New Strategy to Determine Batch Size of the Batch Method for Real Variance Estimation in the Monte Carlo Eigenvalue Calculations

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1. Introduction

In the most MC calculations, it is assumed that each particle is independent of all others. This assumption gives the simple evaluation of variance of tallied value. However, in the MC eigenvalue calculation based on the power iteration method, this assumption occurs biased variance of tallied value. In the power iteration method, a fission reaction causes the birth of the neutron in the next cycle. Therefore, some neutrons are correlated with each other. If this correlation is not considered, the variance of tallied value will be biased.

To estimate the real variance of tally values, several studies have been performed. Among them, the most widely used method is the Gelbard's batch method [1]. The Gelbard's batch method is easy to implement. However, it is difficult to set appropriate batch size [2]. The batch size is important parameter in the Gelbard's batch method to estimate the variance. It is well known that the increase of the batch size will give the variance which is close to the real variance. In general, the batch size is determined empirically after several MC calculations with different batch sizes. These are inefficient and time-consuming works. More efficient method to find batch size is required. In this study, the new simple method to determine batch size for the reliably estimated variance is proposed.

2. Methods and Results

2.1 Review of the Background

The Gelbard's batch method is developed to calculate the real variance in the MC calculation. In the Gelbard's batch method, the total number of active cycle N is divided into L batches. Each batch consists of successive M active cycles.

$$L = \frac{N}{M},\ (0 < M < N). \tag{1}$$

The tally value is estimated in every batch. For example, in the i-th batch, the tally is estimated as

$$Q_i = \frac{1}{M} \sum_{j=(i-1)\times M+1}^{i\times M} q_j\ , \tag{2}$$

where q_j is the estimated tally value in j-th active cycle. The final estimated tally value is determined by averaging the tally values of each batches, i.e.

$$\bar{Q} = \frac{1}{L}\sum_{i=1}^{L} Q_i\ . \tag{3}$$

The estimated real variance is calculated as follows:

$$\sigma^2[\bar{Q}] = \frac{1}{L(L-1)}\sum_{j=1}^{L}\left(\frac{1}{M}\sum_{i=(j-1)\times M+1}^{j\times M} q_i - \frac{1}{N}\sum_{i=1}^{N} q_i\right)^2. \tag{4}$$

2.2 The Proposed Strategy to Determine the Batch Size of the Gelbard's Batch Method

The main idea of the new approach is to choose the batch size of which the correlation between cycles is negligible. It is well known that the correlation of cycles causes under-estimated variance and the cycle-to-cycle correlation is decreased as the gap of the cycle is increased. To select the batch size as the sufficient cycle gap of which correlation is negligible, the estimated variance will be close to the real variance.

In general, the correlation between cycles is calculated from tallied values of each cycle [3]. Through this method, the desirable gap of the cycle cannot be acquired before the end of MC calculation. To determine the cycle gap for the negligible correlation, the new method without full eigenvalue MC calculation was developed.

The fission probability matrix was utilized to obtain the gap of cycle. The fission probability matrix is the square matrix which is composed of the probability of the generation of a neutron [4]. The element of the fission probability matrix P_{ij} means the probability of a neutron born in i region caused a fission reaction in j region.

It is possible to calculate the probability that a neutron causes fission in the next cycles by utilizing the fission probability matrix. For example, the probability that a neutron which is generated in i region causes fission in j region after 2 cycles is as follows:

$$P_{ij}^{\ 2} = P_{i1}\times P_{1j} + P_{i2}\times P_{2j} + \ldots + P_{in}\times P_{nj} \tag{5}$$

where superscript of P_{ij}^2 means that the probability after 2 cycles, i and j denote indices of the fission region and the size of fission probability matrix is n by n. In the

same way, the probability that a neutron which is generated in *i* region causes fission in *j* region after 3 cycles is expressed as follows:

$$P_{ij}^{3} = P_{i1}^{2} \times P_{1j} + P_{i2}^{2} \times P_{2j} + \ldots + P_{in}^{2} \times P_{nj} = \sum_{l=1}^{n} (P_{il}^{2} \times P_{lj}). \quad (6)$$

Finally, the equation for the probability that a neutron in *i* region causes fission in *j* region after *k* cycles is as follows:

$$P_{ij}^{k} = \sum_{l=1}^{n} (P_{il}^{k-1} \times P_{lj}). \quad (7)$$

Hereafter, P_{ij}^{k} will be called the fission cumulative probability matrix after *k* cycles. As P_{ij}^{k-1} and P_{ij} are less than one, P_{ij}^{k} will be converged to some values with the increase of *k*. It is assumed that if P_{ij}^{k} is converged, the correlation between a certain cycle and the cycle after *k* is negligible. The main idea of the proposed method is to determine batch size as the gap of cycles of which correlation is negligible.

2.3 Verification

To apply the proposed strategy for determining batch size, simple problems were solved.

2.3.1 Three Thick One-dimensional Slabs Problem

Three thick one-dimensional slabs problem [5] was solved to apply the proposed strategy. The geometry of this problem is shown in Fig. 1. The unit 1 and unit 2 are consist of uranyl solution.

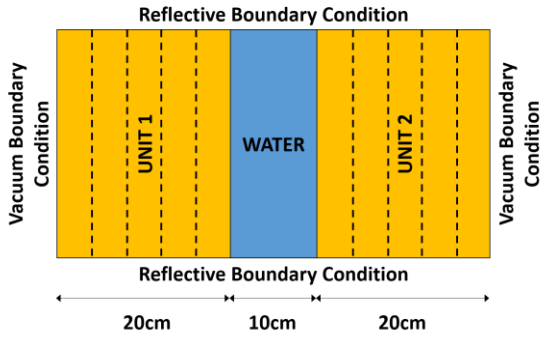

Fig. 1. The Geometry of Three Thick One-dimensional Slabs Problem

The fission probability matrix of the problem was calculated by McCARD [6] and shown in Fig. 2. The unit 1 and unit 2 were divided into 10 regions for the fission probability matrix. Ten thousands of neutrons were utilized to estimate the fission probability matrix.

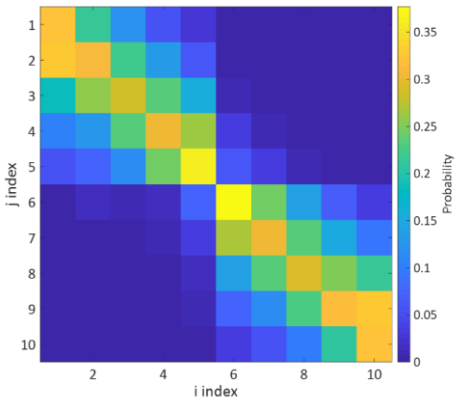

Fig. 2. The Fission Probability Matrix of the Three Thick One-dimensional Slabs Problem

As shown in Fig. 3, the fission cumulative probability was converged after 60th cycle. Thus, the batch size was set to 60.

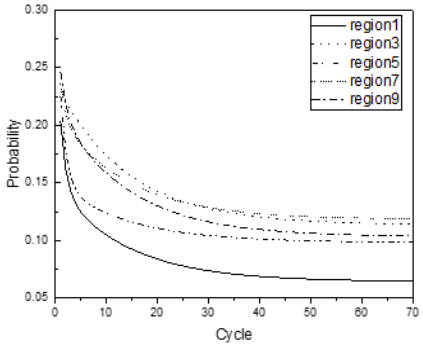

Fig. 3. The Fission Cumulative Probability of the Three Thick One-dimensional Slabs Problem

The fission reaction rates were tallied in each region by changing the batch size for the verification of the proposed strategy. The results were tabulated in Table I.

The estimated standard deviations (SD) of the tallies were compared to the real SD. The real SD was calculated by McCARD. To calculate the real SD, one hundreds of MC calculations were performed changing random seed. As shown in Table I, the estimated SD approaches to the real SD with the increase of batch size. When the batch size is 60, the relative error of estimated SD is 3.85% in average. It was considered that the appropriate batch size was determined by the proposed method.

2.3.2 Homogenized Cylindrical Reactor

Fig. 4 shows the homogenized cylindrical reactor. The homogenized reactor region is composed of uranium oxide and zircaloy. The water is used as the reflector.

Table I: Relative Errors of the SDs for the Three Thick One-dimensional Slabs Problem by the Batch Size

Tally Region	Fission Reaction Rate ($\times 10^{-6}$ / *particle*)	Real Standard Deviation ($\times 10^{-9}$)	[a]Relative Error of Estimated Real Standard Deviation (%)				
			Batch Size 1	10	30	60	100
1	1.18	5.78	-70.7	-29.32	-8.34	6.76	5.00
2	2.51	12.22	-78.65	-31.93	-10.38	3.93	2.07
3	3.28	15.31	-80.73	-33.61	-10.68	5.24	1.16
4	3.54	15.52	-80.43	-35.15	-12.19	3.35	-1.42
5	3.83	13.62	-75.92	-30.67	-9.35	1.02	-3.86
6	3.83	13.18	-75.1	-31.68	-12.3	3.24	0.48
7	3.55	14.88	-79.57	-31.29	-8.04	8.62	5.66
8	3.29	15.93	-81.45	-35.51	-12.66	2.71	-2.15
9	2.52	12.83	-79.64	-35.06	-12.84	-0.95	-4.12
10	1.19	6.13	-72.32	-33.35	-12.95	-2.67	-5.21
Average of | relative error | (%)			77.45	32.76	10.97	3.85	3.11

[a] *Relative Error is calculated by* $(estimated\ SD - real\ SD) \big/ (real\ SD) \times 100$

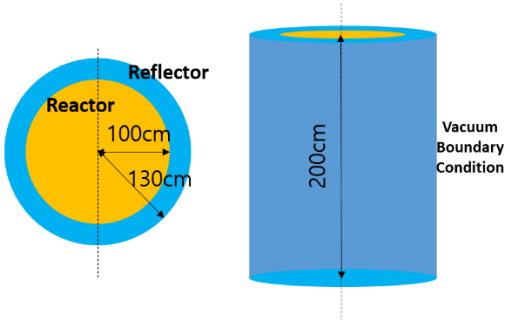

Fig. 4. The Geometry of the Homogenized Cylindrical Reactor

The homogenized reactor was divided into 20 concentric regions to calculate the fission probability Matrix. The fission probability matrix was calculated with 20,000 neutrons and shown in Fig. 5.

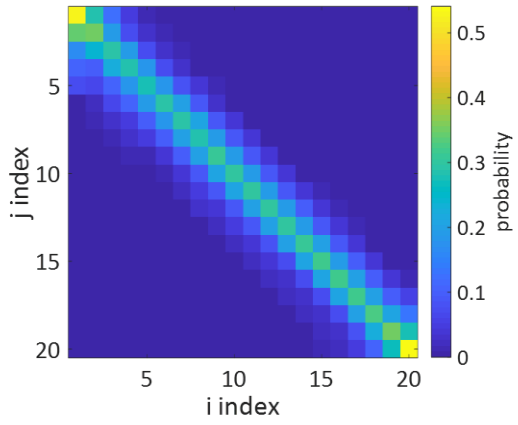

Fig. 5. The Fission Probability Matrix of the Homogenized Cylindrical Reactor

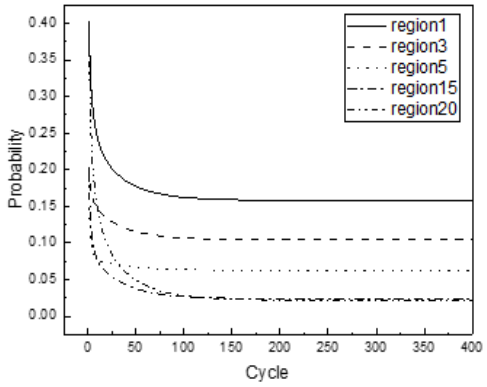

Fig. 6. The Fission Cumulative Probability Matrix of the Homogenized Cylindrical Reactor

In the Fig. 6, the fission cumulative probability of region 20 was converged for the last and it was converged after 200 cycles. By the proposed strategy, the batch size was set to 200. Fluxes of 20 regions were tallied, and the estimated SDs were calculated by changing the batch size. The real SD was calculated by 100 independent MC calculations with different random seed. The results were tabulated in Table II. Two thousands of neutrons per cycle, 500 inactive cycles, and 50,000 active cycles were utilized in the calculations.

When the Gelbard's batch method was not utilized, the estimated SDs of flux were different from the real SDs over 85% in average. When the batch size was 200, the relative error of the estimated standard deviation was about 10%.

3. Conclusions

In this study, a new method to determine the batch size for the Gelbard's batch method was proposed. The main idea is to select the batch size as the gap of cycles of which the cycle-to-cycle correlation is negligible. To calculate the gap of cycles, the fission probability matrix

Table II: Relative Errors of the SDs for the Homogenized Cylindrical Problem by the Batch Size

Tally Region	Flux (10^{-9} / $cm^2 \cdot particle$)	Real Standard Deviation ($\times 10^{-9}$)	[a]Relative Error of Estimated Real Standard Deviation (%)						
			Batch Size 1	10	20	50	100	200	400
1	9.74	54.4	-81.86	-43.31	-33.47	-21.17	-19.09	-18.96	-20.10
2	9.71	49.3	-87.89	-45.98	-34.85	-21.01	-17.6	-18.08	-19.79
3	9.60	44.2	-89.8	-48.52	-36.54	-22.80	-17.92	-17.02	-17.29
4	9.43	38.6	-90.35	-49.83	-37.29	-23.80	-18.05	-15.10	-13.37
5	9.18	32.5	-90.13	-49.99	-37.36	-23.71	-17.11	-12.63	-10.93
6	8.89	26.6	-89.34	-48.41	-35.36	-20.99	-14.60	-8.70	-7.18
7	8.55	21.6	-88.26	-48.14	-35.63	-21.68	-16.08	-10.88	-12.79
8	8.16	17.0	-86.48	-46.53	-34.77	-21.33	-15.34	-10.11	-13.03
9	7.72	12.3	-83.05	-39.18	-28.06	-15.83	-9.89	-6.41	-9.60
10	7.25	9.02	-78.88	-30.14	-20.23	-9.59	-4.35	-2.97	-4.22
11	6.75	6.76	-74.18	-20.39	-9.79	-0.46	4.46	3.36	6.07
12	6.2	6.04	-73.55	-17.93	-6.57	2.31	5.37	0.90	9.83
13	5.63	7.32	-80.05	-34.42	-23.79	-12.03	-11.05	-11.41	-6.42
14	5.04	8.79	-84.84	-44.82	-33.85	-21.07	-18.16	-14.99	-13.96
15	4.43	9.45	-87.18	-48.60	-37.1	-23.95	-19.9	-15.54	-18.55
16	3.81	9.34	-88.30	-49.26	-36.83	-22.73	-16.68	-11.62	-15.00
17	3.18	8.72	-88.83	-48.49	-35.72	-21.95	-15.14	-9.44	-12.01
18	2.55	7.75	-88.99	-47.85	-35.59	-23.30	-16.67	-11.10	-11.77
19	1.93	6.22	-88.31	-45.14	-33.25	-21.69	-16.05	-9.33	-8.06
20	1.35	4.45	-86.41	-40.28	-28.29	-16.26	-10.12	-2.98	0.52
Average of | relative error | (%)			85.33	42.36	30.72	18.38	14.18	10.58	11.52

[a] *Relative Error is calculated by* $(estimated\ SD - real\ SD) \big/ (real\ SD) \times 100$

was utilized. For the verification of proposed strategy, the two problems in the Section 2.3 were solved to apply the proposed method. As a result, the proposed method can provide the batch size for the reliable variance.

To determine the optimum batch size was difficult by the proposed method. It was considered that only correlations between cycles were counted in the proposed method although the real variance is a function of several parameters. However, it is possible to give the guidance of the use of the Gelbard's batch method by the new method. It is expected that the proposed method can be actively utilized for the estimation of the real variance in MC calculations.

4. Acknowledgement

This work was supported by the Energy Efficiency & Resources of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Knowledge Economy (project number: 20171510300470) and the Innovative Technology Center for Radiation Safety (iTRS).

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