Implementation of History-based Batch Method in the iMC Monte Carlo Code for an Improved Variance Estimation

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1. Introduction

In reactor analysis, the Monte Carlo (MC) method is widely recognized as one of the most accurate and realistic simulation techniques, particularly because it effectively models continuous-energy cross sections and complex geometries with minimal assumptions. Given its stochastic nature, the MC method yields both mean values and their associated uncertainties—an inclusion that is essential for a meaningful interpretation of the simulation results.

For steady-state (eigenvalue) Monte Carlo simulations, neutron behavior is modeled stochastically by updating the fission source distribution (FSD) through successive cycle by cycle iterations, and employs a normalization method that scales with the fission source count [1]. Due to the intercycle correlations inherent in the FSDs, the estimates obtained for a tally from individual cycles become interdependent, which in turn biases the sample standard deviation (SD) calculated for the tally's mean value [2].

Several methods have been proposed to quantify the variance bias—that is, the discrepancy between the true variance and the sample variance of the tally mean [3-6]. Notably, the history-based batch method (HBM) [7] has demonstrated considerable success and has been recently adapted for Dynamic Monte Carlo simulations in transient calculations [8].

Recently, the history-based batch method was integrated into the iMC code developed at the Korea Advanced Institute of Science and Technology (KAIST) [9-10]. This paper provides a concise overview of the method, details its implementation within the iMC framework, and presents preliminary results that highlight its effectiveness in enhancing uncertainty estimation.

2. History-based Batch Method

Consider a Monte Carlo eigenvalue simulation with N active cycles, each comprising M neutron histories. Let Q_{ij} represent the tally Q estimate obtained from the j'th neutron history in the i'th cycle. The mean value of Q and its sample variance are computed as follows:

$$\bar{Q} = \frac{1}{NM}\sum_i \sum_j Q_{ij} \,, \tag{1}$$

$$\sigma_S^2[\bar{Q}] = \frac{1}{NM(NM-1)}\sum_i \sum_j \left(Q_{ij} - \bar{Q}\right)^2 . \tag{2}$$

The real variance of the tally mean $\bar{Q}$ is written as

$$\begin{aligned} \sigma^2[\bar{Q}] &= E[\bar{Q}^2] - E[\bar{Q}]^2 \\ &= \frac{1}{NM}\sigma^2[Q_{ij}] \\ &+ \frac{1}{(NM)^2}\sum_{i,j} \sum_{i',j' \neq i,j} \mathrm{cov}\left[Q_{ij}, Q_{i'j'}\right] , \end{aligned} \tag{3}$$

where $\mathrm{cov}[Q_{ij}, Q_{i'j'}]$ denotes the covariance between Q_{ij} and $Q_{i'j'}$ and E [·] is the estimate of variable within the brackets.

The estimate of the sample variance is referred to as the apparent variance $\sigma_A^2[\bar{Q}] = E\left[\sigma_S^2[\bar{Q}]\right]$, which always underestimates the real variance. The discrepancy between the two can be expressed as

$$\begin{aligned} &\sigma^2[\bar{Q}] - \sigma_A^2[\bar{Q}] \\ &= \frac{1}{NM(NM-1)}\sum_{i,j} \sum_{i',j' \neq i,j} \mathrm{cov}\left[Q_{ij}, Q_{i'j'}\right] . \end{aligned} \tag{4}$$

Further details concerning the derivation of Eq. (4) can be found elsewhere [7].

The history-based batch method addresses this discrepancy by reinterpreting a Monte Carlo eigenvalue simulation with N active cycles and M histories per cycle as N_B separate batch runs, each comprising N active cycles and M/N_B histories per cycle. However, this straightforward re-partitioning does not guarantee preservation of the original tally mean $\bar{Q}$ since the normalization of fission source weights is performed using M/N_B histories per cycle rather than the full M. Note that the weight of fission sources for cycle i in the conventional MC run is calculated as

$$w_i = M/M_i \,, \tag{5}$$

where M_i is the number of fission sources generated from the previous (i-1)'th cycle.

To exploit the multiple-run strategy for enhancing sample independence while maintaining the original tally mean value, the history-based batch method with weight correction organizes batches by grouping histories that share common ancestors. To compute each batch tally Q^k

(k = 1, 2, …, N_B) that remain intact from the normalization dependency, we introduce a weight correction factor, f_i^k, for each batch.

$$f_i^k = \frac{w_i^k}{w_i} = \frac{(M_i/N_B)}{M_i^k}, \tag{6}$$

where w_i^k and M_i^k denotes source weight and number for k'th history batch in the i'th cycle respectively. Note that w_i^k is defined as

$$w_i^k = (M/N_B)/M_i^k, \tag{7}$$

which resembles Eq. (5).

The weight correction factor adjusts the source weight for each batch based on a batch size of M/N_B during the tallying of Q^k, where the batch size denotes the number of histories assigned to each batch. Notably, the original transport process remains unaltered; only the particle weights used in the tallying of Q^k are modified by f_i^k.

Then, the obtained batch tally can be expressed as

$$Q^k = \frac{1}{N(M/N_B)} \sum_{i=1}^{N} \sum_{j\in k} f_i^k Q_{ij}, \tag{8}$$

and its mean and sample variance can be obtained as

$$\bar{Q}_{HB} = \frac{1}{N_B} \sum_{k=1}^{N_B} Q^k = \frac{1}{NM} \sum_{i=1}^{N} \sum_{k=1}^{N_B} \sum_{j\in k} f_i^k Q_{ij}, \tag{9}$$

$$\sigma^2[\bar{Q}_{HB}] = \frac{1}{N_B(N_B-1)} \sum_{k=1}^{N_B} (Q^k - \bar{Q}_{HB})^2. \tag{10}$$

In summary, the $\bar{Q}_{HB}$ obtained using the history-based batch method is unaffected by both genealogical and normalization effects, and its variance, $\sigma^2[\bar{Q}_{HB}]$, serves as a close approximation of the true variance, $\sigma^2[\bar{Q}]$. Additional details on the history-based batch method are provided in Ref. 7.

3. Numerical Results

The history-based batch method for enhanced variance estimation has been integrated into the iMC code. During its implementation, significant fluctuations in batch sizes were observed as cycles progressed, with some batches even receiving no source allocations. To address this issue, the number of fission banks, n, stored during the Monte Carlo run was adjusted as follows:

$$n = \mathrm{int}\left[w_i \cdot \frac{1}{k_{eff}} \frac{\nu\sigma_f}{\sigma_t} \cdot f_i^k + \xi \right], \tag{11}$$

where k_{eff} is the multiplication factor, ξ is the uniform random number, int[·] is the integer operator, and the other notations are that of the convention. Excluding f_i^k from Eq. (11) reverts the simulation to a conventional MC run. The impact of incorporating this weight correction factor on determining the number of stored fission banks will be discussed.

To evaluate the accuracy of the history-based batch method implemented in the iMC code, this study employs an expanded version of the C5G7 benchmark. Figure 1 illustrates the overall configuration of the problem, which utilizes the multi-group cross section data specified in the OECD/NEA C5G7 benchmark report [11].

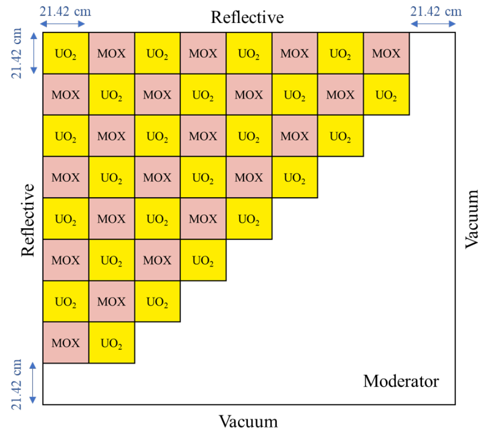

Fig 1. Enlarged C5G7 benchmark layout.

The MC run was executed using 500,000 histories per cycle, comprising 50 inactive cycles followed by 200 active cycles. The pCMFD acceleration technique was applied during the inactive cycles to expedite fission source convergence [12]. The reference result, representing the true variance, was derived from 50 independent batch runs.

Figure 2 shows the calculated multiplication factor for different history-based batch sizes. The label "apparent" denotes the conventional tally mean and its associated apparent variance, i.e., Eq. (2), with HBM-related treatment being employed. The "history batch" refers to the mean and variance obtained from history-based batch-wise values. The blue lines indicate the mean and the real variance, along with a 2σ range, as determined from independent batch runs without any HBM-related treatment being employed.

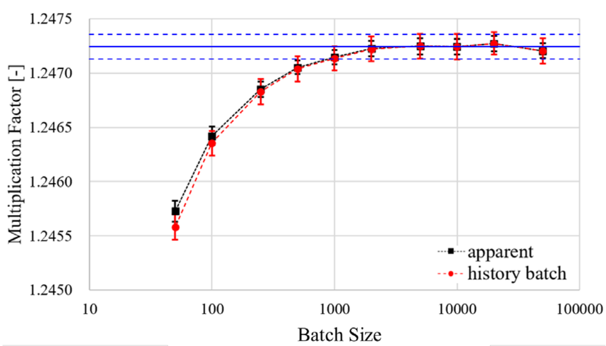

Fig 2. Calculated k_{eff} values for different batch sizes.

It is important to note that when relatively few particles are allocated to each history batch, the conventional tally mean, $\bar{Q}$, tends to be underestimated. This bias arises from the inclusion of the weight correction factor, f_i^k, in Eq. (11) when estimating the number of stored fission banks. A similar trend is observed for the batch tally mean, $\bar{Q}_{HB}$. These observations suggest that ensuring a sufficiently large number of particles per history batch is crucial for preserving the tally mean while achieving reliable variance estimation. Figure 3 illustrates 10 independent runs with a batch size of 5,000, where all trials yield acceptable tally means and improved variance estimates. Note that mean value obtained from Eq. (1) is portrayed in the cartoon.

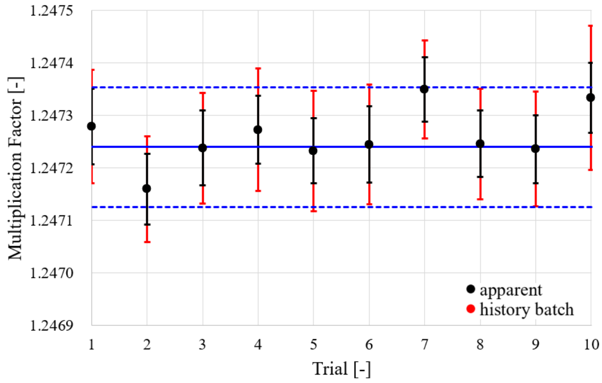

Fig 3. Independent MC runs with batch size of 5,000.

The tallied power density distribution was also examined. Figures 4 and 5 display the mean distribution and its corresponding real variance, respectively. The power distribution along the red axis in Fig. 4 was evaluated for a history batch size of 5,000, as illustrated in Figs. 6 and 7. The results indicate that while the tally means are preserved, the uncertainty from the history-based batch method closely approximates that of the reference. To assess the effect of varying batch sizes, the power density at the position with the highest value was compared, with Fig. 8 showing changes in the estimates similar to those observed in Fig. 2.

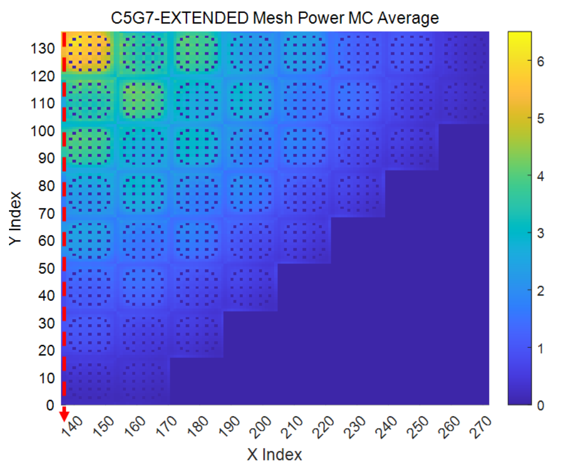

Fig 4. Reference power density distribution (mean value).

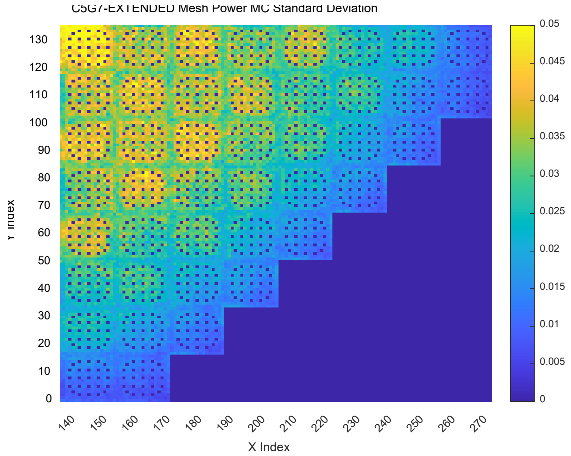

Fig 5. Reference power density distribution (uncertainty).

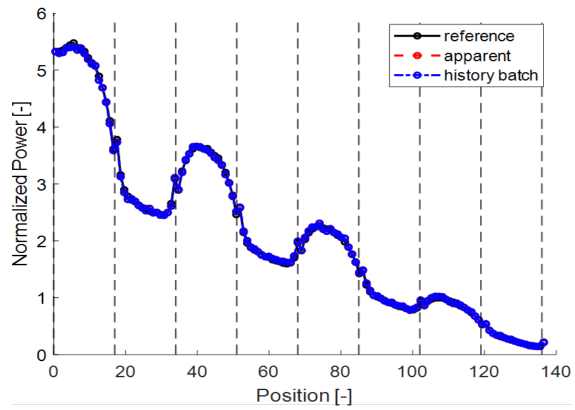

Fig 6. Power density distribution along the red axis (mean value) with batch size of 5,000.

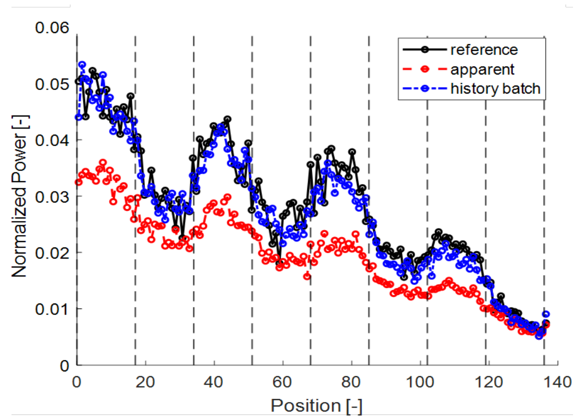

Fig 7. Power density distribution along the red axis (uncertainty) with batch size of 5,000.

Both the conventional tally mean, $\bar{Q}$, and the batch tally mean, $\bar{Q}_{HB}$, tend to decrease as the batch size decreases. To assess the normality of the batch-wise tallies, Q^k, we performed a p-value test based on the D'Agostino-Pearson K² test [13]. Table 1 lists the calculated p-values for both the multiplication factor and the power density at the location with the highest value across various batch sizes.

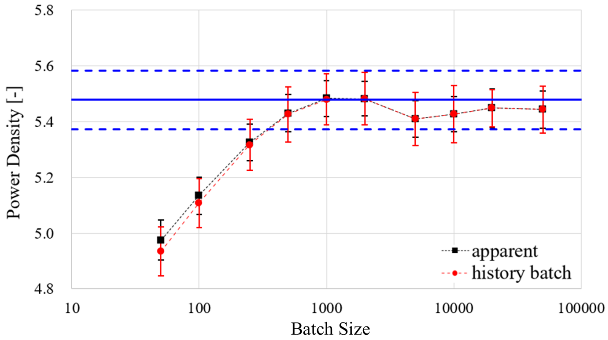

Fig 8. Calculated power density value at the largest position for different batch size.

Table 1. P-values for k_{eff} and power density

Batch size	k_{eff}	Power density
50,000	0.63	0.10
20,000	0.52	0.72
10,000	0.90	0.70
5,000	0.44	0.84
2,000	0.74	0.27
1,000	0.95	0.20
500	0.76	0.00
250	0.03	0.00
100	0.00	0.00
50	0.00	0.00

Analysis indicates that when using a small batch size—say, fewer than 1,000 for this run—the p-value drops below 0.05, which is the typical threshold for rejecting the null hypothesis. Although the variance obtained from the batch tallies, $\sigma^2[\bar{Q}_{HB}]$, appears acceptable even with reduced batch sizes, it is important to note that the distribution deviates from normality. Using a larger batch size sometimes leads to a reduction in the p-value; however, this is not a concern since it always remains above the prescribed significance level of 0.05. In summary, selecting a sufficiently large batch size is essential for maintaining the tally mean and ensuring reliable uncertainty estimates in the history-based batch method currently implemented in the iMC code.

4. Conclusions

In this work, the overall concept of the history-based batch method has been revisited, and its implementation in the iMC code is presented. Grouping source banks into batches initially resulted in significant fluctuations in the number of stored fission banks as the simulation cycles progressed. To address this issue, a weight correction factor was introduced during the determination of the fission bank count, which had led to bias in the tally mean when small batch sizes were employed.

Nevertheless, analysis of the enlarged C5G7 benchmark demonstrates the effectiveness of the implemented history-based batch method in improving the accuracy of uncertainty estimation. With a moderate batch size, the tally mean is maintained and the estimated uncertainty closely approximates the reference (real variance). Future research will explore the applicability of this method to fast spectrum reactors, along with further refinement of the algorithm to reliably preserve the tally mean.

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