Inter-cycle Correlation Estimation in Monte Carlo Criticality Calculations

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1. Introduction

In Monte Carlo computation, many practitioners estimate statistical error through sample variance. But the sample variance is biased in Monte Carlo criticality calculations because the fission source distributions (FSDs) are correlated cycle-to-cycle [1,2,3,4]. When the dominance ratio is close to unity, the inter-cycle correlation becomes strong and the sample variance is quite different from the real variance [3].

A mathematical model for the correlation between FSDs in successive cycles was developed by Gelbard and Prael [1]. In this model, the error of FSD at a certain cycle is expressed by the stochastic errors that propagates cycle-by-cycle. The cycle-by-cycle error propagation model has been used for predicting the behavior of the inter-cycle correlation of *k* or local region's tallies [2,3].

This paper is designed to demonstrate that inter-cycle correlation coefficient between FSDs can be calculated by utilizing cycle-by-cycle error propagation model in combination with the fission matrix constructed from a single Monte Carlo run. To do so, an estimation method for stochastic errors has been presented. Both the stochastic error's covariances and correlation coefficients are calculated to validate the suggested method. It is shown that the combination of error propagation model with the fission matrix method facilitates estimation correlation coefficients between FSD's *L* cycle apart, which are key parameters characterizing the FSD convergence criteria.

2. Methods and Results

2.1 Cycle-by-cycle Error Propagation Model

The discrete Monte Carlo calculations can be expressed by the fission matrix eigenvalue equation of zone-wise FSD as follows:

$$\mathbf{S} = \frac{1}{k}\mathbf{H}\mathbf{S} . \qquad (1)$$

$\mathbf{H}$ and k are the fission matrix and the multiplication factor, respectively.

Due to statistical nature of fission source sampling and the enthusing particle history tracking, the FSDs are unavoidably associated with errors. The errors of FSD in the cycle-to-cycle error propagation model [1,3] can be given by

$$\mathbf{e}^t = \sum_{t'=0}^{t-1} \left(\mathbf{A_0}\right)^{t'} \boldsymbol{\varepsilon}^{t-t'} + \left(\mathbf{A_0}\right)^t \mathbf{e}^0 \qquad (2)$$

where

$\mathbf{e}^t =$ fluctuating component of FSD at *t*-th cycle

$\boldsymbol{\varepsilon}^t =$ stochastic errors generated at cycle number *t*

$\mathbf{A_0}$ is defined by

$$\mathbf{A_0} = \frac{1}{k_0}\left[\mathbf{H} - \mathbf{S}_0 \tau^T\right]. \qquad (3)$$

where $\tau^T = (1,1,\cdots,1)$. k_0 and $\mathbf{S}_0$ are a maximum eigenvalue and corresponding eigenvector of Eq. (1).

From Eq. (2), the FSD error of *m*-th cell is written as

$$e_m^t = \sum_{t'=0}^{t-1}\sum_{m'} a_{mm'}^{t'} \varepsilon_{m'}^{t-t'} + \sum_{m'} a_{mm'}^{t} e_{m'}^0 . \qquad (4)$$

where $a_{mm'}^{t'}$ is a *m*-th row and m'-th column element of matrix $(\mathbf{A_0})^{t'}$ and it means a error propagation ratio at *m*-th cell by a error generated at m'-th cell and t' previous cycle.

2.2 FSD Variance and Covariance

It is assumed that the stochastic error generated at cycle *t* is independent with the accumulated errors of previous cycles and the stochastic errors generated at other cycles: This means

$$E\left[\varepsilon_m^i e_{m'}^j\right] = 0, \quad i > j$$
$$E\left[\varepsilon_m^i \varepsilon_{m'}^j\right] = 0, \quad i \neq j \qquad (5)$$

where *i* and *j* are cycle indexes, *m* and m' are cell indexes.

Then, from Eqs. (4) and (5), the covariance between S_m^t and $S_{m'}^{t+l}$ can be expressed as

$$\begin{aligned}\mathrm{cov}\left[S_m^t, S_{m'}^{t+l}\right] &= E\left[e_m^t e_{m'}^{t+l}\right] \\ &= \sum_{t'=0}^{t-1}\sum_{n}\sum_{n'} a_{mn}^{t'} a_{m'n'}^{t'+l} E\left[\varepsilon_n^{t-t'} \varepsilon_{n'}^{t-t'}\right] + \sum_{n}\sum_{n'} a_{mn}^{t} a_{m'n'}^{t+l} E\left[e_n^0 e_{n'}^0\right]\end{aligned} \qquad (6)$$

In the following analysis, it is assumed that $E[\varepsilon_m^t \varepsilon_{m'}^{t+l}]$ is independent of the cycle number *t* at stationary cycles from the property of equilibrium. Then assuming the covariance of FSDs *l* cycles apart depends only on the cycle difference *l*, one can introduce the lag *l* covariance as

$$\begin{aligned}C_l\left[S_m, S_{m'}\right] &\equiv \mathrm{cov}\left[S_m^t, S_{m'}^{t+l}\right] \\ &= \sum_{t'=0}^{\infty}\sum_{n}\sum_{n'} a_{mn}^{t'} a_{m'n'}^{t'+l} E\left[\varepsilon_n \varepsilon_{n'}\right]\end{aligned} \qquad (7)$$

$E[\varepsilon_n \varepsilon_{n'}]$ in Eq. (7) means the covariance between ε_n and $\varepsilon_{n'}$ because $E[\varepsilon_n] = 0$. Then, it follows

$$C_l\left[S_m, S_{m'}\right] = \sum_{t'=0}^{\infty}\sum_{n}\sum_{n'} a_{mn}^{t'} a_{m'n'}^{t'+l}\, \mathrm{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] . \qquad (8)$$

By the definition of variance, the variance of S_m is the same as the covariance at $l = 0$ for the same cell.

$$\operatorname{cov}\left[S_m^t, S_m^t\right] \equiv \sigma^2\left[S_m\right] = \sum_{t'=0}^{\infty}\sum_n\sum_{n'} a_{mn}^{t'} a_{mn'}^{t'} \operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right]. \quad (9)$$

2.3 Covariance of Stochastic Error

E. M. Gelbard and R. E. Prael suppose that in each generation the probability that a typical particle will be assigned to the *n*-th cell is equal to $\bar{M}_n / M$ where $\bar{M}_n$ is an average number of fission source neutrons which are generated in the *n*-th cell and *M* is the total number of fission sources per cycle [1]. Under these assumption, $\operatorname{cov}[\varepsilon_n, \varepsilon_{n'}]$ can be expressed as

$$\begin{aligned} \operatorname{cov}\left[\varepsilon_n, \varepsilon_n\right] &= \frac{1}{M^2}\left\{\bar{M}_n\left(1 - \frac{\bar{M}_n}{M}\right)\right\} \\ \operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] &= -\frac{1}{M^2}\left(\frac{\bar{M}_n \bar{M}_{n'}}{M}\right) \end{aligned}. \quad (10)$$

Using the eigenvector of Eq. (1) corresponding to the maximum k, Eq. (10) can be calculated by

$$\begin{aligned} \operatorname{cov}\left[\varepsilon_n, \varepsilon_n\right] &= \frac{S_{0n}\left(1 - S_{0n}\right)}{M} \\ \operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] &= -\frac{S_{0n} S_{0n'}}{M} \end{aligned} \quad (11)$$

where S_{0n} is the *n*-th element of the eigenvector.

However, in the realistic Monte Carlo particle simulations the probability that a particle will be assigned to the *n*-th cell varies from the source particle's location, energy, and direction.

Therefore, $\operatorname{cov}[\varepsilon_n^t, \varepsilon_{n'}^t]$ should be estimated from the simulation results of fission sources composing *t*-th cycle as

$$\begin{aligned} \operatorname{cov}_S\left[\varepsilon_n^t, \varepsilon_{n'}^t\right] &= \frac{1}{M(M-1)}\sum_{i=1}^{M}\left(\left(S_n^t\right)_i - \bar{S}_n^t\right)\left(\left(S_{n'}^t\right)_i - \bar{S}_{n'}^t\right) \\ \bar{S}_m^t &= \frac{1}{M}\sum_{i=1}^{M}\left(S_m^t\right)_i; \quad m = n \text{ or } n' \end{aligned} \quad (12)$$

where $(S_m^t)_i$ is the fission source density of *m*-th cell by *i*-th source at *t*-th cycle.

And $\operatorname{cov}[\varepsilon_n, \varepsilon_{n'}]$ can be estimated as

$$\operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] = \frac{1}{N}\sum_{t=1}^{N}\operatorname{cov}_S\left[\varepsilon_n^t, \varepsilon_{n'}^t\right] \quad (13)$$

where *N* is a active cycle number.

$\operatorname{cov}[\varepsilon_n, \varepsilon_{n'}]$ can be calculated indirectly by the simple simultaneous equation of the sample covariances of FSDs.

$$\begin{aligned} \operatorname{cov}_S\left[S_{m'}, S_{m''}\right] = \sum_n\sum_{n'}\Bigg[\sum_{t'=0}^{\infty}\Bigg\{ & a_{m'n}^{t'} a_{m''n'}^{t'} - \frac{1}{N(N-1)}\sum_{l=1}^{N-1}(N-l) a_{m'n}^{t'} a_{m''n'}^{t'+l} \\ & - \frac{1}{N(N-1)}\sum_{l=1}^{N-1}(N-l) a_{m''n}^{t'} a_{m'n'}^{t'+l}\Bigg\}\Bigg]\operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right] \end{aligned} \quad (14)$$

Table 1 shows the comparison of the standard deviations calculated by three methods in the SMART core problem. From the table, we can see that the standard deviations by Eq. (13) and (14) are similar.

Table 1 Comparison of variance of stochastic error for SMART core

Assem. Idx.	by Eq. (14)	by Eq. (13)	by Eq. (11)
1	6.72E-04	6.69E-04	4.58E-04
2	1.25E-03	1.31E-03	8.95E-04
3	1.25E-03	1.30E-03	8.73E-04
4	1.27E-03	1.28E-03	8.60E-04
5	1.60E-03	1.75E-03	1.16E-03
6	1.27E-03	1.24E-03	8.57E-04
7	1.20E-03	1.24E-03	8.48E-04
8	1.58E-03	1.64E-03	1.11E-03
9	1.41E-03	1.49E-03	1.06E-03
10	9.28E-04	9.38E-04	6.98E-04
11	1.03E-03	1.12E-03	8.77E-04

2.4 Inter-cycle Correlation Coefficient

From Eq. (8) and (9), the inter-cycle correlation coefficient of FSDs can be calculated by

$$\rho\left[S_m, l\right] \equiv \frac{\operatorname{cov}\left[S_m^t, S_m^{t+l}\right]}{\sigma\left[S_m^t\right]\sigma\left[S_m^{t+l}\right]} = \frac{\sum_{t'=0}^{\infty}\sum_n\sum_{n'} a_{mn}^{t'} a_{mn'}^{t'+l}\operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right]}{\sum_{t'=0}^{\infty}\sum_n\sum_{n'} a_{mn}^{t'} a_{mn'}^{t'}\operatorname{cov}\left[\varepsilon_n, \varepsilon_{n'}\right]} \quad (15)$$

Figure 1 shows the correlation coefficient of FSD calculated by Eq. (15) using Eq. (13) as the stochastic error's covariance.

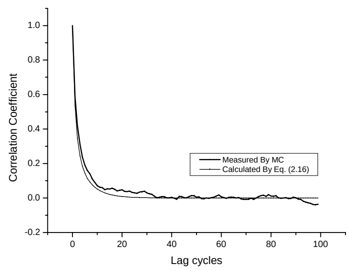

Figure 1 Inter-cycle correlation coefficient for the SMART core

3. Conclusion

The inter-cycle correlation coefficient was calculated by the cycle-to-cycle error propagation model from the precise stochastic error's covariance. From the numerical results, we can see that the correlation coefficient by the cycle-to-cycle error propagation model can predict the real correlation really well.

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