Sample Variance Estimation for Fission Source Distribution in Monte Carlo Eigenvalue Calculations Under Cross Section Feedback

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1. Introduction

In reactor physics, the importance of multi-physics analysis is increasing as computational power grows rapidly and various advanced reactor designs are being developed. As a result, substantial progress has been made in integrating multi-physics into Monte Carlo transport analysis. Various codes, such as MC21 [1], Serpent [2], McCARD [3], RMC [4], and MCS [5], have demonstrated their successful capabilities in multi-physics steady-state core analysis. For neutronics calculations, sharing computational results for multi-physics analysis can be viewed as a fixed-point iteration in a feedback-coupled system, where the feedback is reflected through cross-section updates.

Such feedback updates are known to influence not only the solution of Monte Carlo calculations but also their uncertainty. For instance, a previous study reported that xenon equilibrium feedback could accelerate the convergence of Monte Carlo calculations [6]. To explain this stabilizing behavior when feedback is applied, Shim [7] derived a feedback-considered error propagation model based on prior studies [8][9], which describe how the normalized error of the FSD in eigenvalue calculations propagates and affects subsequent cycles.

To more directly quantify the effect of uncertainty changes due to cross-section feedback, we reformulated the feedback-considered error propagation model described above. We then set up a 2-cell Kinetics Monte Carlo problem with cross-section feedback to analytically estimate the sample variance of the normalized FSD in our error propagation model and validate it with the calculated values.

2. Derivation of Feedback-Considered Error Propagation Model

2.1 Cycle-wise Feedback-Updated Fission Operator

Consider a feedback-coupled system in which the feedback update has reached a steady state. Denoting this steady state with the subscript 0, the Time-Independent Boltzmann Transport Equation can be expressed as follows:

$$\mathbf{T}_0\psi = \frac{1}{k_0}\mathbf{F}_0\psi, \tag{1}$$

where k_0 is the main mode eigenvalue, and $\mathbf{T}_0, \mathbf{F}_0$ are operators that are defined by

$$\begin{aligned}\mathbf{T}_0\psi &= \left[\Omega\cdot\nabla + \Sigma_t\left(r,E\right)\right]\psi\left(r,E,\Omega\right)\\ &\quad -\int dE'\int d\Omega\,\Sigma_s\left(r;E',\Omega'\rightarrow E,\Omega\right)\psi\left(r,E',\Omega'\right),\\ \mathbf{F}_0\psi &= \frac{\chi\left(E\right)}{4\pi}\int dE'\int d\Omega'\nu\left(E'\right)\Sigma_f\left(r,E'\right)\psi\left(r,E',\Omega'\right),\end{aligned} \tag{2}$$

where $\psi\left(r,E,\Omega\right)$ is the angular flux. Note that the cross-sections in Eq. (2) represent the steady state cross-sections for feedback.

By introducing $\mathbf{H}_0 = \mathbf{F}_0\mathbf{T}_0^{-1}$, one can rewrite Eq. (1) for fission source density S,

$$S = \frac{1}{k_0}\mathbf{H}_0 S. \tag{3}$$

And the cycle-wise normalized fission source distribution(FSD) is updated in Monte Carlo eigenvalue calculation by

$$S^{i+1} = \frac{\mathbf{H}_0 S^i}{\left\langle \mathbf{H}_0 S^i\right\rangle} + \varepsilon^{i+1}, \tag{4}$$

where the angle bracket $\langle\ \rangle$ represents integration over phase space $\left(r,E,\Omega\right)$, i is cycle index, and ε^{i+1} is the stochastic error of S^{i+1} resulting from Monte Carlo calculation at cycle i, defined by

$$\varepsilon^{i+1} \equiv S^{i+1} - E\left[S^{i+1}\,|\,S^i\right], \tag{5}$$

where $E\left[S^{i+1}\,|\,S^i\right]$ is the conditional mean of S^{i+1}, given S^i.

Now consider the cycle-wise feedback-updating process before calculating $\left(i+1\right)^{th}$ cycle, using $\left(i\right)^{th}$

cycle result. Regarding the cross-section feedback applied in the form of a function of the fission source density, S^i, the above operator $\mathbf{F}$ and $\mathbf{T}$ can be written using first-order Taylor's series expansion as

$$\mathbf{F}^i \cong \mathbf{F}_0 + \frac{\partial \mathbf{F}}{\partial S}\left(S^i - S_0\right) = \mathbf{F}_0 + \frac{\partial \mathbf{F}}{\partial S} e^i,$$
$$\mathbf{T}^i \cong \mathbf{T}_0 + \frac{\partial \mathbf{T}}{\partial S}\left(S^i - S_0\right) = \mathbf{T}_0 + \frac{\partial \mathbf{T}}{\partial S} e^i, \qquad (6)$$

where S_0 is the main mode solution of FSD, and e^i is the error of S^i, defined by

$$e^i \equiv S^i - S_0. \qquad (7)$$

Accordingly, the cycle-wise feedback-updated fission operator $\mathbf{H}^i$ can be expressed, and its relationship with $\mathbf{H}_0$ can further be derived using the Neumann's series expansion as follows:

$$\begin{aligned}
\mathbf{H}^i &= \mathbf{F}^i \left(\mathbf{T}^i\right)^{-1} \\
&\cong \left(\mathbf{F}_0 + \frac{\partial \mathbf{F}}{\partial S} e^i\right)\left(\mathbf{T}_0 + \frac{\partial \mathbf{T}}{\partial S} e^i\right)^{-1} \\
&= \left(\mathbf{I} + \frac{\partial \mathbf{F}}{\partial S} e^i \mathbf{F}_0^{-1}\right)\mathbf{F}_0 \mathbf{T}_0^{-1}\left(\mathbf{I} + \frac{\partial \mathbf{T}}{\partial S} e^i \mathbf{T}_0^{-1}\right)^{-1} \\
&= \left(\mathbf{I} + \frac{\partial \mathbf{F}}{\partial S} e^i \mathbf{F}_0^{-1}\right)\mathbf{H}_0 \sum_{n=0}^{\infty}\left(-\frac{\partial \mathbf{T}}{\partial S} e^i \mathbf{G}_0\right)^n. \qquad (8)
\end{aligned}$$

where $\mathbf{G}_0 = \mathbf{T}_0^{-1}$ is the Green's function of the feedback-coupled system in which the feedback update has reached a steady state.

2.2 Feedback-Considered Error Propagation Model

We defined the feedback-considered fission operator, $\mathbf{H}_g$, as the total derivative of the fission source density, which is generated from the cycle-wise feedback-updated fission operator $\mathbf{H}^i$, and S^i, with respect to S^i, as follows:

$$\mathbf{H}_g \equiv \left.\frac{d\mathbf{H}^i S^i}{dS^i}\right|_{S^i = S_0} = \mathbf{H}_0 + \frac{\partial \mathbf{H}^i}{\partial S} S_0. \qquad (9)$$

Subsequently, we can derive the feedback-considered error propagation model from Eq. (4) using a first-order Taylor's series expansion.

$$\begin{aligned}
S_0 + e^{i+1} &= \frac{\mathbf{H}^i S^i}{\left\langle \mathbf{H}^i S^i \right\rangle} + \varepsilon^{i+1} \\
&\cong \frac{\mathbf{H}_0 S_0}{\left\langle \mathbf{H}_0 S_0 \right\rangle} + \frac{\mathbf{H}_g}{\left\langle \mathbf{H}_0 S_0 \right\rangle} e^i - \frac{\mathbf{H}_0 S_0}{\left\langle \mathbf{H}_0 S_0 \right\rangle^2}\left\langle \mathbf{H}_g e^i \right\rangle + \varepsilon^{i+1} + O\left(\left(e^i\right)^2\right) \\
&= S_0 + \frac{1}{k_0}\left(\mathbf{H}_g e^i - S_0 \left\langle \mathbf{H}_g e^i \right\rangle\right) + \varepsilon^{i+1} + O\left(\left(e^i\right)^2\right).
\end{aligned} \qquad (10)$$

By eliminating S_0 from both sides, we can finally rewrite Eq. (10) as follows:

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

$$\mathbf{A} e^i \equiv \frac{1}{k_0}\left(\mathbf{H}_g e^i - S_0 \left\langle \mathbf{H}_g e^i \right\rangle\right). \qquad (12)$$

Shim presented the above derivation in Ref. [7]. As seen in Eqs. (11) and (12), the feedback-considered fission operator $\mathbf{H}_g$ allows the error propagation of the cycle-wise feedback-updated system to be expressed in the form of the existing error propagation model, while also serving as a key factor in determining its characteristics. The relationship between cross-section feedback and $\mathbf{H}_g$ will be discussed in the next section.

2.3 Feedback-Considered Fission Operator

The feedback-considered fission operator $\mathbf{H}_g$, defined in Eq. (9), can be further derived using Eq. (8) as follows:

$$\begin{aligned}
\mathbf{H}_g &\equiv \left.\frac{d\mathbf{H}^i S^i}{dS^i}\right|_{S^i = S_0} \\
&= \mathbf{H}_0 + \frac{\partial\left(\mathbf{I} + \frac{\partial \mathbf{F}}{\partial S} e^i \mathbf{F}_0^{-1}\right)\mathbf{H}_0 \sum_{n=0}^{\infty}\left(-\frac{\partial \mathbf{T}}{\partial S} e^i \mathbf{G}_0\right)^n}{\partial e^i} S_0 \\
&= \mathbf{H}_0 + \left(\frac{\partial\left(\frac{\partial \mathbf{F}}{\partial S} e^i \mathbf{F}_0^{-1} \mathbf{H}_0\right)}{\partial e^i} - \frac{\partial\left(\mathbf{H}_0 \frac{\partial \mathbf{T}}{\partial S} e^i \mathbf{G}_0\right)}{\partial e^i}\right) S_0 \\
&= \mathbf{H}_0 + \left(\frac{\partial \mathbf{F}}{\partial S}\mathbf{G}_0 - \mathbf{H}_0 \frac{\partial \mathbf{T}}{\partial S}\mathbf{G}_0\right) S_0.
\end{aligned} \qquad (13)$$

Eq. (13) describes how the cross-section feedback affects the error propagation. $\partial \mathbf{F} / \partial S$ represents the feedback sensitivity of the fission rate operator with respect to the fission source density, which can be defined as the product of the χ distribution and the feedback sensitivity of $\nu\Sigma_f$. $\partial \mathbf{T} / \partial S$ represents the feedback sensitivity of the transport operator with respect to the fission source density. Especially for the absorption cross-section feedback, the feedback sensitivity of Σ_a would be the diagonal term of the operator. In Section 3, we will demonstrate the determination of $\mathbf{H}_g$ in the 2-cell problem with cross-section feedback.

2.4 Sample Variance of FSD

To evaluate the change in uncertainty, the FSD is integrated into a discrete form by dividing the entire region of the nuclear system into N_m non-overlapping regions with spatial volume $V_m\left(m=1,2,\ldots,N_m\right)$,

$$S_m^i=\int_{V_m}dV\int_0^\infty dE\int_{4\pi}d\mathbf{\Omega}S^i\left(\mathbf{r},E,\mathbf{\Omega}\right), \tag{14}$$

$$S_{0,m}=\int_{V_m}dV\int_0^\infty dE\int_{4\pi}d\mathbf{\Omega}S_0\left(\mathbf{r},E,\mathbf{\Omega}\right). \tag{15}$$

For the stationary cycles, assuming that $E\left[S_m^i\right]=E\left[S_m\right]=S_{0,m}$ and the covariance of the stochastic error is independent of the cycle, the sample variance of the FSD can be written as follows:

$$\begin{aligned}\mathrm{var}\left[S_m\right]&=E\left[\left(S_m^i-S_{0,m}\right)^2\right]\\&=E\left[\left(e_m^i\right)^2\right]\\&=\varsigma_m^T\cdot\sum_{t=0}^{\infty}\mathbf{A}^t\sum_{t'=0}^{\infty}E\left[\varepsilon^i\left(\varepsilon^i\right)^T\right]\left(\mathbf{A}^t\right)^T\cdot\varsigma_m\\&=\sum_{t=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m}A_{mn}^tA_{mn'}^t\,\mathrm{cov}\left[\varepsilon_n,\varepsilon_{n'}\right],\end{aligned} \tag{16}$$

where ς_m is a unit vector of dimension N_m with the only nonzero element being unity at the m'th position, and A_{mn}^t is the m'th row and n'th column element of the matrix $\mathbf{A}^t$. The detailed derivation is presented in Ref. [10]. Note that Eq. (16) can also be regarded as a different form of the Lyapunov equation, given the covariance of the stochastic error, $\mathrm{cov}[\varepsilon_n,\varepsilon_{n'}]$.

3. Application to One-Group Two-Cell Problem

3.1 Definition of the Problem

To evaluate our reformed feedback-considered error propagation model, we conducted Kinetics Monte Carlo calculations for a hypothetical one-group, two-cell symmetric problem. The $\mathbf{F}_0,\mathbf{T}_0$ matrices are defined as follows:

$$\mathbf{F}_0=\begin{pmatrix}1.0&0\\0&1.0\end{pmatrix}\times10^{-2}, \tag{17}$$

$$\mathbf{T}_0=\begin{pmatrix}0.9&-0.1\\-0.1&0.9\end{pmatrix}\times10^{-2}, \tag{18}$$

satisfying

$$\mathbf{H}_0=k_0\begin{pmatrix}0.9&0.1\\0.1&0.9\end{pmatrix}; \tag{19}$$

with $k_0=1.25,$ and $S_0=\left(0.5,0.5\right)^T$.

The corresponding cross-sections, $v\Sigma_f=0.01,$ and $\Sigma_a=0.008$ can be calculated from Eqs. (17) and (18). This problem can be viewed as a simplified model of a nuclear system with two symmetric fissionable regions, providing a useful approach to analytically analyze the behavior of sample variance in relation to cross-section feedback through our error propagation model. The feedback sensitivities are defined as $\partial v\Sigma_f/\partial S=0.001$ and $\partial\Sigma_a/\partial S=0.002$ to represent the increase in cross-section due to temperature rise, such as thermal-hydraulic feedback. Consequently, the corresponding $\partial\mathbf{F}/\partial S$ and $\partial\mathbf{T}/\partial S$ would be diagonal matrices as follows:

$$\frac{\partial\mathbf{F}}{\partial S}=\begin{pmatrix}0.1&0\\0&0.1\end{pmatrix}\times10^{-2}, \tag{20}$$

$$\frac{\partial\mathbf{T}}{\partial S}=\begin{pmatrix}0.2&0\\0&0.2\end{pmatrix}\times10^{-2}, \tag{21}$$

and the $\mathbf{H}_g$ and $\mathbf{A}$ matrices are obtained from Eqs. (13) and (12), respectively,

$$\mathbf{H}_g=\begin{pmatrix}1.053125&0.103125\\0.103125&1.053125\end{pmatrix}, \tag{22}$$

$$\mathbf{A}=\begin{pmatrix}0.38&-0.38\\-0.38&0.38\end{pmatrix}. \tag{23}$$

Note that if we exclude any cross-section feedback for the above system, the matrix $\mathbf{A}$ would be

$$\mathbf{A}_0=\begin{pmatrix}0.4&-0.4\\-0.4&0.4\end{pmatrix}. \tag{24}$$

3.2 Calculation Result

A calculation of 20,000,000 active cycles with 100,000 histories was performed. The stochastic error is directly computed at every cycle using Eq. (25) below to obtain the covariance of the stochastic error.

$$\varepsilon^{i+1}=S^{i+1}-\frac{\mathbf{H}^iS^i}{\tau^T\mathbf{H}^iS^i}, \tag{25}$$

where $\tau^T = (1,1)$.

Table 1 presents the obtained covariance of the stochastic error for the two regions of the problem, depending on the feedback. It shows that the effect of cross-section feedback on the covariance of the stochastic error is negligible.

Table 1. The Covariance of the Stochastic Error Depending on the Feedback

	$\mathrm{cov}[\varepsilon_1,\varepsilon_1]$	$\mathrm{cov}[\varepsilon_1,\varepsilon_2]$
Without Feedback	9.00×10^{-7}	-9.00×10^{-7}
With Feedback	9.00×10^{-7}	-9.00×10^{-7}

The variance of the FSD is calculated in two different ways: using the feedback-considered error propagation model and the direct tally method. Table 2 presents a comparison of the estimated sample variances obtained from both methods. The variance of the FSD calculated by both methods shows good agreement within two significant figures. In particular, the results when cross-section feedback is applied demonstrate the validity of our error propagation model.

Table 2. Comparison Between Feedback-Considered Error Propagation Model and Direct Tally

	Error Propagation Model	Direct Tally
Without Feedback	2.50×10^{-6}	2.50×10^{-6}
With Feedback	2.13×10^{-6}	2.13×10^{-6}

4. Conclusions and Future Works

The feedback-considered error propagation model is derived and validated using a hypothetical problem with cross-section feedback. A good agreement is observed between the analytical estimation and the tally value for the sample variance of the FSD.

Especially for xenon equilibrium feedback, which increases the absorption cross-section while keeping the fission cross-section unchanged, the proposed model is expected to explain the reduction in uncertainty. Expanding the problem to cases with continuous energy and a large number of cells, as well as verifying the validity of the model in such scenarios, will be a task for future work. Alternatively, predicting and explaining changes in uncertainty due to different types of feedback or code coupling can enhance understanding and aid in designing more efficient computations.

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