Monte Carlo Fission Source Convergence Diagnosis by Skewness and Kurtosis Estimation Method for Various Benchmark Problems

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Seung-Ah Yang* and Ho Jin Park

Kyung Hee University

*seunga@khu.ac.kr

몬테칼로 노물리 연구실 경희대학교 KYUNG HEE UNIVERSITY

01 Introduction

- Background
- Previous Study

Background

❑ Determining Inactive Cycles in MC Eigenvalue Calculations

- In a Monte Carlo (MC) eigenvalue transport calculation, so-called "**inactive cycle**" MC runs are performed to provide stationary or fundamental-mode fission source distribution (FSD).
- Fission Source Distributions (FSDs) converge by the Dominance Ratio (DR) which is the convergence rate of an iterative numerical solution. In the nuclear system with a high dominance ratio, MC solutions are very slowly converged.
  - ➢ Difficult to determine whether the FSD iteration has converged or not in a high DR problem.
  - ➢ **Insufficient convergence** of FSDs can result in bias.
- **Accurately determining the number of inactive cycles is crucial to obtaining an unbiased Monte Carlo solution.**

Previous Study

❑ Convergence Diagnosis Methodology

- There are various studies for the convergence criteria in MC eigenvalue calculations.
  - ➢ Ueki's posterior source convergence method [1]
  - ➢ Shim's on-the-fly stopping criterion [2]
  - ➢ Center of Mass method [3]

- Recently, we propose a way in which the skewness and kurtosis can be used to test for convergence criteria in MC eigenvalue calculations [4].
  - ➢ Skewness estimation method (**SEM**)
  - ➢ Kurtosis estimation method (**KEM**)

- In this study, we will test the SEM and KEM analyses to determine the FSD convergence cycle or the number of inactive cycles in MC eigenvalue calculations for various benchmark problems
  - ➢ AGN- 201K [5], 1D Slab Problem [6], and OECD/NEA Slow Convergence Benchmark [7]

02

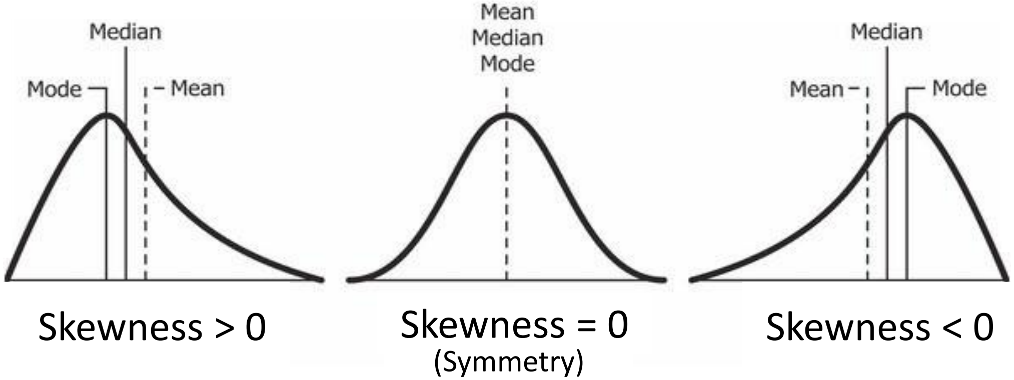
SEM and KEM

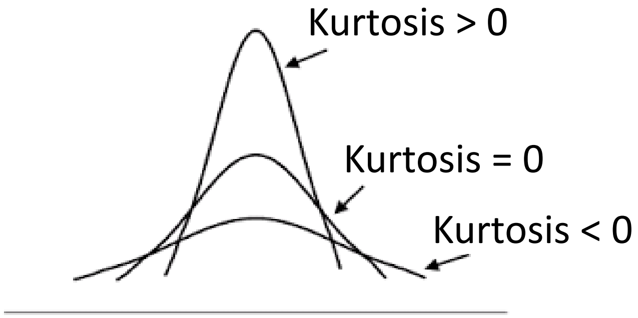
- Skewness and Kurtosis
- Skewness and Kurtosis Estimation Method

Skewness and Kurtosis

❑ What is Skewness and Kurtosis?

- **Skewness** is the measure of the symmetry or distortion from a **normal distribution**.
- **Kurtosis** is the measure of whether the data has outliers, including heavy tails or light tails.





Skewness, g_1

$$g_1 = E\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{E[(X-\mu)^3]}{E[(X-\mu)^2]^{3/2}}$$

Kurtosis, g_2

$$g_2 = E\left[\left(\frac{X-\mu}{\sigma}\right)^4\right] - 3 = \frac{E[(X-\mu)^4]}{E[(X-\mu)^2]^2} - 3$$

Sample Skewness, G_1

$$G_1 = \frac{\sqrt{n(n-1)}}{(n-2)} g_1$$

Sample Kurtosis, G_2

$$G_2 = \frac{n-1}{(n-2)(n-3)}((n+1)g_2 + 6)$$

Skewness and Kurtosis Estimation Method(1/2)

❑ Fission Source Convergence Diagnosis by SEM and KEM

- In MC eigenvalue transport calculations, the MC tallies based on a fully converged FSD should be symmetrically and normally distributed.
- Accordingly, skewness (G_1) and kurtosis (G_2) can be used as convergence criteria where the values of Eqs. (1) and (2) fall below a predetermined threshold value, ε_1 and ε_2.

$$\max_m \left| G_1\left[S_m^p, L, N\right]\right| < \varepsilon_1 \ , \qquad \cdots (1)$$

$$\max_m \left| G_2\left[S_m^p, L, N\right]\right| < \varepsilon_2 \ , \qquad \cdots (2)$$

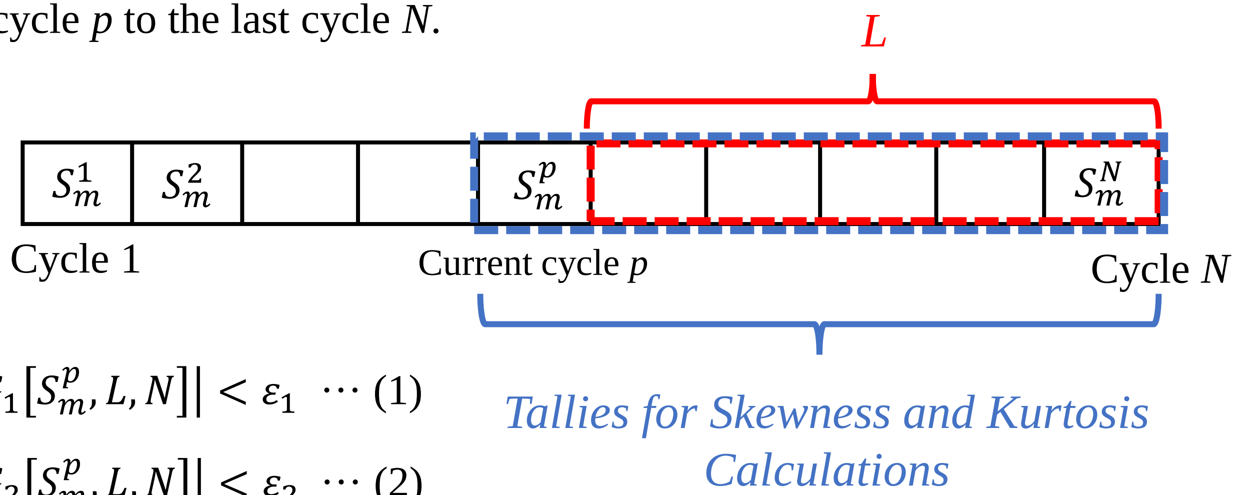
$$S_m^p = \int_{V_m} d\boldsymbol{r} S^p(\boldsymbol{r}) \qquad \cdots (3)$$

- ✓ $S^p(\boldsymbol{r})$ is the FSD of neutrons born at any energy, $\boldsymbol{r}$, and cycle index p.
- ✓ m refers to the cell or region index for MC tally
- ✓ L indicates the minimum cycle length for skewness and kurtosis calculations.

Skewness and Kurtosis Estimation Method(2/2)

❑ Fission Source Convergence Diagnosis by SEM and KEM

- $G_1[S_m^p, L, N]$ and $G_2[S_m^p, L, N]$ indicate the skewness and kurtosis by the distribution of FSDs from the current cycle *p* to the last cycle *N*.



$$\max_m \left|G_1[S_m^p, L, N]\right| < \varepsilon_1 \quad \cdots (1)$$

$$\max_m \left|G_2[S_m^p, L, N]\right| < \varepsilon_2 \quad \cdots (2)$$

- In this study, all McCARD calculations are performed as below conditions:
  - ➢ 100,000 #/cycle and 10,000 cycles
  - ➢ L = 4000 and $\varepsilon_1 = \varepsilon_2 = 0.5$ [8]

03 Numerical Results

- AGN-201K and 1D Slab Problems
- OECD/NEA Slow Convergence Benchmark Problem

AGN-201K and 1D Slab Problems

❑ AGN-201K Problem

- **Low DR** of about **0.59**.
- Initial fission sources are placed at the lowest part among the fuel disks (**Fuel 9**).
- Nevertheless, as shown in Figs. 2 and 3, the FSDs converged immediately.

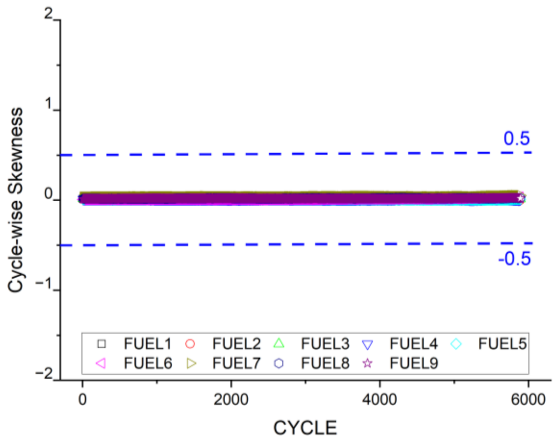


Figure 2. Cycle-wise cumulative skewness of AGN

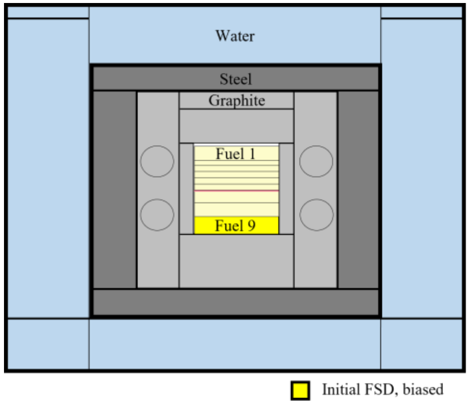


Figure 1. Vertical cross section of AGN-201K

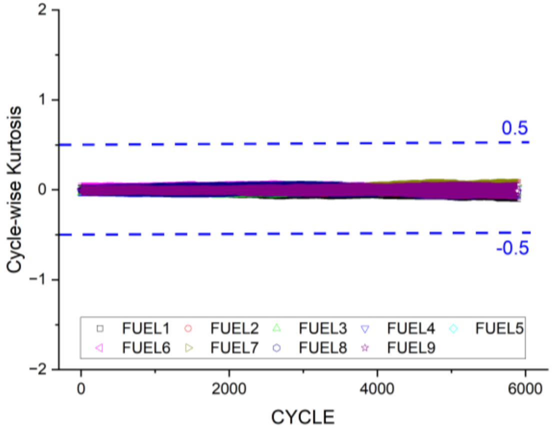


Figure 3. Cycle-wise cumulative kurtosis of AGN

AGN-201K and 1D Slab Problems

❑ 1D Slab Problem(1/2)

- **Intermediate DR** of about **0.9188**.
- Figures 5 and 6, as the cycle proceeds, the skewness and kurtosis are closer to 0.0.
- The skewness and kurtosis come within the convergence criteria (=0.5) on the 31st and 39th cycle.

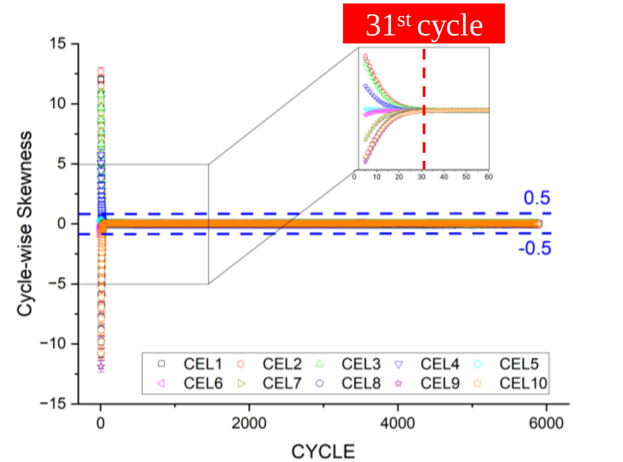


Figure 5. Cycle-wise cumulative skewness of slab

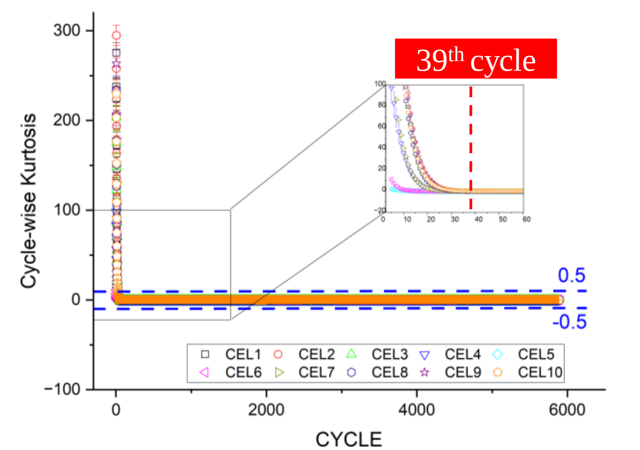


Figure 6. Cycle-wise cumulative skewness of slab

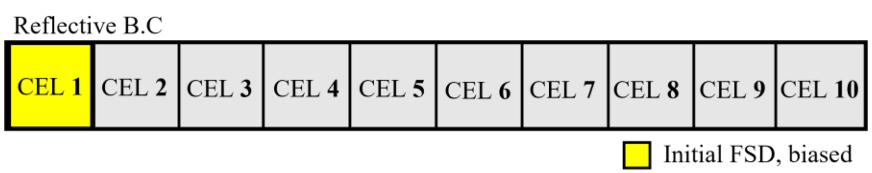


Figure 4. Vertical cross section of slab

AGN-201K and 1D Slab Problems

❑ 1D Slab Problem(2/2)

- The number of convergence cycles by the SEM and KEM was determined as **31st and 39th**.
- It was noted that the convergence cycle by the SEM (ε_1=0.5) and KEM (ε_2=0.5) was similar to the behavior of FSD in Fig. 7, which converges at about 40 cycles.

Table I: Convergence cycle results for the 1D slab problem

Method	Convergence Cycle
	1D Slab
Ueki's posterior	56
Type-A stopping criterion	97
Type-B stopping criterion	100
SEM	**31**
KEM	**39**

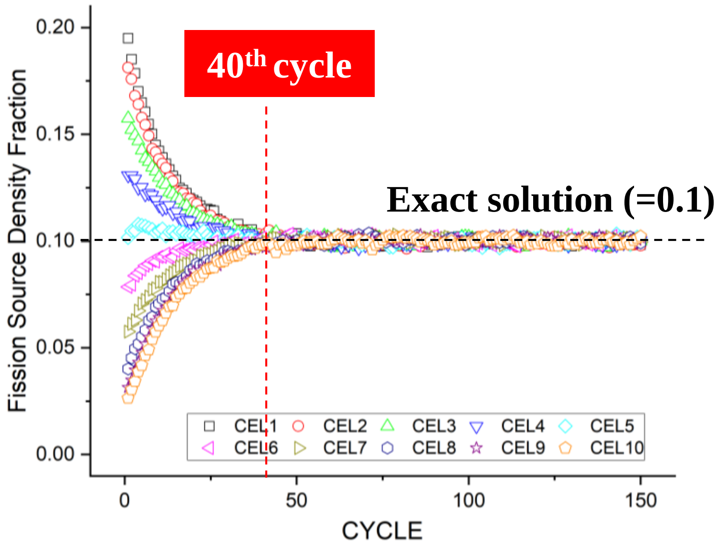


Figure 7. Fission source density fraction of slab

OECD/NEA Slow Convergence Benchmark Problem

❑ Checkerboard storage of assemblies (1/4)

- In the checkerboard problem, fuel and water are stored alternately, surrounded by concrete on three sides. Because of its asymmetry and the superior reflecting properties of concrete, the FSDs were converged biased towards the upper-left corner, resulting in a **high DR of 0.997**
- We consider the **10 fuels** on the left side among all fuels.

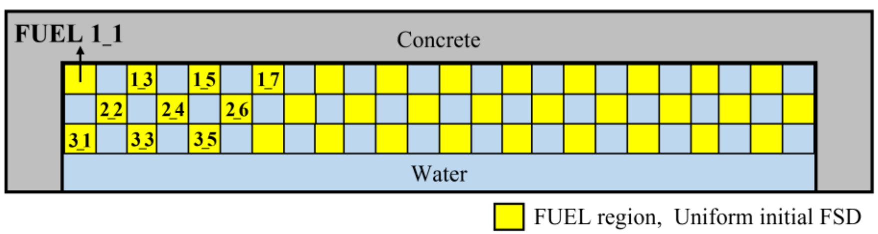


Figure 8. Checkerboard storage of assemblies

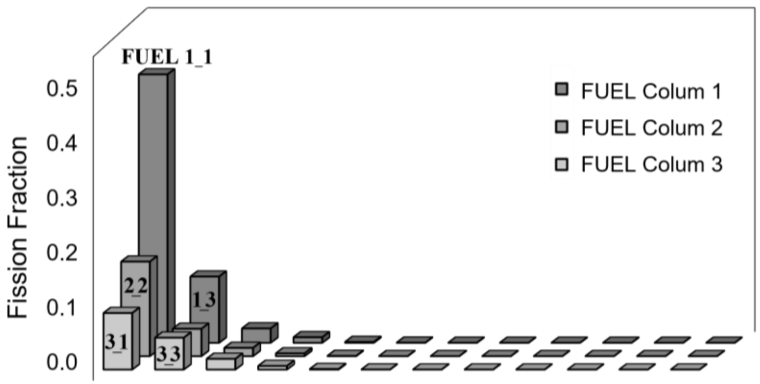


Figure 9. Fission distribution after FSD convergence

OECD/NEA Slow Convergence Benchmark Problem

❑ Checkerboard storage of assemblies (2/4)

- Calculated average skewness and kurtosis through ten calculations using different initial seeds.
- The SEM converged at the **1007th cycle**, while the KEM converged at the **1127th cycle**.

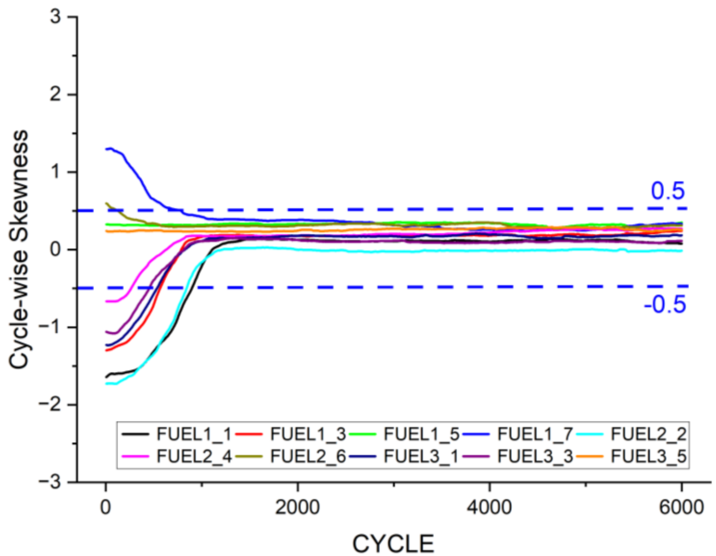


Figure 10. Cycle-wise cumulative skewness

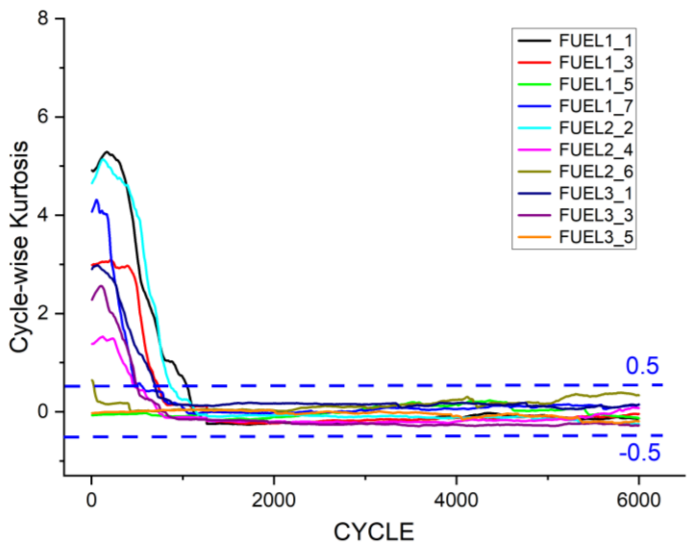
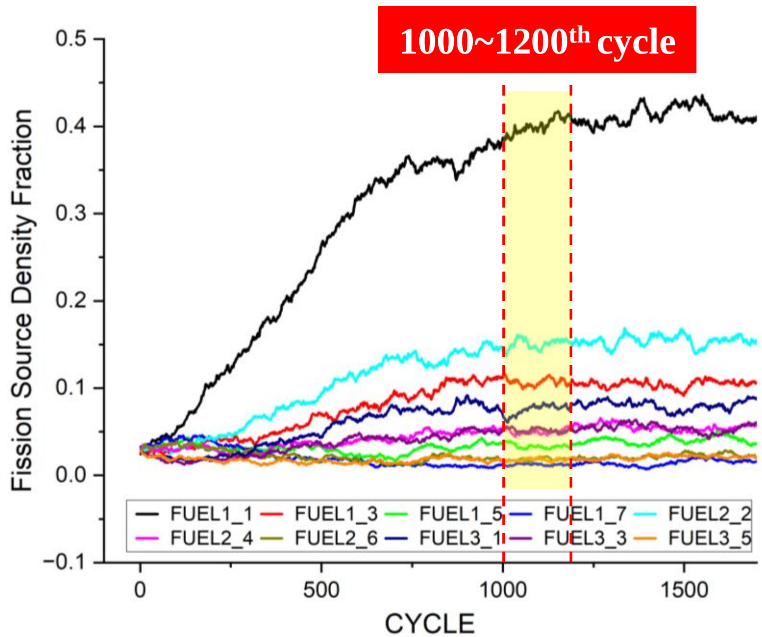


Figure 11. Cycle-wise cumulative kurtosis

OECD/NEA Slow Convergence Benchmark Problem

❑ Checkerboard storage of assemblies (3/4)

- Figure shows the cycle-wise fission source density fraction of Problem 1.
- Considering the statistical uncertainty and noise, it can be confirmed that the FSDs tend to converge at around 1000 cycles.
  - ➢ The convergence cycles diagnosed by SEM (1007th) and KEM (1127th) were similar.



Method	Convergence Cycle
	Prob. 1
SEM	1007
KEM	1127
Observed FSD value	1000 ~ 1200

OECD/NEA Slow Convergence Benchmark Problem

❑ Checkerboard storage of assemblies (4/4)

- Figures 12 and 13 show the probability distribution of FUEL1_1 respectively before and after FSD convergence at the 100th and 2000th cycle.
- After convergence, the distribution of FUEL1_1 appears to resemble a normal distribution.

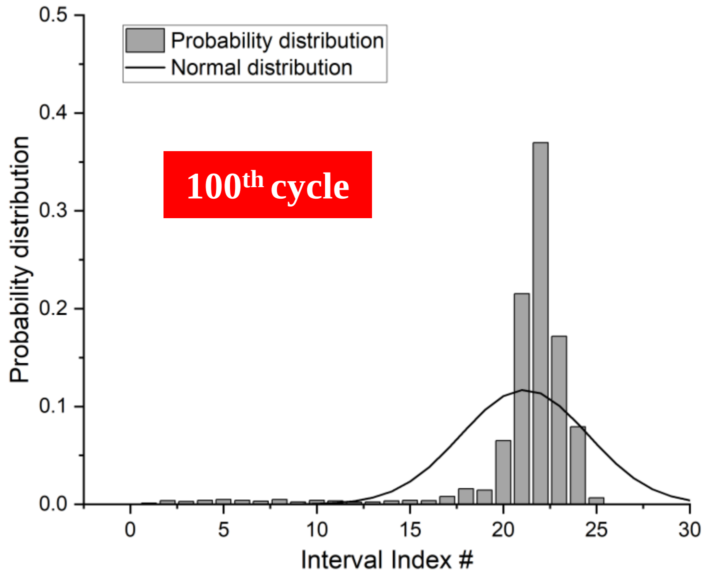


Figure 12. Probability distribution before FSD converged

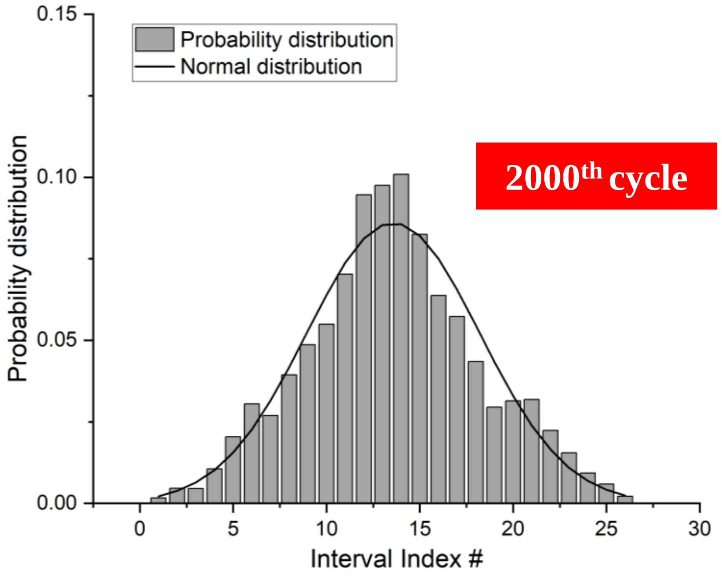


Figure 13. Probability distribution after FSD converged

OECD/NEA Slow Convergence Benchmark Problem

❑ Pin-cell array with irradiated fuel (1/4)

- Problem 2 is the light water reactor fuel pin with a non-symmetric idealized burnup distribution.
  - ➢ We used Case 1-3, low-multiplication section in the center Fuel 5 with Natural UO_2.
  - ➢ Fuel 1~4 and 6~7 are fresh fuels UO_2(4.5wt.%). Fuel 8~9 are fresh fuels UO_2 (4.0wt.%).
- It has a **high DR of 0.976**.
- Due to the small FSDs in the lower parts (Fuel 6 ~ Fuel 9) shown in Figure 15, skewness and kurtosis values from Fuel 1 to Fuel 5 were used.

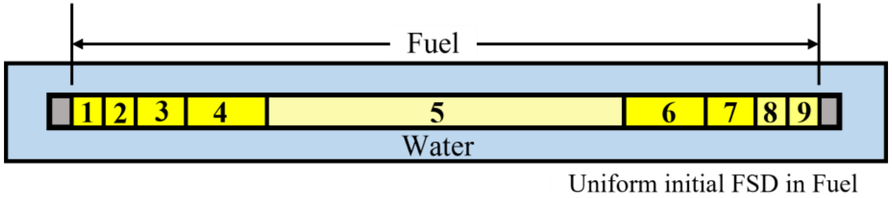


Figure 14. Pin-cell array with irradiated fuel

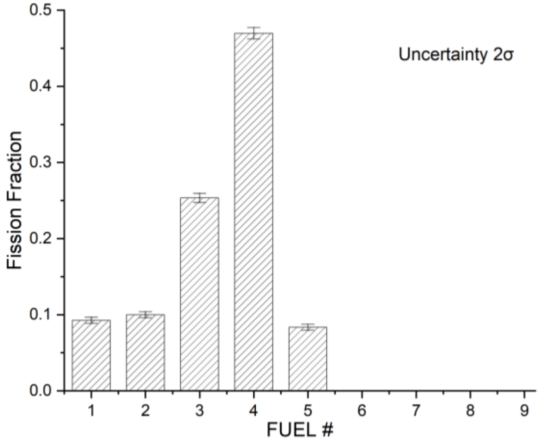


Figure 15. Fission distribution after FSD convergence

OECD/NEA Slow Convergence Benchmark Problem

❑ Pin-cell array with irradiated fuel (2/4)

- Figures 16 and 17 presents the cycle-wise cumulative skewness and kurtosis of Problem 2.
- By the SEM and KEM, the convergence cycle is determined as **752nd** and **881st**.

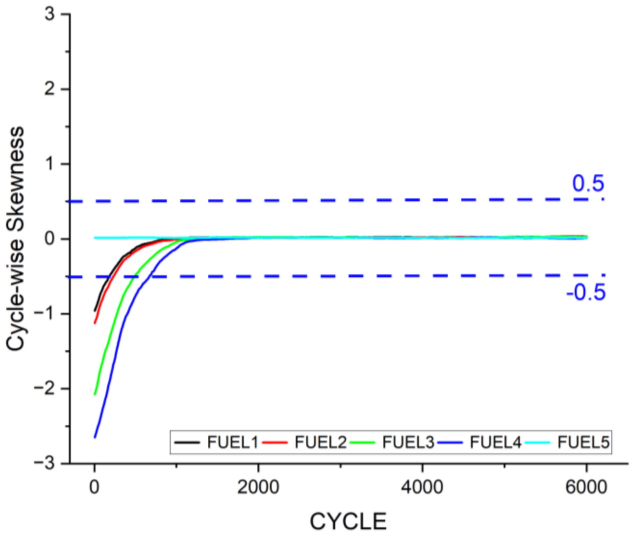


Figure 16. Cycle-wise cumulative skewness

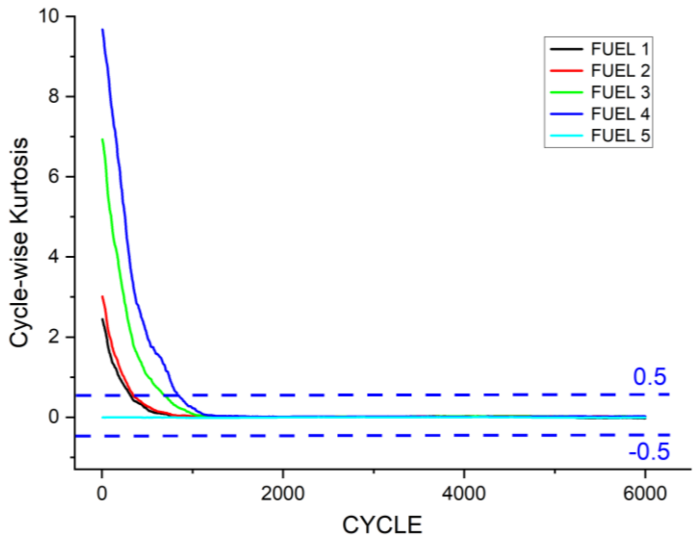
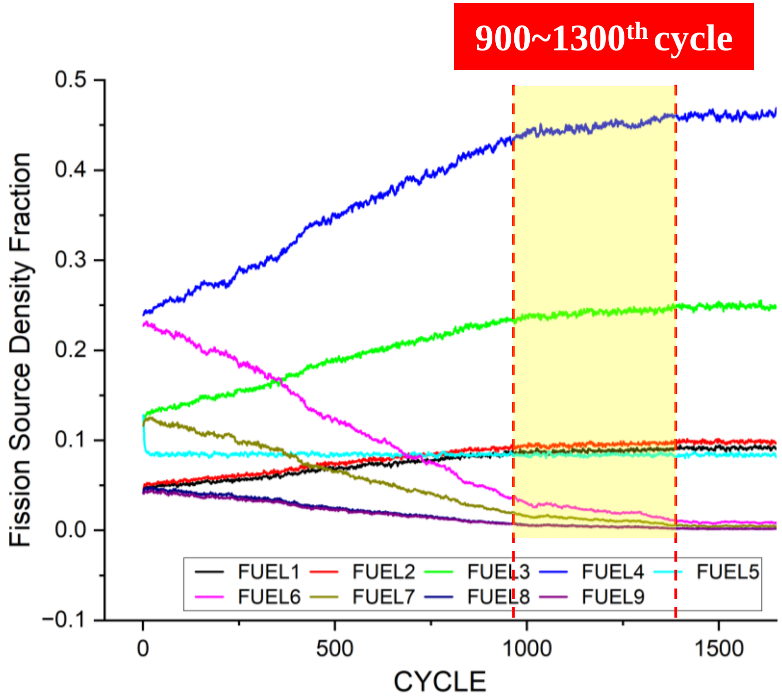


Figure 17. Cycle-wise cumulative kurtosis

❑ Pin-cell array with irradiated fuel (3/4)

- Figure shows a slowly changing behavior of FSD and indicates that it converges at about 900 cycles.
  - ➢ The number of convergence cycles diagnosed by SEM(752nd) and KEM(881st) were similar.



Method	Convergence Cycle
	Prob. 2
SEM	752
KEM	881
Observed FSD value	900 ~ 1300

❑ Pin-cell array with irradiated fuel (4/4)

- Figure 18 shows the probability distribution of FUEL4 in the 100th cycle before FSD convergence, while Figure 19 confirms its normal distribution in the 2000th cycle after convergence.

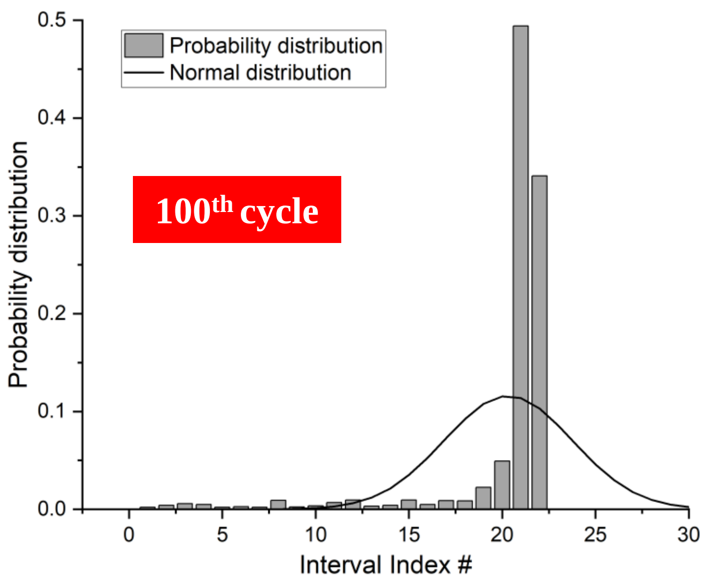


Figure 18. Probability distribution before FSD converged

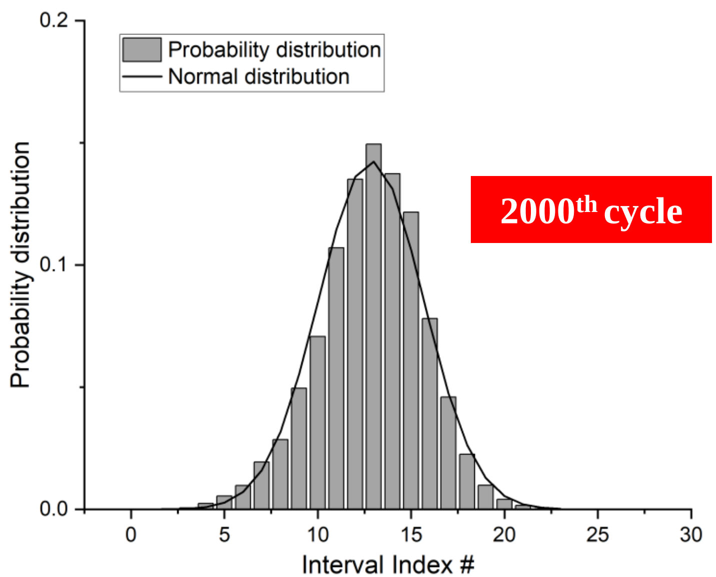


Figure 19. Probability distribution after FSD converged

OECD/NEA Slow Convergence Benchmark Problem

❑ OECD/NEA Benchmark Summary

- Both the SEM (ε_1 =0.5) and KEM (ε_2 =0.5) showed similar convergence cycles to Ueki's posterior and the Shim's type B. In Problem 2, SEM and KEM converged at 752nd and 881st cycles, which falls between Ueki's posterior and the Shim's types A and B stopping criterion.
- The SEM and KEM methods reliably diagnose the fission source convergence cycle.

Table II: Convergence cycle results for OECD/NEA Slow Convergence Benchmark

Method	Convergence Cycle	
	Prob. 1	Prob. 2
Ueki's posterior	1160	1865
Type-A stopping criterion	163	36
Type-B stopping criterion	1075	48
SEM	**1007**	**752**
KEM	**1127**	**881**

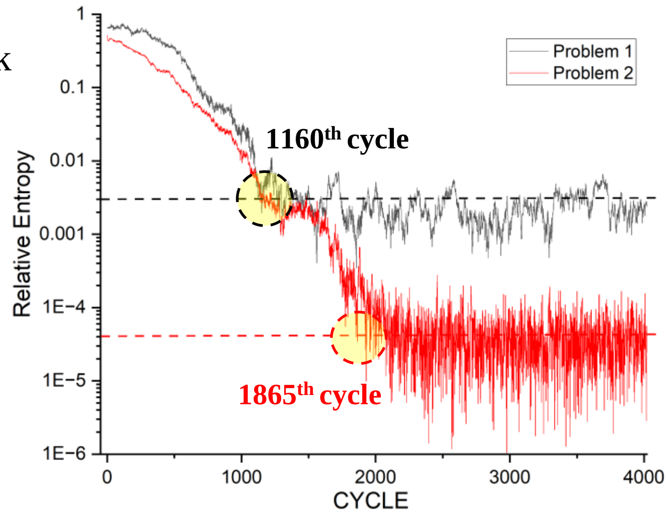


Figure 20. Ueki's posterior source convergence diagnosis

04 Conclusion

Conclusion

❑ Summary

- Confirm the performance and reliability of the SEM and KEM for **various DR problems**

  - AGN-201K, 1D Slab, and OECD/NEA Slow Conv. Benchmarks.

    - **SEM and KEM provided effective and reliable convergence cycles** when compared to other method and fission source density fraction trends.
    - Concluded that a criterion value of **0.5 for both ε_1 and ε_2** is reasonable.

- In this study, large neutron histories and long cycles (i.e., 100,000 #/cycle and 10,000 cycles) were used for skewness and kurtosis calculations to reduce the statistical fluctuations caused by FSD noise.

❑ Future work

- We will study the modified SEM and KEM that combines Kalman filter to reduce the statistical fluctuation of FSDs.

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2. H. J. Shim, C. H. Kim, Stopping criteria of inactive cycle Monte Carlo calculations, Nucl. Sci. Eng., Vol.157, p. 132, 2007.
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6. H. J. Park, H. C. Lee, “Application of Higher Order Fission Matrix for Real Variance Analysis in McCARD Monte Carlo Eigenvalue Calculation,” M&C2017, Apr. 16-20, 2017, Jeju, Korea.
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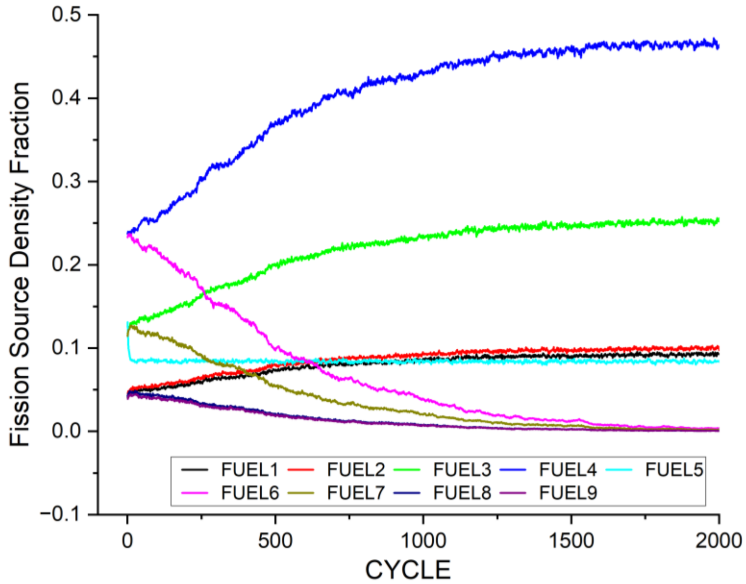
8. D. N. Joanes, C. A. Gill, “Comparing Measures of Sample Skewness and Kurtosis,” The Statistician, Vol.47, 1, p.183, 1998.

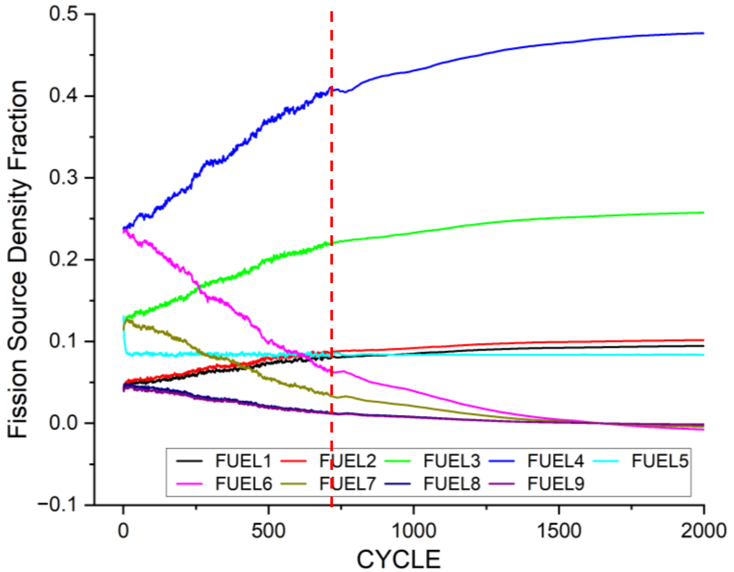
THANK YOU

Appendix

❑ Kalman filter



Cycle-wise cumulative FSD fraction



FSD fraction with Kalman filter after 700 cycle