Real Variance Estimation using Spectral Analysis Method in Monte Carlo Criticality Calculation with p-CMFD Feedback

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1. Introduction

The framework of the continuous-energy Monte Carlo (MC) criticality calculation with the partial current-based coarse-mesh finite difference (p-CMFD) feedback (MC/p-CMFD) have been proposed [1,2]. The effects of the MC/p-CMFD are 1) acceleration of the convergence speed in the fission source distributions (FSDs) and 2) real variance reduction in the local MC tallies by reducing the inter-cycle correlation.

On the other hand, the estimation of the real variance of the sample mean has been a big challenge in the MC criticality calculation [3]. The conventional way to estimate variance from a single batch run neglects the inter-cycle correlation, which leads to the significant underestimation. To estimate the real variance, the inter-cycle covariance of a MC tally should be considered [4,5].

Recently, the spectral analysis method which is widely used in covariance stationary simulation [6] is applied to the MC criticality calculation [7,8]. The discrete Fourier transformation is applied to a MC tally in the time domain (cycle) to estimate the spectral density in the frequency domain. Then, the spectral density at frequency zero is used to estimate the real variance of the sample mean, where the inter-cycle covariance is inherently considered.

The problem in the spectral analysis method is that the periodogram at frequency zero is not a consistent estimator of the spectral density at frequency zero and also biased. Thus, the spectral density at frequency zero is indirectly estimated by the local average over the periodograms near frequency zero. Depending on the number of periodograms used in the local average, there is a trade-off between the bias and the variance of the real variance.

In this paper, the spectral analysis method is applied to estimate the real variances of the local MC tallies in the MC/p-CMFD. In numerical results, it is shown that the p-CMFD feedback not only reduces the real variance itself, but also makes it possible to reduce the variance of the estimated real variance by the spectral analysis method without losing significant accuracy.

2. MC Criticality Calculation with p-CMFD Feedback (MC/p-CMFD)

In this section, the MC/p-CMFD is briefly described. The detailed description is given in Refs. [1,2]. When the reactor problem is discretized into I coarse-mesh cells, the MC/p-CMFD calculation at cycle l can be written as:

$$S_{MC}^{(l)}(\vec{r}) = \frac{1}{k_{pCMFD}^{(l-1)}} \sum_{i=1}^{I} \int_{\vec{r}' \in V_i} dV' \int dE \int dE' \times H(\vec{r}', E' \to \vec{r}, E) \left(\chi(E') S_{MC}^{(l-1)}(\vec{r}') f_i^{(l-1)} \right), \quad (1)$$

where $H(\vec{r}', E' \to \vec{r}, E)$ is the number of fission neutrons born at $(\vec{r}, E)$ produced by a fission neutron born at $(\vec{r}', E')$, $S_{MC}^{(l-1)}(\vec{r})$ is the FSDs being used in the current MC cycle, $f_i^{(l-1)}$ is the weight correction factor for the p-CMFD feedback, $S_{MC}^{(l)}(\vec{r})$ is the newly sampled FSDs from the current cycle, and $k_{pCMFD}^{(l-1)}$ is the k-eigenvalue obtained from the previous p-CMFD calculation.

For each MC cycle, the p-CMFD equation is constructed based on the coarse-mesh MC tallies, as:

$$\frac{1}{V_i} \sum_j A_{ij} \left(\left(\tilde{D}_{MC,ij}^{(l)} + \hat{D}_{MC,ij}^{+,(l)} \right) \phi_{pCMFD,i}^{(l)} - \left(\tilde{D}_{MC,ij}^{(l)} + \hat{D}_{MC,ij}^{-,(l)} \right) \phi_{pCMFD,j}^{(l)} \right) + \Sigma_{MC,removal,i}^{(l)} \phi_{pCMFD,i}^{(l)} = \frac{\Sigma_{MC,production,i}^{(l)} \phi_{pCMFD,i}^{(l)}}{k_{pCMFD}^{(l)}}, \quad \text{for } i = 1 \text{ to } I, \quad (2)$$

where $\Sigma_{MC,removal,i}^{(l)}$ and $\Sigma_{MC,production,i}^{(l)}$ are the removal and production homogenized cross sections, respectively. $\hat{D}_{MC,ij}^{+,(l)}$ and $\hat{D}_{MC,ij}^{-,(l)}$ are the outgoing and incoming partial current correction factors, respectively, at the coarse-mesh cell interface j, while $\tilde{D}_{MC,ij}^{(l)}$ is an arbitrary diffusion coupling coefficient. In these notations, the subscript "MC" and superscript "(l)" indicates that the quantities are obtained from the MC cycle l

The solution of the p-CMFD equation, which are $k_{pCMFD}^{(l)}$ and $\vec{\phi}_{pCMFD}^{(l)} = \left[\phi_{pCMFD,1}^{(l)},...,\phi_{pCMFD,I}^{(l)}\right]^T$ is obtained by the usual power iteration method. Then the weight correction factor for the next MC cycle is updated as:

$$f_i^{(l)} = \frac{S_{pCMFD,i}^{(l)} \Big/ \sum_{i=1}^{I} S_{pCMFD,i}^{(l)}}{S_{MC,i}^{(l)} \Big/ \sum_{i=1}^{I} S_{MC,i}^{(l)}} , \quad (3)$$

where $S_{pCMFD,i}^{(l)} = V_i \Sigma_{MC,production,i}^{(l)} \phi_{pCMFD,i}^{(l)}$ is the number of fission neutrons in coarse-mesh cell *i* obtained from the p-CMFD calculation, $S_{MC,i}^{(l)}$ is that obtained from the MC calculation.

It is noted that the p-CMFD feedback accelerates the convergence of the FSDs during inactive cycles and reduces the real variance in the local MC tallies by reducing the inter-cycle covariances.

3. Estimation of Real Variance using Spectral Analysis Method

From a single batch run, the sample mean of the MC tally is expressed as:

$$\bar{Q} = \frac{1}{L_{active}} \sum_{l=1}^{L_{active}} Q^{(l)} , \quad (4)$$

where L_{active} is the number of active cycles, and $Q^{(l)}$ is the MC tally obtained from *l*-th active cycle.

Then, the real variance of the sample mean is expressed as:

$$\begin{aligned} \sigma_{real}^2(\bar{Q}) &= \frac{1}{{L_{active}}^2} \sigma^2 \left(\sum_{l=1}^{L_{active}} Q^{(l)} \right) \\ &= \frac{1}{{L_{active}}^2} \left(\sum_{l=1}^{L_{active}} \sum_{m=1}^{L_{active}} \gamma^{(l-m)} \right) , \\ &= \frac{1}{L_{active}} \left(\sum_{h=-L_{active}}^{L_{active}} \left(1 - \frac{|h|}{L_{active}} \right) \gamma^{(h)} \right) , \end{aligned} \quad (5)$$

where $\gamma^{(h)}$ is lag-covariance of $Q^{(l)}$ and $Q^{(l+h)}$ with *h* lagging cycles. As L_{active} goes to infinity, $L_{active}\sigma_{real}^2(\bar{Q})$ becomes $\sum_{h=-\infty}^{\infty} \gamma^{(h)}$. Thus, the real variance can be asymptotically approximated as

$$\sigma_{real}^2\left[\bar{Q}\right] \approx \frac{1}{L_{active}} \sum_{h=-\infty}^{\infty} \gamma^{(h)} . \quad (6)$$

In spectral analysis, $\gamma^{(h)}$ is considered as a signal in the time domain, which can be decomposed into a number of discrete frequencies. The spectral density at certain frequency is expressed as:

$$f(\omega) = \frac{1}{2\pi} \sum_{h=-\infty}^{\infty} \gamma^{(h)} e^{ihw} \quad \omega \in (-\pi, \pi) , \quad (7)$$

where *i* is the imaginary number.

The spectral density at frequency ω = 0 gives

$$f(0) = \frac{1}{2\pi} \sum_{h=-\infty}^{\infty} \gamma^{(h)} . \quad (8)$$

Then, the real variance based on the spectral analysis method is expressed as:

$$\sigma_{spec}^2\left[\bar{Q}\right] = \frac{2\pi f(0)}{L_{active}} . \quad (9)$$

To estimate the spectral density, the periodogram based on the Fourier transformation of the discrete time domain data $Q^{(l)}$ is used as:

$$\begin{aligned} I(\omega_k) &= \frac{1}{2\pi L_{active}} \left| \sum_{l=1}^{L_{active}} Q^{(l)} e^{-il\omega_k} \right|^2 \\ &= \frac{1}{2\pi L_{active}} \left(\left(\sum_{l=1}^{L_{active}} Q^{(l)} \cos(l\omega_k) \right)^2 + \left(\sum_{l=1}^{L_{active}} Q^{(l)} \sin(l\omega_k) \right)^2 \right) \end{aligned} \quad (10)$$

where $\omega_k = \frac{2\pi k}{L_{active}}$ is the *k*-th Fourier frequency.

Referring to Ref. [9], the periodogram at non-zero frequency is an asymptotically unbiased estimator of the spectral density as L_{active} goes to infinity, while the variance is proportional to the square of the periodogram, which does not decrease as L_{active} increases. Furthermore, the periodogram at frequency zero is even biased.

For the consistent estimation of the spectral density at frequency zero, the local average of the periodograms near frequency zero is used as:

$$\hat{f}(0) = \frac{1}{M} \sum_{m=1}^{M} I(\omega_m) , \quad (10)$$

where *M* is the number of the periodograms used to estimate the local average.

Using the Taylor series analysis, Ref. [8] shows that the bias of $\hat{f}(0)$ is approximated as:

$$E\left[\hat{f}(0)\right]-f(0)\approx\frac{\pi f'(0)(M+1)}{L_{active}}, \qquad (11)$$

while the variance of $\hat{f}(0)$ is approximated as:

$$\sigma^2\left[\hat{f}(0)\right]\approx\frac{1}{M^2}\sum_{m=1}^{M}f^2(w_k). \qquad (12)$$

As M increases, the bias increases and the variance decreases. Thus, there is a trade-off between the bias and the variance of the real variance. The memory requirement for the spectral analysis method is M times larger than that for the conventional sample variance which neglects the inter-cycle covariance.

4. Numerical Results

The benchmark problem is one-dimensional, one-group reactor problem, as show in Fig. 1. The cross section of artificial fuel material is shown in Table I.

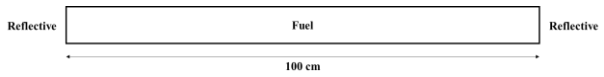

Figure 1 Configuration of benchmark problem.

Table I Cross sections for benchmark problem

Cross Sections	Value	Cross Sections	Value
Σ_t	0.50 cm^{-1}	Σ_f	0.06 cm^{-1}
Σ_s*	0.40 cm^{-1}	ν	2.0
Σ_c	0.04 cm^{-1}	k_{eff}	1.2

*Scattering is isotropic.

For both the conventional MC and the MC/p-CMFD, 1,000 history per cycle, 20 inactive cycles, 1,000 active cycles, and 50 independent batch runs are performed, where the flux tally bins are set as 1cm x 100. For the p-CMFD feedback, five coarse mesh cells are used.

Figure 2 shows the flux distributions averaged over 50 independent batch runs with an error bar indicating the real standard deviation (SD). The real SD of the MC/p-CMFD becomes 2.88 times smaller in average, compared to that of the conventional MC.

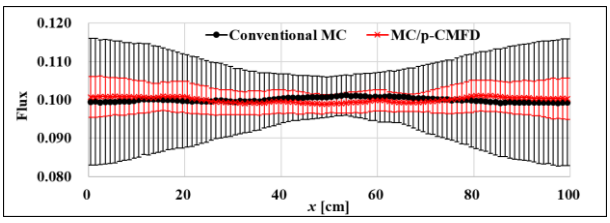

Figure 2 Flux distributions averaged over 50 independent batch runs, where error bar indicates real SD.

Figure 3 shows the periodograms obtained from the conventional MC and the MC/p-CMFD at tally bins 1 (0 ~ 1 cm), 15 (14 ~ 15 cm), 30 (29 ~ 30 cm), 50 (49 ~ 50 cm). The p-CMFD feedback reduces the periodogram near frequency zero and makes the periodogram flat over the frequency.

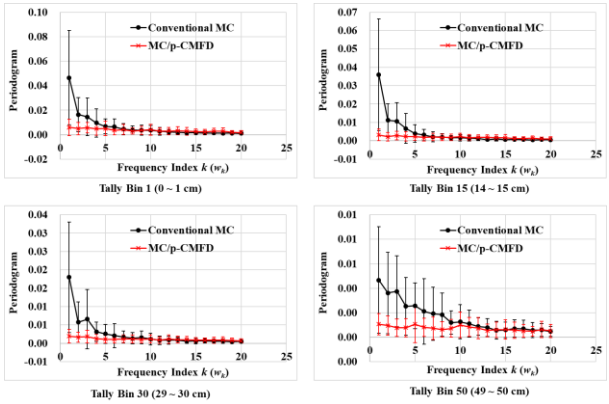

Figure 3 Periodograms averaged over 50 independent batch runs, where error bar indicates sample standard deviation of periodogram.

Figure 4 shows the real SD, apparent SD, and the SDs estimated by the spectral analysis method (spectral SDs) with M = 1, 5, 10, and 20 in the conventional MC, where the spectral SDs are averaged over the 50 independent batch runs. Figure 5 shows the corresponding quantities for the MC/p-CMFD. As M increases, the spectral SD underestimates the real SD in the conventional MC, while the accuracy of the spectral SD is almost maintained in the MC/p-CMFD.

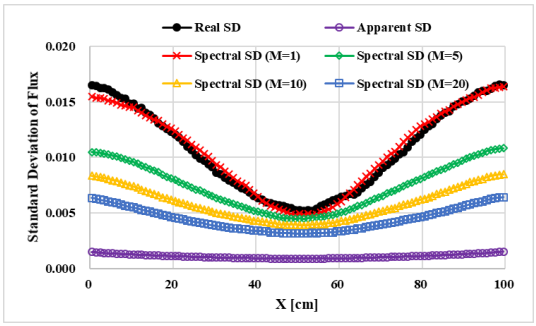

Figure 4 Comparisons of real SD, apparent SD, and spectral SDs (M= 1, 5, 10, and 20) in conventional MC.

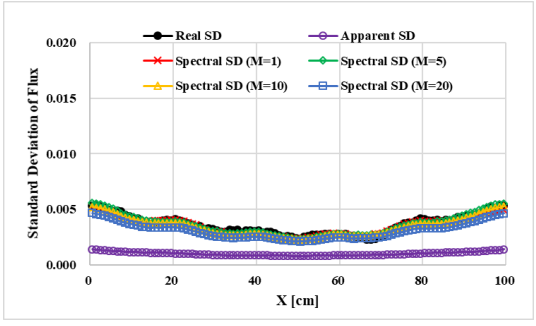

Figure 5 Comparisons of real SD, apparent SD, and spectral SDs (M= 1, 5, 10, and 20) in MC/p-CMFD.

Figures 5 and 6 compares the relative SD [%] of the spectral SDs, estimated by the 50 independent batch runs for different M (M = 1, 5, 10, and 20) in the conventional MC and the MC/p-CMFD, respectively. For both the conventional MC and the MC/p-CMFD, the relative SD of the spectral SD decreases, as M increases. For M = 20, the relative SD of the spectral SD in the conventional MC is around 18%, while that in the MC/p-CMFD is around 12%.

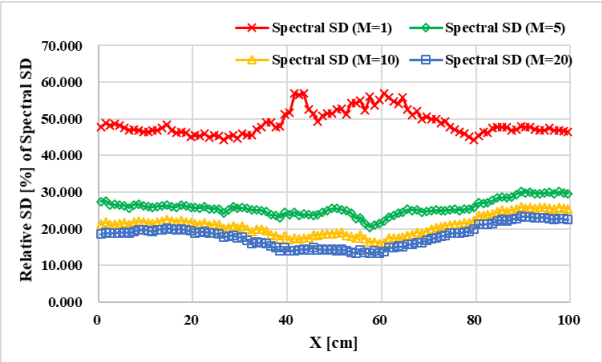

Figure 6 Comparisons of relative SD [%] of spectral SD for different M (M = 1, 5, 10, and 20) in conventional MC.

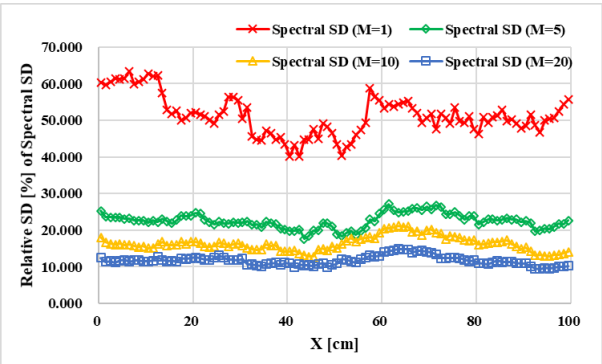

Figure 7 Comparisons of relative SD [%] of spectral SD for different M (M = 1, 5, 10, and 20) in MC/p-CMFD.

5. Summary and Conclusions

The spectral analysis method was applied to estimate the real variances of the local MC tallies in the MC/p-CMFD. It was shown that the p-CMFD feedback not only reduces the real variance itself, but also makes it possible to reduce the variance of the spectral SD by averaging the periodogram near frequency zero without losing significant accuracy.

In the time domain (cycle), the p-CMFD feedback efficiently accelerates the convergence of the FSDs by reducing slowly decaying error component, which is the low frequency error component in the frequency domain [10]. Thus, the periodogram near frequency zero is reduced and the periodogram becomes flat over the frequencies. Equation (11) explains that the flattened periodogram reduces the bias, which is proportional to $f'(0)$.

It should be also noted that the bias is inversely proportional to the active cycle length. For the accurate estimation of real variance by the spectral analysis method, a sufficient number of active cycles is required.

As further studies, the cycle length control in terms of the accuracy of the spectral SD will be performed. Of course, a synergetic application of the p-CMFD feedback and the spectral analysis method will be investigated in the continuous-energy whole-core problem. Furthermore, the investigation of the appropriate filter for the spectral analysis method is also viable.

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