A New Approach for Real Variance Estimation Using Local Tally Correlation Between Neighboring Cells

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1. Introduction

It is well-known that the standard deviation for a local tally in Monte Carlo (MC) eigenvalue calculations is underestimated. [1,2] In previous study [3], it was observed that the real-to-apparent standard deviation (SD) ratios for fuel assembly-wise fission powers ranged from 4 to 11 whereas those for pin-wise or core-wise fission powers were close to 1.0. To investigate the cause of the different behaviors of the real-to-apparent SD ratios, the correlation coefficients between the pin and fuel assembly (FA) fission powers were calculated. From the results, it was noted that the correlation coefficients between the pin fission powers in the FA were primarily large positive values. This led to the large positive covariance terms between the pin fission powers without cancellation, and it could explain the large real-to-apparent SD ratio of the FA power. In this study, a new approach for real variance estimations based on the consideration of the local MC tally correlation between neighboring sub-cells are suggested.

2. Methods and Results

2.1 Correlation Coefficients Between Local MC Tallies

To confirm the correlation coefficients between local MC tallies, simple 1D slab problems were considered. We took a 1D slab problems from Ref. [4] and its cross sections are shown in Table I. The slab regions were divided equally into 10 cells, and each cell was also divided equally into 10 sub-cells for local tally estimations. The length of the slab was 10cm. Therefore, the length of a cell and a sub-cell were 1cm and 0.1 cm, respectively.

Table I: Cross sections in 1D slab problem [4]

Case	B.C.*	Width	Σ_t	$\Sigma_{s,0}$	$\nu\Sigma_f$
I	Reflective	10.0	1.0	0.6	0.48

* B.C. = Boundary Condition

The correlation coefficients were calculated from 100 replicas with different random number sequences using 5 active cycles with 200,000 neutron histories per cycle and 100 inactive cycles by McCARD [5] to minimize the inter-cycle correlation. Figure 1 shows the correlation coefficient matrix between cell fission powers, and Fig. 2 displays the correlation coefficient matrix between sub-cell fission powers in Cell 1. In Fig. 2, (X,Y) indicates the Y-th sub-cell in the X-th cell. Accordingly, (1,1) and (10,10) sub-cells locate at the left and right side, respectively.

	Cell 1	Cell 2	Cell 3	Cell 4	Cell 5	Cell 6	Cell 7	Cell 8	Cell 9	Cell 10
Cell 1	1.00	0.90	0.69	0.34	-0.02	-0.46	-0.73	-0.75	-0.66	-0.67
Cell 2	0.90	1.00	0.86	0.51	0.04	-0.51	-0.73	-0.80	-0.74	-0.74
Cell 3	0.69	0.86	1.00	0.76	0.24	-0.38	-0.68	-0.80	-0.80	-0.78
Cell 4	0.34	0.51	0.76	1.00	0.59	-0.05	-0.45	-0.68	-0.75	-0.72
Cell 5	-0.02	0.04	0.24	0.59	1.00	0.48	-0.06	-0.43	-0.52	-0.46
Cell 6	-0.46	-0.51	-0.38	-0.05	0.48	1.00	0.60	0.16	-0.01	0.04
Cell 7	-0.73	-0.73	-0.68	-0.45	-0.06	0.60	1.00	0.73	0.48	0.42
Cell 8	-0.75	-0.80	-0.80	-0.68	-0.43	0.16	0.73	1.00	0.84	0.71
Cell 9	-0.66	-0.74	-0.80	-0.75	-0.52	-0.01	0.48	0.84	1.00	0.87
Cell 10	-0.67	-0.74	-0.78	-0.72	-0.46	0.04	0.42	0.71	0.87	1.00

Fig. 1. Correlation coefficient matrix between cell fission powers.

	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	(1,10)
(1,1)	1.00	0.97	0.95	0.94	0.92	0.92	0.89	0.90	0.89	0.88
(1,2)	0.97	1.00	0.97	0.94	0.92	0.92	0.90	0.91	0.88	0.88
(1,3)	0.95	0.97	1.00	0.97	0.94	0.93	0.91	0.91	0.89	0.89
(1,4)	0.94	0.94	0.97	1.00	0.97	0.95	0.92	0.92	0.89	0.88
(1,5)	0.92	0.92	0.94	0.97	1.00	0.98	0.94	0.92	0.91	0.89
(1,6)	0.92	0.92	0.93	0.95	0.98	1.00	0.97	0.94	0.93	0.91
(1,7)	0.89	0.90	0.91	0.92	0.94	0.97	1.00	0.96	0.94	0.94
(1,8)	0.90	0.91	0.91	0.92	0.92	0.94	0.96	1.00	0.96	0.94
(1,9)	0.89	0.88	0.89	0.89	0.91	0.93	0.94	0.96	1.00	0.96
(1,10)	0.88	0.88	0.89	0.88	0.89	0.91	0.94	0.94	0.96	1.00

Fig. 2. Correlation coefficient matrix between sub-cell fission powers in Cell 1.

As shown in Fig. 1, it was observed that the cell power correlation between neighboring cells is positive, while that between cells positioned far from each other were either negative or close to 0. In contrast, the power correlation between the sub-cells in a cell was strongly all positive, as shown in Fig. 2. Because a cell power is defined as the sum of the sub-cell powers in the cell, a cell power and its uncertainty can be expressed by

$$P^i = \sum_{m=1}^{10} P_m^i, \tag{1}$$

$$\sigma(P^i) = \sqrt{\sum_{m=1}^{10} \sigma^2(P_m^i) + \sum_{m'=1}^{10} \sum_{\substack{m''=1 \\ (m' \neq m'')}}^{10} \operatorname{cov}(P_{m'}^i, P_{m''}^i)}. \tag{2}$$

where P^i and P^i_m are the fission power of the i-th cell and the m-th sub-cell fission power in the i-th cell. By the definition of a correlation coefficient, Eq. (2) can be rearranged by

$$\sigma(P^i) = \sqrt{\sum_{m=1}^{10} \sigma^2(P_m^i) + \sum_{m'=1}^{10} \sum_{\substack{m''=1 \\ (m' \neq m'')}}^{10} \rho(P_{m'}^i, P_{m''}^i) \cdot \sigma(P_{m'}^i) \cdot \sigma(P_{m''}^i)} \quad (3)$$

where $\rho(P_{m'}^i, P_{m''}^i)$ indicates the correlation coefficients between the m'-th and m''-th sub-cell fission power in the *i*-th cell. Therefore, the covariance terms in Eqs. (2) or (3) primarily have large positive values, because the power correlation coefficients between the sub-cells in a cell are strongly all positive as shown in Fig 2.

2.2 Real-to-Apparent SD Ratio Estimation Using Local Tally Correlation Between Neighboring Cells

Because the region-wise or inter-cycle correlations were not considered in the calculation of an apparent SD, the uncertainties of medium-sized region-wise MC tallies (i.e., cell fission power, as shown in Fig. 2) were underestimated by the covariance term. To estimate a real SD, the correlations between sub-cell MC tallies should be exactly considered. That is, an apparent SD should be calculated without consideration of the correlation. From this, the real-to-apparent for a cell-wise tally can be calculated by

$$\frac{\sigma^R(P^i)}{\sigma^A(P^i)} \approx \frac{\sqrt{\sum_{m=1}^{10} \sigma^2(P_m^i) + \sum_{m'=1}^{10} \sum_{\substack{m''=1 \\ (m' \neq m'')}}^{10} \mathrm{cov}(P_{m'}^i, P_{m''}^i)}}{\sqrt{\sum_{m=1}^{10} \sigma^2(P_m^i)}} \quad (4)$$

Assuming that we already know sub-cell fission powers and their statistical uncertainties, the covariance terms are only unknown terms in Eq. (4). These covariance terms can be predicted using the following two approaches:

- Two approaches for real variance estimation
  - (1) Assumption of all correlation coefficients
  - (2) Calculations of covariance terms
    - (2.A) from cycle-wise tallies
    - (2.B) from independent run tallies

First, the assumption of the first approach (Approach 1) means conservative results. If all correlation coefficients are assumed as +1.0 values, larger uncertainties may be calculated by the first approach. In the second approach, the correlation coefficients can be estimated using cycle-wise tallies or independent run tallies for sub-cells. Figure 3 shows the real-to-apparent SD ratio results from the two approaches and reference results for the 1D slab problem using the same neutron history condition. In Fig. 3, the dashed lines represent the real-to-apparent SD ratio calculated by assuming single correlation coefficients (Approach 1). The reference solutions distributed across the results calculated by assuming that all correlation coefficients are +0.75 and +0.25. Therefore, this approach with the assumption of all correlation coefficients may provide a helpful guideline for users to recognize the range of real-to-apparent SD ratios.

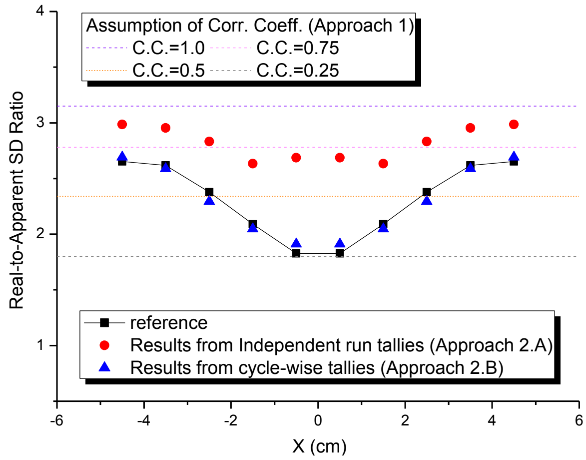

Fig. 3. Real-to-Apparent SD ratios using the two approaches based on the local tally correlation for the 1D slab problem.

In Fig. 3, the blue triangles and red cycle points indicate the results calculated by the covariance terms from cycle-wise tallies (Approach 2.A) and independent run tallies (Approach 2.B), respectively. It was noted that the real-to-apparent SD ratios from cycle-wise tallies agree well with the reference solutions. Meanwhile, the real-to-apparent SD ratios from independent run tallies at both boundary cells are close to the reference. All calculations are performed by McCARD except the calculations of the correlation coefficients from cycle-wise tallies, which are herein calculated by the in-house multi-group MC code Roulette. [6]

2.3 Dependency of Real Variance on the Number of Active Cycles

To examine the dependence of the real variance of the local tallies and their correlation between neighboring sub-cells on the number of active cycles with a fixed total neutron history, the real-to-apparent SD ratios of Cell 1 for the slab problem were calculated. The detailed calculation conditions for the real variance estimation are:

- Number of inactive cycles: 100
- Total neutron histories for active cycles: 1,000,000 (fixed).
- N (number of active cycles): 1, 2, 5, 10, 20, 100, 1000

For a representative unit value for local tally correlation, a root-sum-square (RSS) of correlation coefficient is defined by

$$RSS(P^{i}) = \sqrt{\sum_{m'=1}^{10}\sum_{m''=1}^{10}\left(\rho(P_{m'}^{i}, P_{m''}^{i})\right)^{2}}. \quad (5)$$

In a 10x10 correlation matrix case, the maximum RSS is 10.0 whereas the minimum is $\sqrt{10}$.

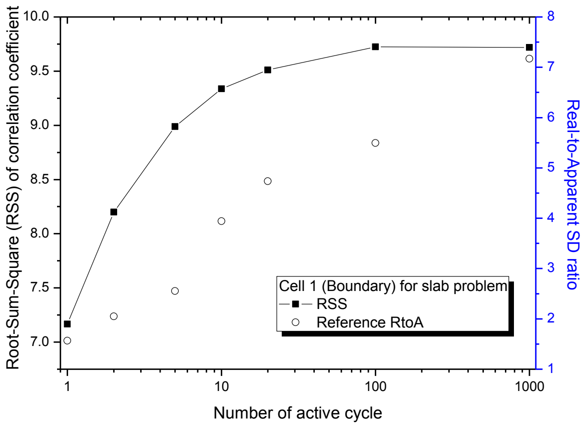

Fig. 4. Root-Sum-Square (RSS) of correlation coefficients and reference Real-to-Apparent SD ratios due to the number of active cycles with a fixed neutron history for Cell 1.

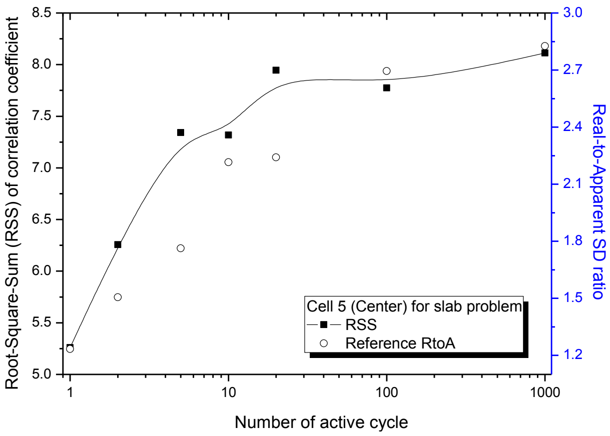

Fig. 5. Root-Sum-Square (RSS) of correlation coefficients and reference Real-to-Apparent SD ratios due to the number of active cycles with a fixed neutron history for Cell 5.

Figures 4 and 5 show the RSS values and reference real-to-apparent SD ratio values in Cell 1 and Cell 5, respectively. As explained in previous study [7], it was observed that the variance bias and the RSS value decrease as the number of active cycles (N) decreases. To understand the behaviors of the RSS value of correlation coefficients, the correlation coefficient matrix between neighboring sub-cells in Cell 1 is presented in Figs. 6a and 6b for N=1000 and N=1, respectively. It is noted that the effect by region-wise correlation decreased.

	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	(1,10)
(1,1)	1.00	0.98	0.98	0.97	0.96	0.96	0.95	0.95	0.95	0.94
(1,2)	0.98	1.00	0.99	0.98	0.97	0.97	0.96	0.96	0.96	0.94
(1,3)	0.98	0.99	1.00	0.99	0.98	0.97	0.96	0.96	0.96	0.95
(1,4)	0.97	0.98	0.99	1.00	0.99	0.98	0.97	0.97	0.96	0.95
(1,5)	0.96	0.97	0.98	0.99	1.00	0.99	0.98	0.98	0.96	0.96
(1,6)	0.96	0.97	0.97	0.98	0.99	1.00	0.99	0.98	0.97	0.97
(1,7)	0.95	0.96	0.96	0.97	0.98	0.99	1.00	0.99	0.97	0.96
(1,8)	0.95	0.96	0.96	0.97	0.98	0.98	0.99	1.00	0.98	0.98
(1,9)	0.95	0.96	0.96	0.96	0.96	0.97	0.97	0.98	1.00	0.99
(1,10)	0.94	0.94	0.95	0.95	0.96	0.97	0.96	0.98	0.99	1.00

Fig. 6a. Correlation coefficient matrix between sub-cell fission powers in Cell 1 (N=1,000).

	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	(1,10)
(1,1)	1.00	0.85	0.78	0.64	0.62	0.56	0.48	0.46	0.44	0.48
(1,2)	0.85	1.00	0.86	0.71	0.65	0.59	0.56	0.52	0.43	0.50
(1,3)	0.78	0.86	1.00	0.81	0.74	0.67	0.65	0.64	0.56	0.57
(1,4)	0.64	0.71	0.81	1.00	0.84	0.71	0.69	0.66	0.56	0.60
(1,5)	0.62	0.65	0.74	0.84	1.00	0.83	0.79	0.69	0.64	0.61
(1,6)	0.56	0.59	0.67	0.71	0.83	1.00	0.91	0.81	0.71	0.68
(1,7)	0.48	0.56	0.65	0.69	0.79	0.91	1.00	0.84	0.70	0.66
(1,8)	0.46	0.52	0.64	0.66	0.69	0.81	0.84	1.00	0.80	0.68
(1,9)	0.44	0.43	0.56	0.56	0.64	0.71	0.70	0.80	1.00	0.80
(1,10)	0.48	0.50	0.57	0.60	0.61	0.68	0.66	0.68	0.80	1.00

Fig. 6b. Correlation coefficient matrix between sub-cell fission powers in Cell 1 (N=1).

3. Conclusions

In this study, a new approach for real variance estimation based on the local tally correlation was introduced. In this new approach, the correlation coefficients between neighboring sub-cells are required. The correlation coefficients can be predicted by assumption or the calculations from cycle-wise tallies or independent run tallies. To examine the new approach, a 1D slab problem was considered. The approach by assuming all correlation coefficients (Approach 1) will provide a helpful guideline for users to recognize the range of real-to-apparent SD ratios. The approaches by the covariance terms from cycle-wise tallies (Approach 2.A) and independent run tallies (Approach 2.B) predict the real variance well. There is an additional point to be considered in the real-to-apparent SD ratio estimation with the new approaches. The cell or region should be finely divided into sub-cells so that its real-to-apparent SD should be close to 1.0.

The dependency of the real variance on the number of active cycles was also examined, under the constraint that the total number of neutron histories was fixed. It is observed that the number of active cycles have a large influence in the real-to-apparent SD ratio estimation. In the near future, the inter-cycle correlation should be considered for the new approach additionally.

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