Stochastic Error Propagation Model for Monte Carlo Eigenvalue Calculations with Feedback Updates

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1. Introduction

The Monte Carlo (MC) whole-core transport with considering depletion and multi-physics feedbacks has been actively studied from the last decade. Various MC codes such as MC21 [1], Serpent [2], McCARD [3], RMC [4], MCS [5] have successfully demonstrated their multi-physics steady-state core analysis capabilities. Especially there have been advances [6,7] in developments of efficient and stable convergence algorithms for the thermal-hydraulics (T/H) coupled MC calculations.

In spite of these progress, it is required to better understand the feedback-coupled MC calculations. For example, one of these stability studies interestingly reported [8] that the fixed point iteration scheme with coupling, iteration by iteration, a MC eigenvalue solver and an equilibrium xenon feedback solver shows faster fission source convergence than MC calculations without the feedback. In addition, characteristics of the statistical uncertainty in the feedback-coupled MC eigenvalue calculations is hardly studied although it is inevitably accompanied with a mean estimate in the MC calculations.

It is well-known that the sample variance over cycle-wise estimates in the MC eigenvalue calculations suffers from its bias due to the inter-cycle correlation of the fission source distribution (FSD) [9]. Earlier, the covariance between FSDs in successive cycles was formulated by the Gelbard and Prael's error propagation model [9] in which an error of an FSD, normalized to eigenvalue k, at a certain cycle from the true stationary FSD is expressed in its stochastic error components that propagate cycle by cycle. Shim and Kim [10] developed a real variance estimation method in which the inter-cycle covariance of the MC tally of interest is calculated by a slightly modified cycle-by cycle error propagation model for the FSD normalized to unity.

Here I develop a cycle-by-cycle error propagation model for the MC eigenvalue calculation coupled with a feedback module via the fixed point iteration. The developed model is applied for a simple 2x2 fission matrix problem to investigate behaviors of the variance bias in the feedback-coupled MC eigenvalue calculation.

2. Development of Error Propagation Model

In the MC eigenvalue calculations, the FSD is updated cycle-by-cycle (or generation-by-generation) as [10]

$$S^{(i+1)} = \frac{1}{\langle \mathbf{H} S^{(i)} \rangle} \mathbf{H} S^{(i)} + \varepsilon^{(i+1)} \tag{1}$$

where $S^{(p)}$ ($p = i$ or $i+1$) denotes the FSD, $S(\mathbf{P})$, at cycle p where $\mathbf{P}$ stands for $(\mathbf{r}, E, \mathbf{\Omega})$, the six-dimensional phase space vector representing a neutron state. The angle bracket $\langle\ \rangle$ implies integration over $\mathbf{P}$. The fission operator $\mathbf{H}$ implies

$$\mathbf{H} \cdot = \int d\mathbf{P}' H(\mathbf{P}' \to \mathbf{P}) \cdot \tag{2}$$

$H(\mathbf{P}' \to \mathbf{P})$ means the number of next-generation fission neutrons born per unit phase space volume about $\mathbf{P}$, due to a parent neutron born at $\mathbf{P}'$. $\varepsilon^{(i+1)}$ is the stochastic error components of $S^{(i+1)}$ resulting from a finite number of MC history at cycle i and defined by

$$\varepsilon^{(i+1)}(\mathbf{P}) \equiv S^{(i+1)}(\mathbf{P}) - E[S^{(i+1)}(\mathbf{P}) | S^{(i)}(\mathbf{P})] \tag{3}$$

where $E[S^{(i+1)}(\mathbf{P}) | S^{(i)}(\mathbf{P})]$ is the conditional mean of $S^{(i+1)}(\mathbf{P})$, given $S^{(i)}(\mathbf{P})$.

In the fixed point iteration scheme of this study, MC outputs including the FSD estimated at cycle i is assumed to be inputted to a feedback solver, of which results are used to update the fission operator $\mathbf{H}$ for the next cycle, $\mathbf{H}^{(i+1)}$. By introducing $\mathbf{H}^{(i)}$ into Eq. (1), the MC power iteration formulation considering the feedback updates becomes

$$S^{(i+1)} = \frac{1}{\langle \mathbf{H}^{(i)} S^{(i)} \rangle} \mathbf{H}^{(i)} S^{(i)} + \varepsilon^{(i+1)} \tag{4}$$

Because all the macroscopic cross sections such as $\Sigma_t(\mathbf{r}, E)$ and $\Sigma_s(\mathbf{r}, E)$ used to define the operator $\mathbf{H}$ are determined for a given FSD, $\mathbf{H}$ can be regarded as a function of *S*. When the operator $\mathbf{H}$ at the steady-state system is denoted by $\mathbf{H}_0$, thus, $\mathbf{H}^{(i)}$ can be approximated to its first-order Taylor's series expansion as

$$\mathbf{H}^{(i)} \cdot \cong \mathbf{H}_0 \cdot + \frac{\partial \mathbf{H}}{\partial S}\left(S^{(i)} - S_0\right) \cdot \equiv \int d\mathbf{P}' H_0(\mathbf{P}' \to \mathbf{P}) \cdot + \int d\mathbf{P}' \int d\mathbf{P}'' \frac{\partial H(\mathbf{P}' \to \mathbf{P})}{\partial S(\mathbf{P}'')} \left(S^{(i)}(\mathbf{P}'') - S_0(\mathbf{P}'')\right) \cdot \tag{5}$$

One can define the error of $S^{(i)}$, $e^{(i)}$, as its difference from the true distribution:

$$e^{(i)}(\mathbf{P}) = S^{(i)}(\mathbf{P}) - S_0(\mathbf{P}). \tag{6}$$

S_0 is the fundamental mode FSD to the eigenvalue equation of

$$S_0 = \frac{1}{k_0}\mathbf{H}S_0, \tag{7}$$

where k_0 is the fundamental mode eigenvalue corresponding to S_0 satisfying

$$k_0 = \langle \mathbf{H}S_0 \rangle \tag{8}$$

The cycle-by-cycle error propagation model for the MC eigenvalue calculation with feedback can be derived by introducing Eq. (5) and substituting $S^{(i)} = S_0 + e^{(i)}$ from Eq. (6) into Eq. (4) as

$$S_0 + e^{(i+1)} \cong \frac{1}{\langle\left(\mathbf{H}_0 + \frac{\partial \mathbf{H}}{\partial S}e^{(i)}\right)(S_0 + e^{(i)})\rangle} \cdot \left(\mathbf{H}_0 + \frac{\partial \mathbf{H}}{\partial S}e^{(i)}\right)\left(S_0 + e^{(i)}\right) + \varepsilon^{(i+1)} \tag{9}$$

Taylor's series expansion of the first term on the right side of Eq. (9) in powers of $e^{(i)}$ yields

$$S_0 + e^{(i+1)} \cong \frac{1}{\langle \mathbf{H}_0 S_0 \rangle}\mathbf{H}_0 S_0 + \frac{1}{\langle \mathbf{H}_0 S_0 \rangle}\left(\mathbf{H}_0 + \frac{\partial \mathbf{H}}{\partial S}S_0\right)e^{(i)} - \frac{\mathbf{H}_0 S_0}{\langle \mathbf{H}_0 S_0 \rangle^2}\left\langle\left(\mathbf{H}_0 + \frac{\partial \mathbf{H}}{\partial S}S_0\right)e^{(i)}\right\rangle + \varepsilon^{(i+1)} \tag{10}$$

Using Eqs. (7) and (8), Eq. (10) can be expressed as

$$e^{(i+1)} \cong \mathbf{A}e^{(i)} + \varepsilon^{(i+1)}; \tag{11}$$

$$\begin{aligned}\mathbf{A}\cdot &\equiv \frac{1}{k_0}[\mathbf{H}_\mathrm{g}\cdot - S_0\langle \mathbf{H}_\mathrm{g}\cdot]\\ &= \frac{1}{k_0}\left[\int d\mathbf{P}' H_\mathrm{g}(\mathbf{P}' \to \mathbf{P}) - S_0(\mathbf{P})\int d\mathbf{P}\int d\mathbf{P}' H_\mathrm{g}(\mathbf{P}' \to \mathbf{P})\right]\cdot\end{aligned} \tag{12}$$

$$\begin{aligned}\mathbf{H}_\mathrm{g}\cdot &\equiv \int d\mathbf{P}' H_\mathrm{g}(\mathbf{P}' \to \mathbf{P})\cdot\\ &= \int d\mathbf{P}'\left(H_0(\mathbf{P}' \to \mathbf{P}) + \int d\mathbf{P}'' \frac{\partial H(\mathbf{P}' \to \mathbf{P})}{\partial S(\mathbf{P}'')}S_0(\mathbf{P}'')\right)\cdot\end{aligned} \tag{13}$$

Here $\mathbf{H}_\mathrm{g}$ is named the feedback-considered fission operator.

3. Application to 2x2 Fission Matrix Problem

Now, the variance bias of an arbitrary tally Q in a multiplying system with or without a negative feedback is compared for an eigenvalue problem of an imaginary 2x2 fission matrix defined by [11]

$$\mathbf{H} = \begin{pmatrix} a_{11} & k_0 - a_{22} \\ k_0 - a_{11} & a_{22}\end{pmatrix};\ 0 < a_{11}, a_{22} \le k_0 \tag{14}$$

This problem may be a simplified representation of a nuclear system which contains two fissionable regions arranged symmetrically, and can provide a useful means to examine the variance bias behavior according to a feedback application analytically by the developed error propagation model.

In the matrix of Eq. (14), the parameter a_{nn} ($n = 1$ or 2) means the number of next-generation fission neutrons produced at the same region n as the one where their parent neutron is produced, namely, n. In this problem, a_{nn} is assumed to be changed by a factor of $-\mathrm{g}$ ($\mathrm{g} > 0$) proportional to the region-wise and cycle-wise FSD change at the region n from its reference value at the system without feedback as

$$a_{nn} \cong a_0 - \mathrm{g}(S_n - S_{0n})\ \ (n = 1 \text{ or } 2); \tag{15}$$

$$\mathrm{g} = -\frac{\partial a_{nn}}{\partial S_n}, \tag{16}$$

where S_n denotes the n-th element of the fission source vector S. S_{0n} indicates the n-th element of the fundamental-mode eigenvector of the fission matrix without considering the feedback given by

$$\mathbf{H}_0 = \begin{pmatrix} a_0 & k_0 - a_0 \\ k_0 - a_0 & a_0\end{pmatrix};\ 0 < a_0 \le k_0 \tag{17}$$

By inserting Eq. (14) into Eq. (12), the error propagation matrix $\mathbf{A}$ can be expressed as

$$\mathbf{A} = \frac{1}{k_0}\left[\mathbf{H}_\mathrm{g} - \mathbf{S}_0 \cdot \boldsymbol{\tau}^T \cdot \mathbf{H}_\mathrm{g}\right]; \tag{18}$$

$$\begin{aligned}\mathbf{H}_\mathrm{g} &= \mathbf{H}_0 + \frac{\partial \mathbf{H}}{\partial S}\mathbf{S}_0\\ &= \begin{pmatrix} a_0 & k_0 - a_0 \\ k_0 - a_0 & a_0\end{pmatrix}\\ &+ \begin{pmatrix} \sum_{n=1}^{2}\frac{\partial a_{11}}{\partial S_n}S_{0n} & \sum_{n=1}^{2}\frac{\partial a_{22}}{\partial S_n}S_{0n} \\ \sum_{n=1}^{2}\frac{\partial a_{11}}{\partial S_n}S_{0n} & \sum_{n=1}^{2}\frac{\partial a_{22}}{\partial S_n}S_{0n}\end{pmatrix}.\end{aligned} \tag{19}$$

where $\boldsymbol{\tau}^T$ is the two-dimensional row vector (1,1).

Then, by inserting Eq. (15) into Eq. (18) and using $\mathbf{S}_0 = (0.5, 0.5)^T$, $\mathbf{A}$ becomes

$$\mathbf{A} = \frac{\rho_\mathrm{g}}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1\end{pmatrix}; \tag{20}$$

$$\rho_\mathrm{g} = \frac{2a' - k_0}{k_0} \tag{21}$$

$$a' = a_0 - \frac{\mathrm{g}}{2}, \tag{22}$$

where ρ_g is the dominance ratio (DR) of the feedback-considered fission matrix of

$$\mathbf{H}_\mathrm{g} = \begin{pmatrix} a' & k_0 - a' \\ k_0 - a' & a'\end{pmatrix}; \tag{23}$$

Noting that two eigenvalues of the matrix $\mathbf{H}_\mathrm{g}$ are k_0 and $2a' - k_0$, the DR of the fission matrix without feedback, $\mathbf{H}_0$, is

$$\rho_0 = \frac{2a_0 - k_0}{k_0} \tag{24}$$

Then the error propagation matrix for $\mathbf{H}_0$ becomes [11]

$$\mathbf{A}_0 = \frac{\rho_0}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \qquad (25)$$

In Ref. [11], the variance bias for the same 2x2 fission matrix problem is derived as

$$\mathrm{B}[\bar{Q}] \cong \frac{\left(R_1^Q - R_2^Q\right)^2}{2M} \cdot \frac{\rho}{(1-\rho)^2(1+\rho)} \qquad (26)$$

where $\bar{Q}$ denotes an MC mean estimate of an arbitrary tally Q and R_n^Q ($n = 1$ or 2) means the MC tally response from a unit fission source located at region n. M and N are the numbers of histories per cycle and active cycles, respectively. ρ denotes the dominance ratio of the fission matrix.

By introducing the ρ_g of Eq. (21) and ρ_0 of Eq. (24) into Eq. (26), a variance bias ratio between the 2x2 matrix problem with and without feedback becomes

$$\frac{B_g[\bar{Q}]}{B_0[\bar{Q}]} = \frac{\rho_g}{\rho_0} \cdot \frac{1-\rho_0^2}{1-\rho_g^2} \cdot \frac{1-\rho_0}{1-\rho_g} \qquad (27)$$

Figure 1 shows the comparison of B_g/B_0 according to the g value with changing the parameter a. From the figure, one can see that the variance bias is drastically reduced by the feedback effect especially for a matrix with a large a value.

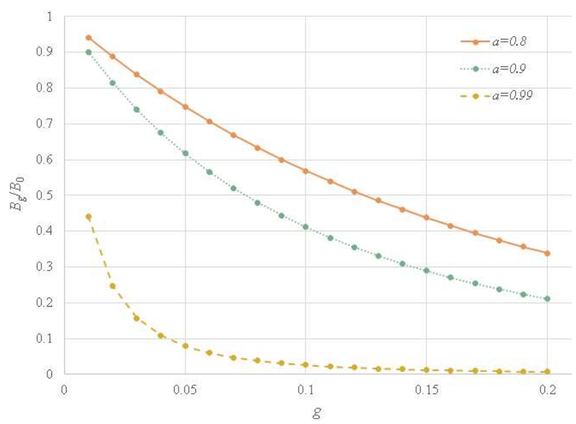

Figure 1. B_g/B_0 Behavior According to *a* and g

4. Conclusion and Future Works

A stochastic error propagation model for the MC eigenvalue calculation considering feedback updates of the fission matrix is derived. The developed formulation is applied for the 2x2 fission matrix problem to investigate a change of the variance bias according to the feedback effect. From the analytical comparisons, it is shown that the variance bias can be drastically reduced by the feedback effect especially for a high DR problem. The effectiveness of the developed error propagation model will be examined for the weakly coupled fissile array problem and da fuel pin problem in the continuous-energy MC transport calculations.

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