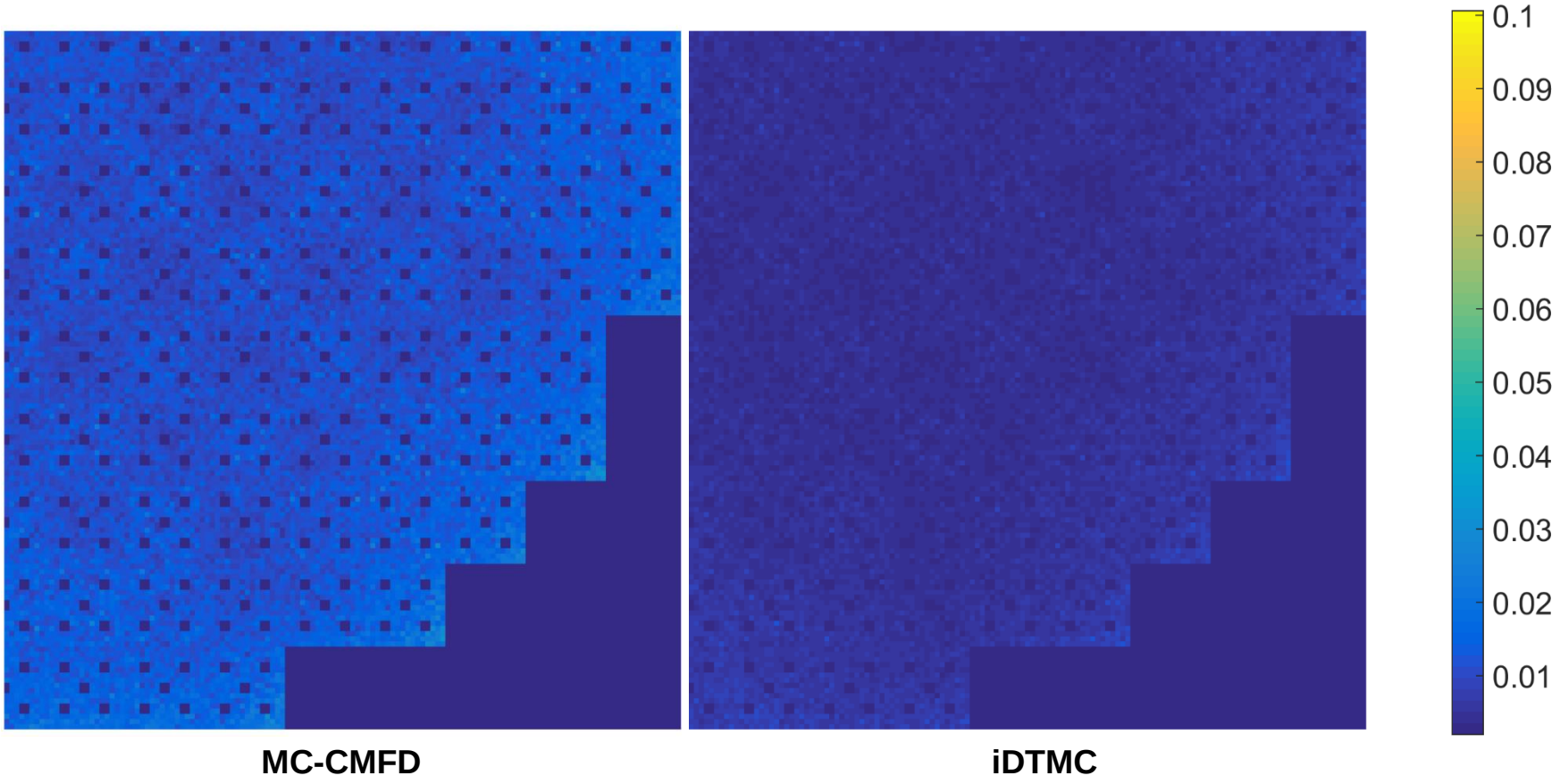
$$\sigma_{i,j} = \frac{1}{N_b}\sum_{b}^{N_b}(p_{i,j}^{b} - \bar{p}_{i,j})^2 \quad \text{where } b: \text{batch number}, N_b: \text{No. of batches} \qquad (44)$$

Numerical Results

Real standard deviation of the 2D pin power

– **At cycle 10**

Cycle 10	MC-CMFD	iDTMC
Avg.	0.013	0.005



MC-CMFD **iDTMC**

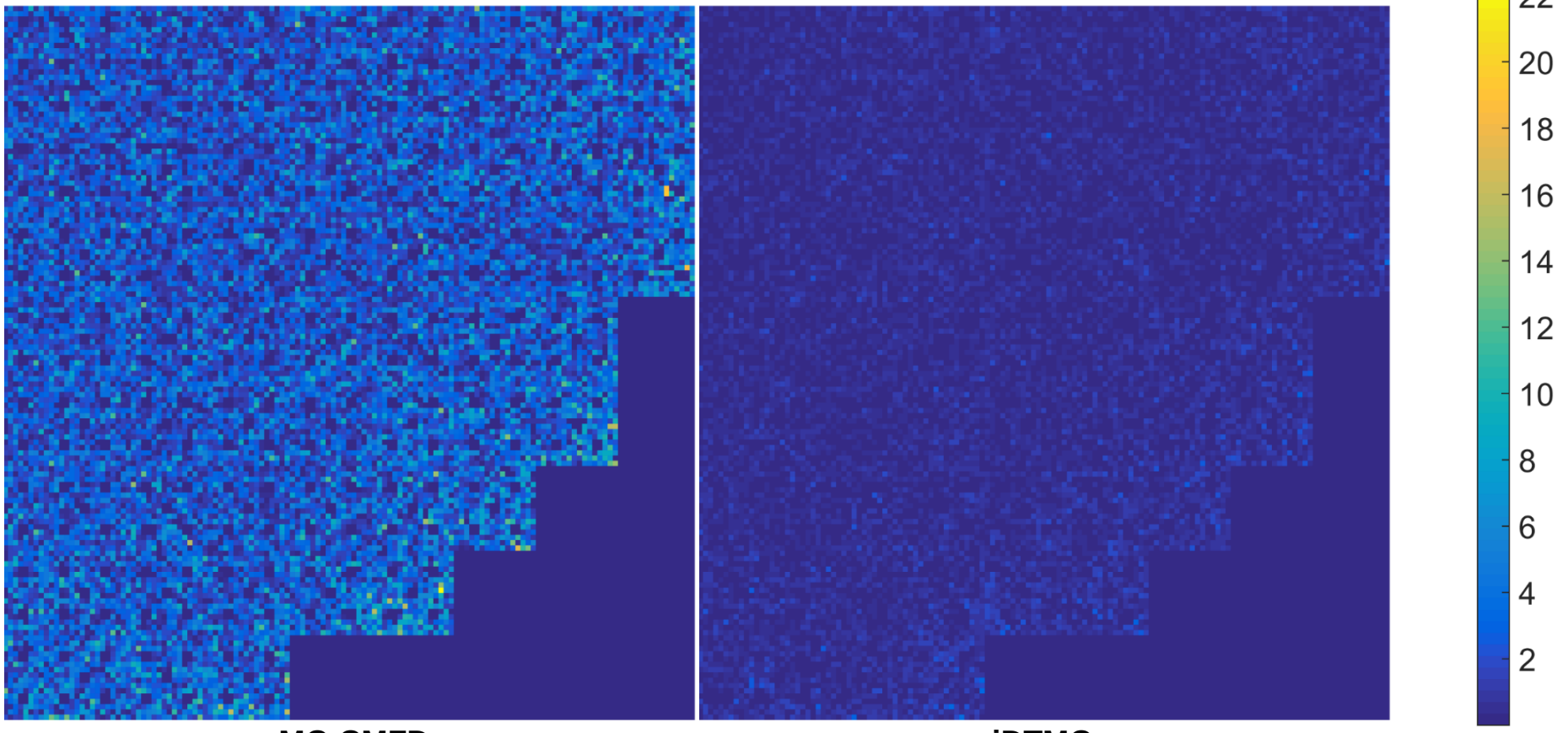
$$\sigma_{i,j} = \frac{1}{N_b}\sum_{b}^{N_b}(p_{i,j}^{b} - \bar{p}_{i,j})^2 \quad \text{where } b: \text{batch number, } N_b: \text{No. of batches} \qquad (45)$$

Numerical Results

Relative error distribution for the 2D pin power

– **At cycle 1**

Error (%)	MC-CMFD	iDTMC
Avg.	2.3	0.42
Max.	22.3	3.8



MC-CMFD **iDTMC**

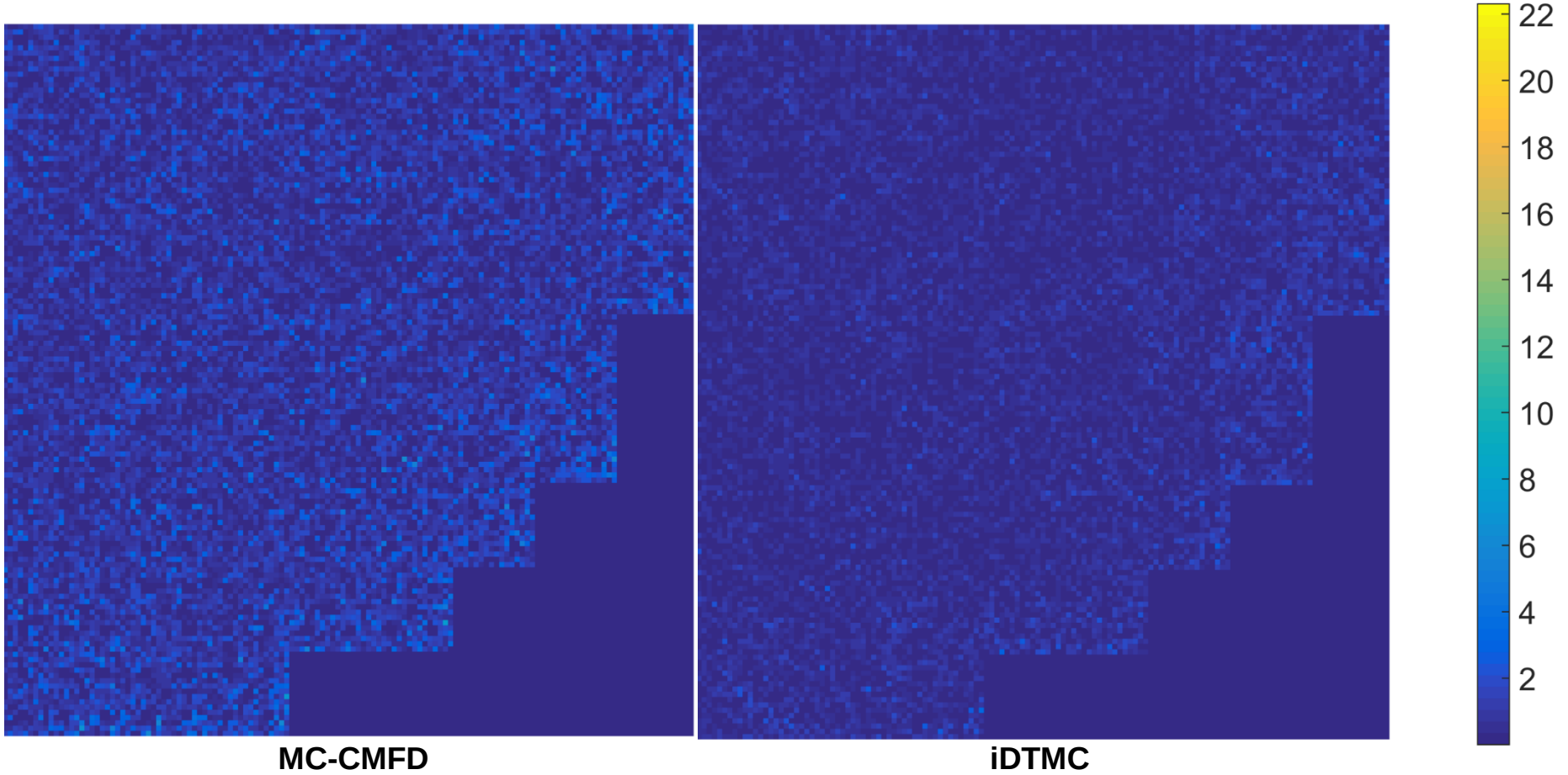
$$\varepsilon_{i,j} = \left| \frac{p_{i,j} - p^*_{i,j}}{p^*_{i,j}} \right| \times 100\ (\%) \qquad \text{where } p^* \text{ : reference pin power} \qquad (46)$$

Numerical Results

Relative error distribution for the 2D pin power

– **At cycle 10**

Error (%)	MC-CMFD	iDTMC
Avg.	0.8	0.4
Max.	7.5	3.5



MC-CMFD **iDTMC**

$$\varepsilon_{i,j} = \left| \frac{p_{i,j} - p^*_{i,j}}{p^*_{i,j}} \right| \times 100\ (\%) \qquad \text{where } p^* \text{ : reference pin power} \qquad (47)$$

Numerical Results

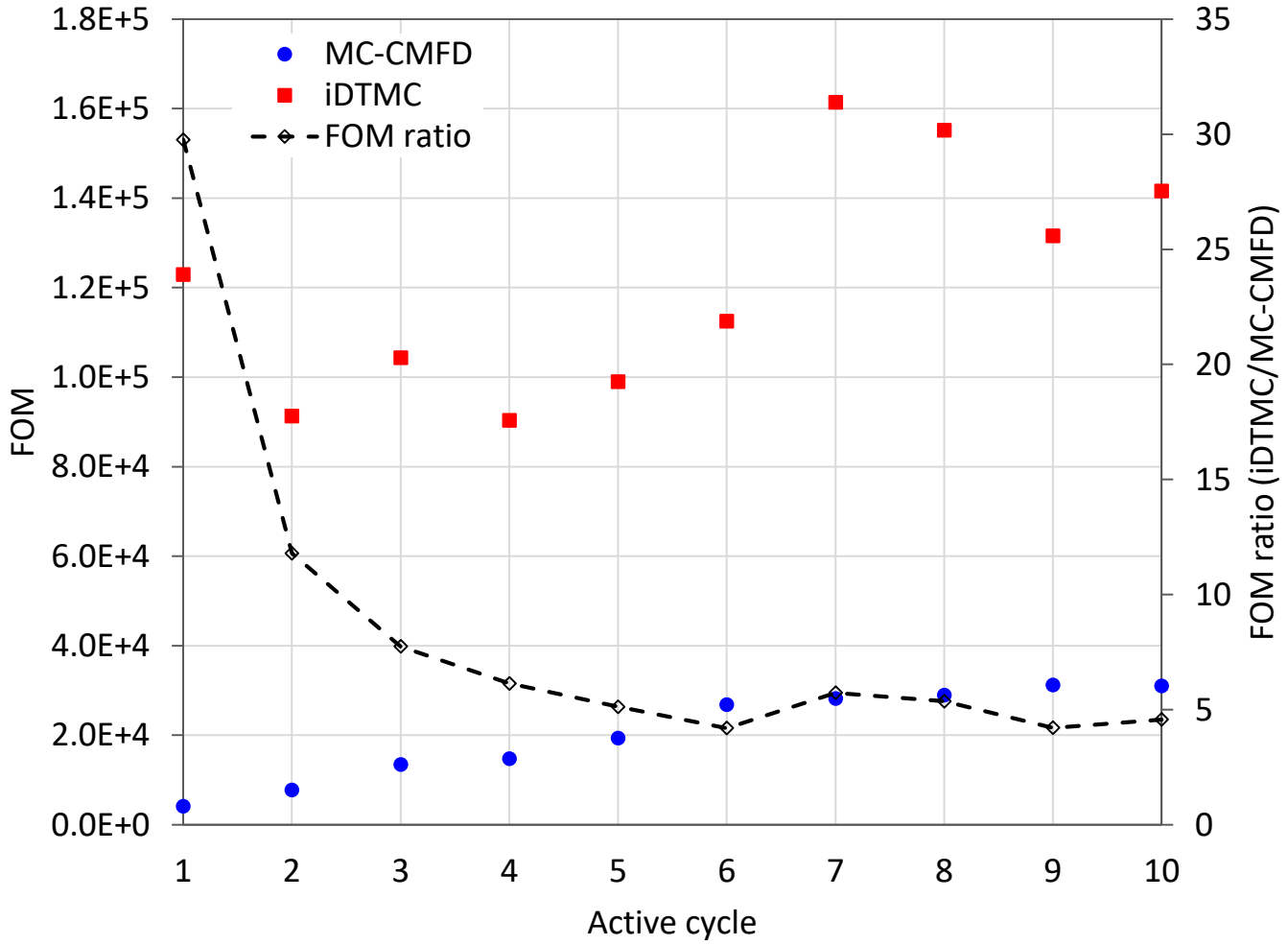
Computing time

– **MC calculation**

	Standard MC	MC-CMFD	iDTMC
No. of inactive cycles	160	24.4	25.5
No. of active cycles	10	10	10
Inactive time (hr.)	14.0	2.4	2.4
Active time (hr.)	0.9	0.9	1.0
Total time (hr.)	15.0	3.3	3.4

Numerical Results

FOM for the multiplication factor



Much higher numerical performance is achieved
with the iDTMC method over 5 to 30 times higher

Conclusions

Conclusions

– **The iDTMC method has been developed for efficient neutornic reactor analysis**

- Potential bias and numerical instability disappear.
- The convergence of the FSD is accelerated and thus the computing time is reduced.
- The stochastic uncertainty is decreased even from the beginning of the active cycle.
- The stochastic error can be reasonably measured by parameter sampling scheme.
- The numerical performance is enhanced by the comparison of the conventional CMFD-assisted MC method.

Future work

– Various applications

- Burn up calculation
- Multi-physics calculation
- Fast reactor analysis

Thank you for your attention