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Real Variance Estimation of BEAVRS whole core benchmark in Monte Carlo Eigenvalue Calculations

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1. INTRODUCTION

As the computing performance of hardware and software advances, Monte Carlo (MC) method have been applied to the neutronic analysis of whole core problem such as the commercial nuclear reactors because the accuracy of the MC calculations benefits from its ability to use continuous energy nuclear data and to handle complex geometric information. For whole core analysis by the MC eigenvalue mode calculations, some severe problems are encountered because these systems have higher dominance ratios (DRs) than a fuel assembly (FA) or critical facilities. It is well known that the apparent variance of a local tally like pin power is differ from the real variance considerably. In McCARD [1] code, four approaches for the real variance estimation were implemented. These are Gelbard's batch method [2], Ueki's method [3], Fission Source Distribution (*FSD*) method [4], and History-based Batch (*HB*) method [5].

Recently, a new whole core benchmark BEAVRS [6] (Benchmark for Evaluation and Validation of Reactor Simulations) was proposed by MIT computational Reactor Physics Group. This benchmark provides a detailed description of fuel assemblies, burnable absorbers, in-core fission detectors, core loading patterns, and numerous in-vessel components with three-dimensional (3D) scale.

In this study, we perform a real variance estimation of MC tally for the design parameter such as k_{eff}, pin fission power, FA-wise fission power for BEAVRS fresh core using McCARD. In addition, this paper presents a new method to estimate the real variance called history-based sampling method, briefly.

2. REAL VARIANCE ESTIMATION FOR BEAVRS

2.1 Source Convergence Diagnosis for BEAVRS

In MC eigenvalue calculation, the inactive cycles are required to obtain the converged FSD. In McCARD, the Ueki's posterior method [7] based on '*Shannon entropy*' of FSD and the Shim's on-the-fly stopping criterion [8] were implemented to determine the number of inactive cycles. Figure 2 shows the relative entropy and the stopped cycle number for BEAVRS. The stopped cycle number by Ueki's posterior method is 206 while those by Shim's on-the-fly stopping criterion of type A and B are 294 and 360, respectively. Considering the results, the number of inactive cycle were set as 400 for all the BEAVRS calculations. It was observed that the cumulative k_{eff} as a function of cycle number converged adequately at round 400-th cycle as shown in Fig. 3. The DR of BEAVRS fresh core by McCARD at cycle 1 is about 0.99.

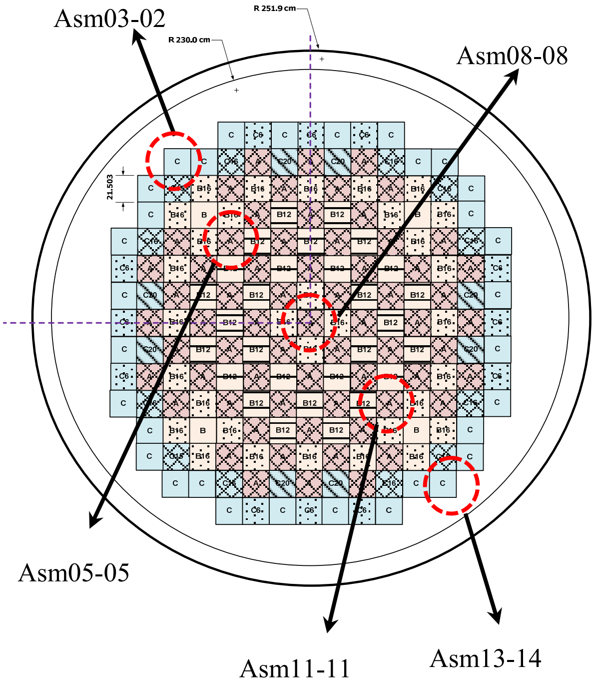

Fig. 1. Core Loading Pattern for BEAVR cycle 1

2.2 Real Variance Estimation for BEAVRS

As mentioned above, McCARD provides the four methods available to estimate real variances of tallied values. Among these methods, the Ueki's covariance method requires the fission matrix (FM) of FSD for analysis of the error propagation. To estimate the real variance by Ueki's method, the 193x193 FA-wise regional discretization was used to build FM for BEAVRS. The batch size for *HB* method was 1,000. The MC eigenvalue calculation was performed on 100 active cycles with 1,000,000 neutron histories per cycle. The reference real standard deviation (SD) was estimated from 26 replicas with different random number sequence.

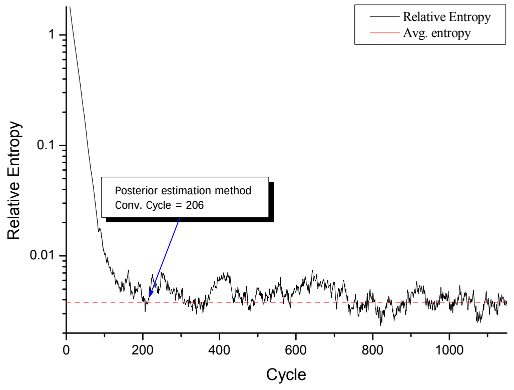

Fig. 2. Ueki's Shannon entropy for BEAVRS cycle 1

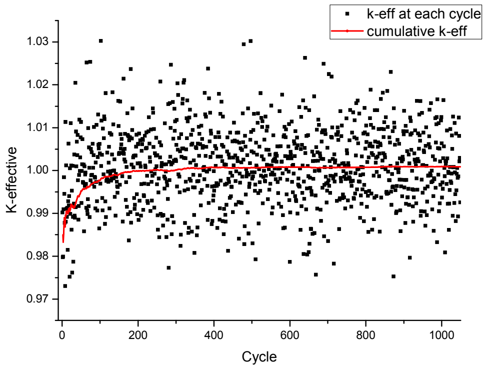

Fig. 3. k_{eff} at each cycle and cumulated k_{eff} for BEAVRS cycle 1

Table I: Comparison of estimated real standard deviation of k_{eff} by each method

σ_{REF}	σ_{APP}	σ_{BAT}	σ_{Ueki}
0.00010	0.00010	0.00010	0.00010

Table I presents the estimated standard deviation of the k_{eff} by each method. σ_{REF} represents the SD from the reference while σ_{APP} is the apparent or sample SD. σ_{BAT} and σ_{Ueki} is the SD by Gelbard's batch method and Ueki's method, respectively. Usually, the apparent SD of a global design parameter such k_{eff} agrees well with the reference value. Table II compares the relative standard deviation (RSD) of pin power at each location. The real variance to apparent variance ratio ($\sigma_{\mathrm{REF}}/\sigma_{APP}$) is 1.21~1.71. Table III shows the RSD of FA-wise power, which is calculated by the fission power of the pins consisting of the FA. The real variance to apparent variance ratio ranges from 4.67 to 10.19. Table IV shows the RSD of core fission power, which can be obtained as the sum of the FA-wise fission power. In this case, there is no significant difference between real variance and apparent variance.

Among the four methods for the real variance estimation, the *HB* method predicts the reference for BEAVRS fresh core most accurately.

Table II: Comparison of estimated real variance of pin-wise fission power each method

Assembly	RSD (%)				
	σ_{REF}	σ_{APP}	σ_{BAT}	σ_{Ueki}	σ_{HB}
Asm03-02 Pin01-01	4.17	3.08	3.32	3.56	3.41
Asm03-02 Pin02-02	3.62	2.78	2.77	2.75	3.27
Asm05-05 Pin01-01	2.13	1.25	1.46	1.38	1.77
Asm08-08 Pin01-01	2.01	1.65	1.55	1.55	1.97
Asm11-11 Pin01-01	2.07	1.41	1.36	1.62	1.81
Asm13-14 Pin01-01	2.05	1.33	1.43	1.25	2.11

Table III: Comparison of estimated real variance of FA-wise fission power each method

Assembly	RSD (%)				
	σ_{REF}	σ_{APP}	σ_{BAT}	σ_{Ueki}	σ_{HB}
Asm13-14	1.75	0.20	0.27	0.39	1.56
Asm05-05	1.52	0.17	0.21	0.30	1.10
Asm03-02	2.04	0.20	0.29	0.45	1.48
Asm08-08	0.96	0.21	0.27	0.40	1.00
Asm11-11	1.44	0.17	0.23	0.35	1.08

Table IV: Comparison of estimated real variance of whole core fission power each method

Core	RSD (%)				
	σ_{REF}	σ_{APP}	σ_{BAT}	σ_{Ueki}	σ_{HB}
Core	0.010	0.010	0.009	0.009	0.010

2.3 Correlation Coefficients between MC tally

In order to examine the reason why the real variance to apparent variance ratio in a FA-wise fission power is larger than that in pin fission power, the correlation coefficients between pin fission power and FA-wise fission power are calculated. The FA-wise fission power (P_k^{Asm}) and its SD ($\sigma\left(P_k^{\mathrm{Asm}}\right)$) can be calculated by Eq.(1) and Eq.(2).

$$P_k^{\mathrm{Asm}} = \sum_{m=1}^{N_m} P_m^{Pin} \tag{1}$$

$$\sigma\left(P_k^{\mathrm{Asm}}\right) = \sqrt{\sum_{m=1}^{N_m} \sigma^2\left(P_m^{\mathrm{Pin}}\right) + 2\sum_{m'=1}^{N_m} \sum_{\substack{m''=1,\\ m'\neq m''}}^{N_m} \mathrm{cov}[P_{m'}^{\mathrm{Pin}}, P_{m''}^{\mathrm{Pin}}]}, \tag{2}$$

where m and k are a cell indices for pin and FA, respectively. $\mathrm{N_m}$ and $\mathrm{N_k}$ is the number of pins in a FA and the total number of FAs in BEAVRS fresh core. From its definition, one can determine the correlation coefficients between pin fission power tallies as follow

$$\rho[P_{m'}^{\mathrm{Pin}}, P_{m''}^{\mathrm{Pin}}] = \frac{\mathrm{cov}[P_{m'}^{\mathrm{Pin}}, P_{m''}^{\mathrm{Pin}}]}{\sigma(P_{m'}^{\mathrm{Pin}}) \cdot \sigma(P_{m''}^{\mathrm{Pin}})} \tag{3}$$

Table V shows the correlation coefficients between pin fission powers. The FA locations are shown in Fig. 1. According to the inter-cycle correlations of the FSDs, it was observed that the correlation coefficients of pin power between neighbor pins is strongly positive. Meanwhile, the correlation coefficients of pin power between two pins far from each other is negative or close to 0. The covariance terms in Eq.(2) have mostly large positive values because a FA-wise fission power is defined as the sum of the fission powers of the pins in the FA and there are strong positive correlations between the fission powers of the pins This explains the large real to apparent variance ratio in the FA-wise fission power.

In the same manner, the core fission power and its SD can be obtained.

$$P^{\mathrm{Core}} = \sum_{k=1}^{N_k} P_k^{\mathrm{Asm}} \tag{4}$$

$$\sigma\left(P^{\mathrm{Core}}\right) = \sqrt{\sum_{m=1}^{N_k} \sigma^2\left(P_k^{\mathrm{Asm}}\right) + 2\sum_{k'=1}^{N_k} \sum_{\substack{k''=1\\ k'\neq k''}}^{N_k} \mathrm{cov}[P_{k'}^{\mathrm{Asm}}, P_{k''}^{\mathrm{Asm}}]} \tag{5}$$

The behavior of correlation coefficients between FA-wise fission powers is similar to that between pin fission powers as shown in Table VI. The covariance terms between two FAs far from each other are more negative. The error of the covariance terms in Eq. (4) cancel out because the core fission power is defined as the sum of the FA-wise fission powers and their correlations are either positive or negative. This explains why the real to apparent variance ratio is close to 1.0 in the core fission power.

Table V: Correlation Coefficients between pin fission power tally

Pin (m'')	$\rho[P_{m'}^{\mathrm{Pin}}, P_{m''}^{\mathrm{Pin}}]$
	Asm03-02>Pin01-01 (m')
Asm03-02>Pin01-01	1.000
Asm03-02>Pin02-02	0.483
Asm05-05>Pin01-01	0.353
Asm08-08>Pin01-01	-0.296
Asm11-11>Pin01-01	-0.365
Asm13-14>Pin01-01	0.047

Table VI: Correlation Coefficients between FA-wise fission power tally

Assembly (k'')	$\rho[P_{k'}^{Asm}, P_{k''}^{Asm}]$
	Asm03-02 (k')
Asm03-02	1.000
Asm05-05	0.808
Asm08-08	-0.367
Asm11-11	-0.619
Asm13-14	-0.529

2.4 New Real Variance Estimation Method by History Sampling – History-based Sampling Method

Overall, the *HB* method can estimate the reference more accurately than other method as shown in the results of BEAVRS in Sec 2.2. However, it is observed that the error of the estimated real variance increase considerably, as the history-based batch size decrease, as presented in the reference 5. Therefore, it must be ensured that the batch size is so enough that the batch average MC tally don't fail to follow the normal distribution.

In order to overcome this problem, the new method called history-based sampling (*HS*) method is proposed in this paper. Figure 4 shows the procedure of the HS method. In the *HS* method, the fission source (FS) data, such as a location and energy of the neutron particle (r, E), are stored in bank files during the additional cycles. Then, the neutron sources are generated by random sampling from the bank files during active cycles.

Figure 5 shows the schematic diagram to understand the *HS* method. In the MC eigenvalue runs on *N* active cycles with *M* histories per cycle, the sample variance of MC tally by the *HS* method can be calculated as follow:

$$\sigma^2\left[\overline{Q}_{HS}\right] = \frac{1}{N(N-1)}\sum_{k=1}^{N}\left(Q^{k,Samp} - \overline{Q}_{HS}\right)^2 \qquad (6)$$

$$\overline{Q}_{HS} = \frac{1}{N}\sum_{k=1}^{N} Q^{k,Samp} \qquad (7)$$

$Q^{k,Samp}$ $(k = 1, 2, \cdots, N)$ indicates the average MC tally calculated by the *M* neutron sources, which are sampled from the bank files at the *k*-th active cycle. The inter-cycle correlations between $Q^{k,Samp}$'s must be weaken by the random sampling of fission sites. Moreover, $Q^{k,Samp}$ may be free from the normalization dependence issue [9] because the number of fission source neutrons at each active cycle is always equal to *M*.

Table VII compares the RSD of FA-wise fission power at each location of BEAVRS core. The MC eigenvalue calculation was performed on 100 active cycles with only 10,000 neutron histories per cycle. In *HB* method, 100 batches were used with a batch size of 100. In *HS* method, 1,000,000 FS data during 100 additional cycles were stored in the bank file. The RSD by the *HS* method are comparable with the reference values in Table III in spite of a small neutron histories per cycle except for the FA at the core center.

Table VII: Comparison of estimated real variance of FA-wise fission power each method in small history problem

Assembly	RSD (%)			
	σ_{REF}	σ_{APP}	σ_{HB}	σ_{HS}
Asm13-14	23.1	1.85	12.5	16.9
Asm05-05	16.2	1.72	11.4	17.4
Asm03-02	21.2	1.95	12.5	17.0
Asm08-08	10.9	1.96	17.1	19.4
Asm11-11	16.4	1.52	10.9	17.4

3. CONCULSION

In this study, the real variance estimations for the BEAVRS whole core benchmark were performed using Gelbard's batch method, Ueki's inter-cycle correction method, and Shim's *HB* method, which were implemented in McCARD. As expected, it was observed that the apparent variance of local MC tally estimate such as pin or FA-wise fission power tends to be smaller than its real variance while that of the global MC tally such as k_{eff} is comparable to the reference.

To investigate the difference of the real to apparent variance ratio between global and local MC tally, the correlation coefficients between each pin or FA fission power are calculated using McCARD. Because the correlation coefficients between neighbor pins is near 1.0, the error by FSD inter-cycle correlation would be propagated.

In addition, this paper presented a new variance estimation method called the *HS* method. The *HS* method has several advantages over the *HB* method. The *HS* method is very easy to implement into a existing MC code and it does not require additional parameters such as batch size in the *HB* method. But the *HS* method requires much more computational effort for the addition cycles to generate the converged FSD. A very limited numerical test using the BEAVRS benchmark was performed with a very small number of neutron histories per cycle to access the applicability of the *HS* method. The *HS* method showed better performance than the *HB* method when the neutron histories per cycle was small. More through verification of the *HS* method should be conducted in the future.

REFERENCES

[1] H. J. Shim, B. S. Han, J. S. Jung, H. J. Park, C. H. Kim, McCARD: Montel Carlo Code for Advanced Reactor Design and Analysis, *Nucl. Eng. Tech.*, **44**, pp161-175, 2012.

[2] E. M. Gelbard and R. E. Prael, Computation of Standard Deviation in Eigenvalue Calculations, *Prog. Nucl. Energy*, **24**, 237, (1990)

[3] T. Ueki, "Batch Estimation of Statistical Errors in the Monte Carlo Calculations of Local Powers, *Ann. Nucl. Energy*, **38**, 2462 (2011)

[4] H. J. Shim and C. H. Kim, Real Variance Estimation Using an Intercycle Fission Source Correlation for Monte Carlo Eigenvalue Calculations, *Nucl. Sci. Eng.*, **162**, 98 (2009)

[5] H. J. Shim, S. H. Choi, C. H. Kim, Real Variance Estimation by Grouping Histories in Monte Carlo Eigenvalue Calculations, *Nucl. Sci. Eng.*, **176**, 58-68 (2014)

[6] N. Horelik, B. Herman, B. Forget, and K. Smith, Benchmark for Evaluation and Validation of Reactor Simulation (BEAVRS), Proc. M&C 2013, Sun Valley, Idaho, May 5-9, 2013.

[7] T. Ueki and F. B. Brown, Stationarity Modelling and Informatics-based Diagnostics in Monte Carlo Criticality Calculations, *Nucl. Sci. Eng.*, **149**, 38 (2005)

[8] H. J. Shim and C. H. Kim, Stopping Criteria of Inactive Cycle Monte Carlo Calculations, *Nucl. Sci. Eng.*, **157**, 132 (2007)

[9] H. J. Shim and S. H. Choi, "History-based Batch Method Preserving Tally Means," Transactions of Korean Nuclear Society Autumn Meeting, Gyeongju, Korea, Oct. 25-26, (2012).

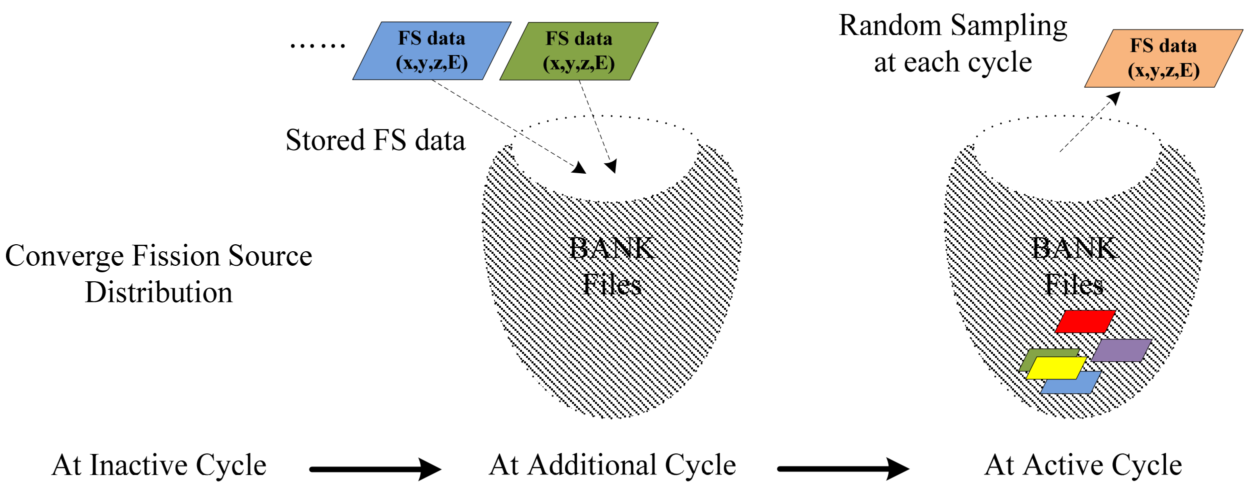

Fig. 4. Procedure of the history-based sampling method

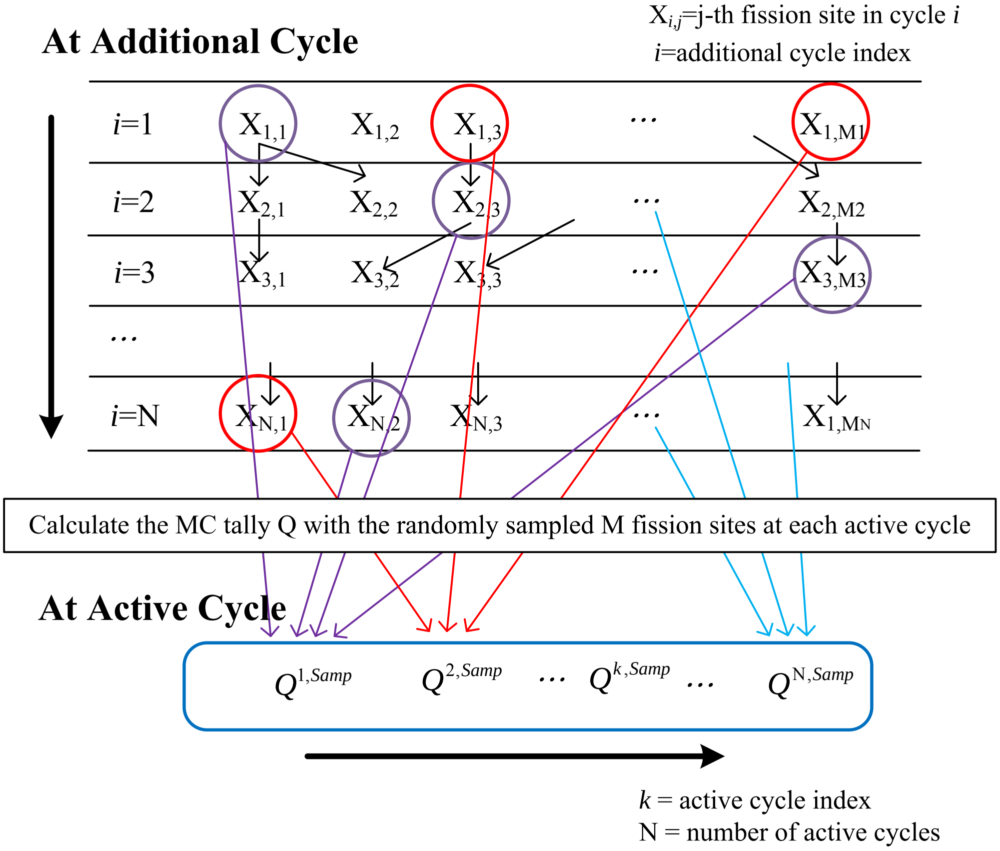

Fig. 5. Schematic diagram of the history-based sampling method