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Technical note

Estimation of errors in the cumulative Monte Carlo fission source

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ABSTRACT

We study the feasibility of estimating the error in the cumulative fission source in Monte Carlo criticality calculations by utilising the fundamental-mode eigenvector of the fission matrix. The cumulative fission source, representing the source combined over active cycles, contains errors of both statistical and systematic nature. Knowledge of the error in the cumulative fission source is crucial as it determines the accuracy of computed neutron flux and power distributions.

While statistical errors are present in the eigenvector of the fission matrix, it appears that these are not (or they are only weakly) correlated to the errors in the cumulative fission source. This ensures the suggested methodology gives error estimates that are distributed around the real errors, which is also supported by results of our numerical test calculations.

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1. Introduction

Conventional Monte Carlo criticality calculations simulate subsequent neutron generations in so-called cycles. The fission source is expected to converge to the steady-state during a certain number of inactive cycles in which no results are being collected. Results of interest are then combined over a number of active cycles. While the fission source is supposed to be converged during the active cycles, there is no diagnostics methodology that could guarantee that with certainty, although progress has been made in this field (Ueki and Brown, 2003). Hence, the fission source may be sampled during the active cycles from a distribution that is far from steady-state; moreover, the fission source may also contain a bias not decaying over the cycles at all (Brissenden and Garlick, 1986). Consequently, the fission source introduces errors into the results sampled over the active cycles (such as the neutron flux and power distributions). We could accept this fact if we had the knowledge of the error in the cumulative fission source (i.e., the error in the fission source that was combined over the active cycles).

The purpose of this paper is to investigate the feasibility of estimating the error in the cumulative fission source. The estimate should reflect not only the error due to the convergence problems; it should also reflect the bias and random errors. We investigate the possibility of achieving this goal via utilising the fundamental-mode eigenvector of the fission matrix. The fission matrix has been already used in a number of unrelated methods (Carter and McCormick, 1969; Kadotani et al., 1991; Kitada and Takeda, 2001; Dufek and Gudowski, 2009; Brown et al., 2013a,b), and a number of established Monte Carlo criticality codes offer the fission matrix as an optional result. Naturally, the fission matrix contains random errors that are also present in its eigenvector; in this paper, we analyse whether these errors allow using the eigenvector for estimating the error in the cumulative fission source.

The paper is organised as follows. Aspects of convergence of the Monte Carlo fission source are briefly described in Section 2. The methodology of estimating the error in the cumulative fission source is suggested in Section 3. Results of the numerical test calculations are given in Section 4. Our conclusions are summarised in Section 5.

2. Aspects of source convergence

The eigenvalue (criticality) equation for the fission source can be written as

$$ks(\mathbf{r}) = Hs(\mathbf{r}), \tag{1}$$

where k is the eigenvalue, $s(\mathbf{r})$ is the concentration of fission neutrons at $\mathbf{r}$, and

$$Hs(\mathbf{r}) \equiv \int_V d^3r' f(\mathbf{r}' \to \mathbf{r}) s(\mathbf{r}'),$$

where $f(\mathbf{r}' \to \mathbf{r})\, d^3r$ is an expected number of first generation fission neutrons produced in the volume element d^3r at $\mathbf{r}$, resulting from a

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fission neutron born at $\mathbf{r}'$. Angular dependence is not considered since fission neutrons are emitted isotropically. The Monte Carlo fission source is represented by a batch of m neutrons with specific positions, energies, and statistical weights.

Eq. (1) has many eigen-pair solutions, s_j and k_j, but only the fundamental-mode solution (corresponding to the largest eigenvalue) has a physical meaning. The respective modes are commonly ordered according to the absolute value of their eigenvalue, from the largest (associated with the fundamental mode $j = 0$) to the smallest. To simplify the notation in the following text, we denote the fundamental-mode fission source as $z; z \equiv s_0$.

To obtain the fundamental-mode solution, Monte Carlo criticality codes apply the power iteration on the fission source; this iteration can be formally described as

$$s^{(i+1)} = \frac{1}{k^{(i)}} H s^{(i)} + \epsilon^{(i)} \tag{2}$$

$$k^{(i)} = \frac{\int_V \mathrm{d}^3 r\, H s(\mathbf{r})}{m} \tag{3}$$

where the steps $i = 0, 1, \ldots$ are commonly referred to as "cycles", $\epsilon^{(i)}(\mathbf{r})$ is the random error component resulting from sampling a finite number of neutron histories in cycle i. The initial fission source $s^{(0)}$ must be guessed. The above iteration assumes that the Monte Carlo fission source is always normalised to m; i.e.,

$$\int_V \mathrm{d}^3 r\, s(\mathbf{r}) = m.$$

In classical Monte Carlo criticality calculations, a number of inactive cycles must be performed just to decay the error present in $s^{(0)}$, while results of interest are sampled over the subsequent active cycles.

As with any Monte Carlo simulation, the random error component $\epsilon^{(i)}(\mathbf{r})$ is of the order $O(1/\sqrt{m})$. Moreover, we can assume that (Gelbard and Gu, 1994)

$$\mathrm{E}[\epsilon^{(i)}] = 0.$$

The random noise in the fission source can thus be reduced by simulating more neutron histories, at the expense of a larger computing time. The random noise in the fission source $\epsilon^{(i)}$ is, however, not a relevant problem as long as the results are combined over a sufficiently large number of active cycles n. The random noise in the cumulative fission source

$$s_c^{(n)} = \sum_{i=i_x+1}^{n} s^{(i)}, \tag{4}$$

being of the order $O(1/\sqrt{mn})$, can then be neglected. In Eq. (4), i_x denotes the number of inactive cycles.

Gelbard and Prael (1974) showed that the random errors propagate over the cycles of Monte Carlo criticality calculations, which results in the presence of a bias in the fission source of the order $O(1/m)$. Thus, the converged Monte Carlo fission source is never sampled from the correct fundamental mode z, but from a biased fundamental mode that we denote as z_m. This bias is indeed reflected in the cumulative fission source. We show an example of a biased cumulative fission source in Section 4.

Ueki et al. (2003) have shown that convergence of the Monte Carlo fission source $s^{(i)}$ to z_m is governed by the dominance ratio k_1/k_0 at the rate of $O((k_1/k_0)^i)$. This is also a well known fact in deterministic calculations (although the solution is not biased there). This has an important consequence to systems with dominance ratio close to unity; if the initial fission source contains a large error then many cycles are necessary to decay this error. There is a risk then that active cycles (and hence the cumulative fission source) will be corrupted.

3. Estimating the error in the cumulative Monte Carlo fission source

In discrete phase-space notation, the eigenvalue (criticality) equation for the fission source can be written as

$$\mathbf{Hs} = k\mathbf{s} \tag{5}$$

where $\mathbf{H}$ is commonly referred to as the fission matrix (Carter and McCormick, 1969). The fission matrix $\mathbf{H}$ is the space-discretised operator H; The $(i,j)^{\text{th}}$ element of $\mathbf{H}$ represents the probability that a fission neutron born in space zone j causes a subsequent birth of a fission neutron in space zone i,

$$\mathbf{H}[i,j] = \frac{\int_{Z_i} \mathrm{d}^3 r \int_{Z_j} \mathrm{d}^3 r' f(\mathbf{r}' \to \mathbf{r}) z(\mathbf{r}')}{\int_{Z_j} \mathrm{d}^3 r'\, z(\mathbf{r}', E')}. \tag{6}$$

The fundamental mode eigenvalue of $\mathbf{H}$ equals k_{eff}, and the corresponding eigenvector $\mathbf{h}$ equals the discretised fundamental mode fission source $z(\mathbf{r})$.

A number of Monte Carlo codes, e.g., TRIPOLI-4 (OECD/NEA, 2008) and KENO V.a (RSICC, 2006), can optionally calculate the fission matrix during standard Monte Carlo calculations. Dufek and Gudowski (2009) showed that the fission matrix becomes less sensitive to errors in the fission source as the mesh zones get smaller. Hence, the errors in the fission source become irrelevant for sampling the fission matrix when the zones are sufficiently small. This means that the fission matrix and its fundamental-mode eigenvector can be correctly evaluated during a Monte Carlo criticality calculation even with a biased fission source. We suggest utilising this quality of the eigenvector of the fission matrix in estimating the error in the cumulative fission source.

We define the relative scalar error ε in the cumulative fission source $\mathbf{s}_c^{(n)}$ discretised over a space mesh as

$$\varepsilon = \left\|\tilde{\mathbf{s}}_c^{(n)} - \tilde{\mathbf{z}}\right\|_1, \tag{7}$$

where $\sim$ denotes a normalisation operator defined for any vector $\mathbf{x}$ as

$$\tilde{\mathbf{x}} = \frac{\mathbf{x}}{\|\mathbf{x}\|_1}.$$

and the one-norm is defined as

$$\|\mathbf{x}\|_1 = \sum_i |x_i|.$$

In Eq. (7), $\mathbf{z}$ is the fundamental-mode source discretised over the same mesh as the cumulative fission source.

The fundamental-mode source $\mathbf{z}$ in Eq. (7) is unknown; hence, the correct value of ε cannot be computed. We suggest to estimate its value as

$$\hat{\varepsilon} = \left\|\tilde{\mathbf{s}}_c^{(n)} - \tilde{\mathbf{h}}^{(n)}\right\|_1, \tag{8}$$

where $\mathbf{h}^{(n)}$ is the eigenvector of the fission matrix $\mathbf{H}^{(n)}$ that was sampled over the same cycles as the cumulative fission source $\mathbf{s}_c^{(n)}$.

Naturally, the fission matrix $\mathbf{H}^{(n)}$ contains random errors of the order $O(1/\sqrt{nm})$ that must also be present in its eigenvector $\mathbf{h}^{(n)}$. We denote the random errors in $\tilde{\mathbf{h}}^{(n)}$ by the vector $\boldsymbol{\delta}^{(n)}$,

$$\boldsymbol{\delta}^{(n)} = \tilde{\mathbf{h}}^{(n)} - \tilde{\mathbf{z}}; \tag{9}$$

while we denote the errors in $\tilde{\mathbf{s}}_c^{(n)}$ by the vector $\boldsymbol{\gamma}^{(n)}$,

$$\boldsymbol{\gamma}^{(n)} = \tilde{\mathbf{s}}_c^{(n)} - \tilde{\mathbf{z}},$$

so that

$$\varepsilon = \sum_i \left|\gamma_i^{(n)}\right|.$$

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