### A Study on Optimization of Albedo Boundary Conditions for the Deterministic Truncation of Monte Carlo Solutions



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## Outline

#### I. Introduction

#### **II. Methods**

- Deterministic truncation of MC solution
- Weight adjustment method
- Vacuum boundary condition with irregular nodes

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- C5G7 benchmark problem
- Multiplication factor
- Pin-wise power distribution
- Computing time
- **IV. Concluding Remarks**



#### Monte Carlo (MC) calculation in a reactor criticality analysis

 A stochastic method to solve a statistical problem finding out the average behavior of the unknown parameters

Pros	Cons
<ul> <li>High accuracy</li> <li>Direct simulation of particles' whole behavior</li> <li>No discretization of variables (energy, angle, space)</li> <li>No constraints on geometry construction</li> <li>Simple parallel calculation</li> </ul>	<ul> <li>Computationally expensive</li> <li>Large memory to describe explicit geometry and to utilize cross section data</li> <li>Long time to track all particles and to get quantities of interest</li> <li>Ever after source convergence, it is important to simulate many particles in active cycles to reduce stochastic uncertainty</li> </ul>

- Several studies have been conducted to accelerate the calculation speed and to reduce stochastic uncertainties more efficiently
  - Diffusion based coarse mesh finite difference (CMFD) method
  - Modified power method
  - Particle ramp-up method



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#### **Coarse mesh finite difference (CMFD) method**

- Acceleration scheme commonly used in a MC eigenvalue problem
- **Preservation of net current and reaction rate** by high fidelity solution (i.e. MC)
- Fast convergence of the fission source distribution (FSD)
  - Shorten the number of inactive cycles and the corresponding computing time
- Weak inter-cycle correlation





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#### **Difference between MC and deterministic methods**

- When solving the neutron transport eigenvalue problem
  - Deterministic calculation : The calculation is finished as soon as FSD converges
  - MC calculation : The main calculation is activated in active cycle when FSD converges
  - MC calculation takes much longer computing time in active cycle than inactive cycle



- Calculation process

• If the FSD truly converges in the inactive MC cycle,

the reactor parameters should be already determined at the end of the inactive cycle



#### **CMFD** solution in MC simulation

- The CMFD method enables a fast convergence of the FSD
- Solution can be truncated from the original MC solution in a systematic / deterministic way
- Combination of the flexible and versatile MC method and the efficient deterministic analysis
  - No limitation in geometry modeling
  - Continuous energy
  - Numerically cheap computation





#### **Concept of deterministic truncation of MC solution (DTMC) method**



- The next FSD in MC simulation is corrected by the CMFD solution
- The deterministic result is a subset of the solution to the original MC approach

#### **Deterministic truncation of MC solution (DTMC) method**

#### - Solving a standard eigenvalue problem

- **Eigenvalue** :  $k_{eff}$
- **Eigenvector** : power distribution
- Generalized equivalence theory confirms that the CMFD solution is equivalent to MC ones

#### - Fine mesh CMFD grid to obtain a detailed pin power profile

- Radial node size : pin (1-2 cm)
- Axial node size : 5-10 cm

#### Characteristics

- Boundary for CMFD domain is confined to the active core where the particle flux is high to get reliable CMFD parameters in pin-sized grid system
- Inter-cycle correlation can be higher in the DTMC method; thus, a minimum of 2 cycles is accumulated to generate the CMFD parameters
- The CMFD solution only retains the uncertainties originating from the CMFD parameters, and is free from the stochastic random process

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#### **Problem description**

- Solved by in-house MC code
- C5G7 rodded A type benchmark problem
- 10-30 inactive cycles, 100 active cycles, 1.0M histories, 60 batches
- Pin-size CMFD mesh
- Reference solution (100 active cycles & 14.0M histories)





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#### **Multiplication factor**

Active cycle	Parameter	MC	CMFD	DTMC	p-CMFD	pDTMC
	$k_{ m eff}$	1.12867	1.12845	1.12821	1.12830	1.12816
1	$\sigma_a$ (pcm)	-	-	-	-	-
	$\sigma_r$ (pcm)	85.7	83.3	43.1	70.5	45.1
	$k_{ m eff}$	1.12783	1.12834	1.12826	1.12766	1.12776
5	$\sigma_a$ (pcm)	39.2	39.9	22.1	40.6	17.2
	$\sigma_r$ (pcm)	53.0	53.6	29.5	44.3	28.7
	$k_{ m eff}$	1.12787	1.12826	1.12842	1.12811	1.12792
10	$\sigma_a$ (pcm)	30.2	31.3	17.1	30.3	13.7
	$\sigma_r$ (pcm)	40.1	37.8	23.0	33.4	21.6
	$k_{ m eff}$	1.12810	1.12807	1.12824	1.12803	1.12807
20	$\sigma_a$ (pcm)	21.9	23.3	12.4	22.4	10.2
	$\sigma_r$ (pcm)	25.7	27.7	16.9	23.7	14.7
100	$k_{ m eff}$	1.12819	1.12811	1.12818	1.12817	1.12812
	$\sigma_a$ (pcm)	10.2	11.0	5.9	10.4	4.7
	σ <sub>r</sub> (pcm)	12.2	12.7	7.0	11.4	7.4

MC : standard MC results CMFD & p-CMFD : MC results with CMFD & p-CMFD DTMC & p-CMFD : Deterministic results with CMFD & p-CMFD  $k_{ref}$  (reference) = 1.12808 ± 1.7 pcm  $\sigma_a$ : apparent standard deviation  $\sigma_r$ : real standard deviation

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#### Cumulative real standard deviation of $k_{eff}$





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#### **Pin-wise power profile**

- Axially integrated 2D distribution





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#### **Errors of 3D pin-wise power distribution**

Cycle	Value	MC	CMFD	DTMC	p-CMFD	pDTMC
	$\sigma_{a}$	-	-	-	-	-
	$\sigma_{\rm r}$	0.038	0.038	0.034	0.038	0.034
1	RMS (%)	4.20	4.22	3.77	4.23	3.74
	$\epsilon_{\rm avg}$ (%)	3.44	3.46	3.09	3.47	3.07
	$\sigma_{a}$	0.021	0.021	0.014	0.021	0.014
5	$\sigma_{\rm r}$	0.022	0.022	0.021	0.022	0.021
3	RMS (%)	2.46	2.47	2.37	2.47	2.37
	$\epsilon_{avg}$ (%)	2.01	2.03	1.95	2.03	1.94
	$\sigma_{a}$	0.016	0.016	0.011	0.016	0.011
10	$\sigma_{r}$	0.016	0.016	0.016	0.016	0.016
10	RMS (%)	1.828	1.828	1.781	1.831	1.785
	$\epsilon_{\rm avg}$ (%)	1.497	1.501	1.463	1.504	1.466
	$\sigma_{a}$	0.0114	0.0115	0.0084	0.0115	0.0081
20	$\sigma_{\rm r}$	0.0119	0.0119	0.0117	0.0119	0.0117
20	RMS (%)	1.327	1.327	1.303	1.329	1.308
	$\epsilon_{\rm avg}$ (%)	1.085	1.089	1.069	1.094	1.078
	$\sigma_{a}$	0.0053	0.0053	0.0040	0.0053	0.0039
100	$\sigma_{r}$	0.0055	0.0055	0.0054	0.0055	0.0054
100	RMS (%)	0.615	0.616	0.609	0.615	0.609
	$\epsilon_{avg}$ (%)	0.503	0.505	0.500	0.505	0.501

 $\sigma_a$ : apparent standard deviation;  $\sigma_r$ : real standard deviation; RMS : root mean square error;  $\epsilon$ : relative error



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#### **RMS error distribution of pin power**





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## Summary

#### Findings

- The DTMC results showed good agreement with the reference solution
- The DTMC solution has lower stochastic uncertainties than the MC solutions
- The DTMC method can estimate the accurate and reliable solution at the early active cycle
- The DTMC solution of **power distribution** is **not improved as much as**  $k_{\text{eff}}$
- The maximum errors appear in the boundary region for each method

#### Next work

#### **Optimization of the boundary condition for solution improvement**



#### **Boundary condition in DTMC method**

- The CMFD domain is confined to the active core region
- The CMFD parameters near the boundary surface are more unreliable
  - Less particles
  - Simpler correction
  - More sensitive to parameters

**Correction factor in the inner region** 

$$\hat{D} = rac{J^{i+1/2} + \tilde{D}^{i+1/2}(\phi^{i+1} - \phi^{i})}{\phi^{i+1} + \phi^{i}}$$

**Correction factor at the boundary surface** 

Albedo boundary condition :  $\hat{D} = J^{i+1/2} / \phi^i$ 



## **Optimization of the boundary condition**

**1.** Weight adjustment method at the boundary region

**2.** Vacuum boundary condition with irregular nodes



## Methods (1)

#### Weight adjustment method at the boundary region

#### - Particle splitting with cell importance



$$-I_{i+1} > I_i: \qquad w_{i+1} = w_i / n$$
  

$$-I_{i+1} < I_i: \qquad \text{kill with probability } 1 - p = 1 - I_{i+1} / I_i$$
  
Track with  $w_{i+1} = w_i \times I_i / I_{i+1}$  with probability  $p = I_{i+1} / I_i$ 



## Methods (1)

#### Weight adjustment method at the boundary region

- Higher importance at the boundary regions
  - ✤ Radial configuration



#### **Multiplication factor**

Cuala	Cuala Daramatar		IMP = 1		<b>IMP</b> = 2		IMP = 3	
Cycle	Parameter	MC	CMFD	DTMC	CMFD	DTMC	CMFD	DTMC
	$\mathbf{k}_{\mathrm{eff}}$	1.12867	1.12845	1.12821	1.12799	1.12790	1.12734	1.12801
1	$\sigma_a$ (pcm)	64.2	68.5	29.3	78.0	25.7	69.6	30.5
	$\sigma_r$ (pcm)	85.7	83.3	43.1	80.8	47.1	83.7	43.8
	$\mathbf{k}_{\mathrm{eff}}$	1.12783	1.12834	1.12826	1.12793	1.12828	1.12817	1.12802
5	$\sigma_a$ (pcm)	39.2	39.9	22.1	45.8	22.6	43.3	21.9
	$\sigma_r$ (pcm)	53.0	53.6	29.5	48.9	28.6	45.1	23.8
	$\mathbf{k}_{\mathrm{eff}}$	1.12787	1.12826	1.12842	1.12771	1.12813	1.12811	1.12784
10	$\sigma_a$ (pcm)	30.2	31.3	17.1	35.0	17.0	33.0	17.0
	$\sigma_r$ (pcm)	40.1	37.8	23.0	36.1	21.4	33.0	16.2
	k <sub>eff</sub>	1.12810	1.12807	1.12824	1.12798	1.12799	1.12792	1.12788
20	$\sigma_a$ (pcm)	21.9	23.3	12.4	25.0	12.7	24.8	12.6
	$\sigma_r$ (pcm)	25.7	27.7	16.9	25.9	15.7	26.2	13.5
	$\mathbf{k}_{\mathrm{eff}}$	1.12819	1.12811	1.12818	1.12793	1.12802	1.12790	1.12796
100	$\sigma_a$ (pcm)	10.2	11.0	5.9	11.4	5.9	11.3	5.7
	$\sigma_r$ (pcm)	12.2	12.7	7.0	12.4	7.1	11.8	6.9



#### Cumulative real standard deviation for $\mathbf{k}_{\text{eff}}$





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#### **Error of power distribution**

Carala	Demonster	Deveryotan MC		<b>IMP</b> = 1		<b>IMP</b> = 2		IMP = 3	
Cycle	Parameter	MC	CMFD	DTMC	CMFD	DTMC	CMFD	DTMC	
1	RMS (%)	4.20	4.22	3.77	4.07	3.64	3.99	3.57	
1	$\epsilon_{avg}$ (%)	3.44	3.46	3.09	3.02	2.70	2.82	2.53	
5	RMS	2.46	2.47	2.37	2.38	2.28	2.34	2.24	
	$\epsilon_{avg}$	2.01	2.03	1.95	1.78	1.71	1.66	1.60	
	RMS	1.83	1.83	1.78	1.78	1.73	1.75	1.70	
10	$\epsilon_{avg}$	1.50	1.50	1.46	1.33	1.30	1.25	1.21	
20	RMS	1.33	1.33	1.30	1.30	1.27	1.28	1.25	
20	$\epsilon_{avg}$	1.09	1.09	1.07	0.98	0.97	0.92	0.91	
100	RMS	0.62	0.62	0.61	0.63	0.63	0.63	0.62	
100	$\epsilon_{avg}$	0.50	0.51	0.50	0.51	0.50	0.49	0.49	



#### **Relative error distribution (%)**

 $- 1^{st} layer, IMP = 3$ 





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#### **Computing time**

- Computing time was increased to track split neutrons, especially fission neutrons

Parameter	Standard MC	CMFD & DTMC			
	Standard MC	IMP = 1	IMP = 2	IMP = 3	
Computing time (min)	49	58	73	81	

 Higher importance can be applied only in the reflector region to minimize the computing time





## Methods (2)

Vacuum boundary condition with irregular nodes

- CMFD domain is extended to actual boundary surface
- The CMFD parameters in reflector can be more reliable with irregular node





#### **Multiplication factor**

Crale	Donomotor	Standard MC -	Albedo BC		Vacuum BC	
	rarameter	Stanuaru MC -	CMFD	DTMC	CMFD	DTMC
	$k_{ m eff}$	1.12867	1.12845	1.12821	1.12805	1.12827
1	σ <sub>a</sub> (pcm)	-	-	-	-	-
	σ <sub>r</sub> (pcm)	86.8	79.1	38.7	69.0	38.4
	$k_{ m eff}$	1.12783	1.12834	1.12826	1.12895	1.12862
5	σ <sub>a</sub> (pcm)	41.4	41.2	23.0	34.8	17.4
	σ <sub>r</sub> (pcm)	54.7	51.4	26.7	35.7	19.5
	$k_{ m eff}$	1.12787	1.12826	1.12842	1.12824	1.12827
10	σ <sub>a</sub> (pcm)	31.4	31.7	17.0	26.9	13.4
	σ <sub>r</sub> (pcm)	41.7	35.5	22.0	24.1	13.8
	$k_{ m eff}$	1.12810	1.12807	1.12824	1.12842	1.12833
20	σ <sub>a</sub> (pcm)	21.8	23.5	12.3	19.8	9.8
	σ <sub>r</sub> (pcm)	26.6	26.4	15.3	20.8	12.3
	$k_{ m eff}$	1.12819	1.12811	1.12818	1.12824	1.12818
100	$\sigma_a$ (pcm)	10.2	11.1	5.9	9.0	4.8
	$\sigma_r$ (pcm)	12.3	13.5	7.0	9.7	6.2



#### Cumulative real standard deviation for $k_{eff}$





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#### **Power distribution**

Cyclo	Donomotor	Stondard MC	Alb	edo	Vacuum	
Cycle	Parameter	Stanuaru MC	CMFD	DTMC	CMFD	DTMC
1	$\epsilon_{avg}$	0.625	0.633	0.563	0.515	0.460
1	$\epsilon_{max}$	4.610	4.370	4.218	3.479	3.255
5	$\epsilon_{avg}$	0.366	0.372	0.356	0.299	0.287
5	ε <sub>max</sub>	2.817	2.768	2.733	2.200	1.977
	$\epsilon_{avg}$	0.274	0.274	0.267	0.223	0.217
10	ε <sub>max</sub>	2.095	2.237	2.096	1.656	1.563
20	$\epsilon_{avg}$	0.198	0.198	0.194	0.163	0.159
20	ε <sub>max</sub>	1.453	1.489	1.449	1.152	1.156
100	ε <sub>avg</sub>	0.092	0.092	0.091	0.076	0.075
100	ε <sub>max</sub>	0.712	0.687	0.696	0.552	0.538

 $\varepsilon_{avg}$ : average relative error

 $\varepsilon_{\max}$ : maximum relative error



#### **RMS error distribution for power distribution**

- Albedo BC





#### **RMS error distribution for power distribution**

- Vacuum BC



#### **Computing time**

- Computing time was somewhat increased for the CMFD computation

Parameter	Standard MC	Albe	Albedo BC Vacuum		ım BC
	Stanuaru MC	CMFD	DTMC	CMFD	DTMC
Computing time (min)	47	52		55	
$\sigma_{\rm a}$ for $k_{\rm eff}$	10.2	11.0	5.9	9.0	4.8
Figure-of-merit	3.41E+04	2.65E+04	9.21E+04	3.74E+04	1.39E+05

Vacuum boundary condition with weight adjustment method can further improve the solution





## **Concluding Remarks**

#### **Summary & Conclusions**

- Method I : weight adjustment method
- The DTMC solution was improved with the optimization of boundary condition
- The power became more reliable especially near boundary with weight adjustment
- The computing time was increased with the higher cell importance
- Method II : vacuum boundary condition
- The weight adjustment only within the reflector can minimize the computing time
- The stochastic uncertainty and error were noticeably decreased with vacuum BC
- It is expected that the weight adjustment with vacuum BC can further improve the solution



## **Concluding Remarks**

#### **Future work**

- Vacuum BC & weight adjustment in the reflector region
- Application n big size reactor problem







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## **Thank you** for your attention

# **Backup Slides**

## CMFD method (1/4)

#### **Basic theory of CMFD method**

- The balance equation by integrating the diffusion equation over a node

$$J^{i+1/2} - J^{i-1/2} + \Sigma_a^i \phi^i = S^i$$
 (1)

where

- J : net current
- $\phi$  : neutron flux
- $\Sigma_a$ : absorption cross section
- S : fission source
- The net neutron flow within the node is preserved by reference net current

$$J^{i+1/2} = -\tilde{D}^{i+1/2}(\phi^{i+1} - \phi^{i}) + \hat{D}^{i+1/2}(\phi^{i+1} + \phi^{i})$$
(2)

where

$$\tilde{D} = \frac{2d^{i+1}d^i}{d^{i+1} + d^i}$$
: effective diffusion coefficient  
$$d = D / \Delta x$$
: unit diffusion coefficient

- The correction factor is calculated by

$$\hat{D} = \frac{\vec{J}_{MC}^{i+1/2} + \tilde{D}^{i+1/2}(\phi_{MC}^{i+1} - \phi_{MC}^{i})}{\phi_{MC}^{i+1} + \phi_{MC}^{i}}$$
(3)



## CMFD method (2/4)

#### **Basic theory of p-CMFD method**

- The balance equation by integrating the diffusion equation over a node

$$J^{i+1/2} - J^{i-1/2} + \Sigma^{i}_{a} \phi^{i} = S^{i}$$
<sup>(1)</sup>

- The net neutron flow within the node is preserved by reference two partial currents

$$J^{+,i+1/2} = -0.5\tilde{D}^{i+1/2}(\phi^{i+1/2} - \phi^{i}) + \hat{D}^{+,i+1/2}\phi^{i}$$
(4.a)

$$J^{-,i+1/2} = +0.5\tilde{D}^{i+1/2}(\phi^{i+1/2} - \phi^{i}) + \hat{D}^{-,i+1/2}\phi^{i+1}$$
(4.b)

- The correction factors are calculated by

$$\hat{D}^{+,i+1/2} = \frac{\vec{J}_{MC}^{+,i+1/2} + 0.5\tilde{D}^{i+1/2}(\phi_{MC}^{i+1} - \phi_{MC}^{i})}{\phi_{MC}^{i}}$$
(5.a)  
$$\hat{D}^{-,i+1/2} = \frac{\vec{J}_{MC}^{-,i+1/2} - 0.5\tilde{D}^{i+1/2}(\phi_{MC}^{i+1} - \phi_{MC}^{i})}{\phi_{MC}^{i+1}}$$
(5.b)



## CMFD method (3/4)

#### **CMFD** parameters

Neutron current

$$\phi = \int \phi(\vec{r}, E) dE dV \tag{6}$$

Neutron flux

$$J^{+} = \int_{\Omega^{+}} \Omega \cdot \varphi(\vec{r}, \Omega, E) d\Omega$$
 (7.a)

$$J^{-} = \int_{\Omega^{-}} \Omega \cdot \varphi(\vec{r}, \Omega, E) d\Omega$$
 (7.b)

- Group constant

$$\Sigma_{\alpha} = \frac{\int \int \Sigma_{\alpha}(\vec{r}, E)\phi(\vec{r}, E)dEdV}{\int \int \phi(\vec{r}, E)dEdV}$$
(8)



## CMFD method (4/4)

#### Numerical treatments for CMFD in MC method

#### Boundary condition

• The correction factor is defined by the ratio of current and flux as in rebalance method

$$\hat{D} = J / \phi \tag{9}$$

#### - Weight adjustment

• Particles' weight is adjusted by the ratio of the fission source probability

$$w_{j}^{'} = w_{j} \times \frac{\nu \Sigma_{f} \phi_{i}^{CMFD} / \sum_{i} \nu \Sigma_{f} \phi_{i}^{CMFD}}{\nu \Sigma_{f} \phi_{j}^{MC} / \sum_{j} \nu \Sigma_{f} \phi_{j}^{MC}}$$
(10)



## **Convergence of FSD**

#### **Shannon entropy with different generation sizes**





## **Simulation Code**

#### **In-house MC code**

- In-house MC code for neutronic analysis
- 3D pin-lattice geometry
- Multi-group energy
- Continuous energy (under development)
- CMFD & p-CMFD acceleration scheme



#### **Real standard deviation distribution of pin power**

- 1<sup>st</sup> layer (near mid-plane)





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#### **Optimal generation size in MC & CMFD calculation**

- Enhances the efficiency of the simulation
- Guarantees the convergence of the calculation





#### Particle ramp-up method (A. L. Lund, P. K. Romano, A. R. Siegel)

- A procedure for accelerating convergence of the source distribution
- Roughly converge using fewer particles per generation and increase the number of particles





#### Algorithm of modified particle ramp-up technique



- $N_0$  : initial number of histories
- i : cycle number
- *e* : Shannon entropy

$$\overline{e}_i^1 = \frac{e_{i-l+1} + \dots + e_i}{l}$$
$$\overline{e}_i^0 = \frac{e_{i-2l+1} + \dots + e_{i-l}}{l}$$

- *l* : accumulation length
- $\Delta N$  : increment of generation size
- j : cycle number before N changes
- $\mathcal{E}_1$  : convergence criterion
- $\varepsilon_2$  : stopping criterion

#### Apparent standard deviation of $k_{\rm eff}$





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#### Cycle-wise multiplication factor with stochastic uncertainty

#### - Standard MC





#### Cycle-wise multiplication factor with stochastic uncertainty







#### Cycle-wise multiplication factor with stochastic uncertainty

#### – DTMC





#### **Cycle-wise multiplication factor with stochastic uncertainty**







#### **Cycle-wise multiplication factor with stochastic uncertainty**

#### – pDTMC





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- Center region; (i,j,k) = (1,2,1)
- Standard MC





- Center region;  $(i_{3}j,k) = (1,2,1)$
- CMFD





Cycle-wise normalized power level at specific cell 1

- Center region;  $(i_{3}j_{1}k) = (1,2,1)$
- DTMC





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- Center region;  $(i_{3}j_{1}k) = (1,2,1)$
- p-CMFD





- Center region;  $(i_{3}j_{1}k) = (1,2,1)$
- pDTMC





- Near boundary region;  $(i_{3}j_{1},k) = (34,34,2)$
- Standard MC





- Near boundary region;  $(i_{,j},k) = (34,34,2)$
- CMFD





- Near boundary region;  $(i_{3}j_{1},k) = (34,34,2)$
- DTMC





- Near boundary region;  $(i_{3}j_{1},k) = (34,34,2)$
- p-CMFD





- Near boundary region;  $(i_{3}j_{1},k) = (34,34,2)$
- pDTMC





#### Computing time and figure-of-merit (FOM) for $k_{eff}$

- The computing time of the MC simulation is estimated with a single core

Method	<b>k</b> <sub>eff</sub>	$\sigma_{a}\left(pcm\right)$	Time (min)	FOM
Reference	1.12808	1.7	1867	3.09E+4
Stand-alone MC	1.12819	9.6	46	3.86E+4
CMFD	1.12813	10.8	<b>7</b> 4	2.62E+4
DTMC	1.12807	5.4	54	1.05E+5
p-CMFD	1.12812	10.7	50	2.76E+4
pDTMC	1.12811	5.0	52	1.22E+5
CRX w/o p-CMFD	1.12822	-	4,708*	-
CRX w/ p-CMFD	1.12822	-	871*	-

\* Indirect estimation

: calculation time is indirectly estimated under the assumption that the parallel efficiency is 60%

#### - CRX : conventional deterministic code

- Whole core 3D transport code based on 2D/1D fusion method
- 32 radial cells per modular fuel pin cell and 36 radial cells per modular reflector pin cell
- 3.57 cm in the axial direction, and 8 azimuthal and 3 polar angles per octant with 50 rays per cell per angle