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Undersampling diagnostics by fission matrix in Monte Carlo criticality calculations

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ABSTRACT

Most Monte Carlo (MC) codes use the power iteration method for criticality calculations, where the fission bank of the previous cycle is taken as the source of the subsequent cycle. If the batch size (i.e. the neutron population per cycle) is insufficient, the power iteration may introduce biases in both k_{eff} and local tallies, which is known as the undersampling problem. Although the undersampling can be examined by independent runs with increasing batch sizes, it is important to diagnose undersampling directly upon a single calculation. In this paper, a method based on the fission matrix is proposed for undersampling diagnostics, and it is implemented in the RMC Monte Carlo code. Numerical results are presented for the "*k*-effective of the world" problem and the MC full-core performance benchmark. The results indicate that the fission matrix method is reliable for undersampling diagnostics. Besides, the effect of the mesh discretization on the fission matrix method is investigated.

1. Introduction

Monte Carlo (MC) methods have been used to compute the multiplication factor and the fundamental mode eigenfunction of critical systems since the 1950s (Kaplan, 1958). Most Monte Carlo codes, e.g. MCNP (X-5 Monte Carlo Team, 2003) and KENO (Oak Ridge National Laboratory, 2011), use the power iteration method to solve *k*-eigenvalue problems. Given an initial k_{eff} and source distribution, a batch or a cycle of neutrons is simulated to estimate a new k_{eff}, and the fission bank of the previous cycle is taken as the source distribution of the subsequent cycle. In order to keep the batch size (i.e. the neutron population per cycle) constant through cycles, the source distribution need be normalized at the end of the previous cycle.

It has been found that the MC power iteration has inherent limitations, known as problems of source convergence (Brown, 2008). The first problem is slow convergence, that is, the power iteration may take a large number of generations to converge in some cases such as those with a high dominance ratio, even as the number of neutrons per generation approaches infinity. Slow convergence occurs in the systems with a high dominance ratio, where the dominance ratio is defined as the ratio of the second-largest to the largest eigenvalues. If insufficient initial cycles (usually called inactive cycles) are discarded prior to beginning the tallies, the results will be contaminated by the fission source which is not converged. Various methods, such as CMFD (Yun and Cho, 2010; Lee and Joo, 2010) and Wielandt method (Yamamoto and Miyoshi, 2004; She et al., 2012), have been proposed to accelerate and diagnose the slow convergence of the fission source. The second problem is undersampling, which causes biases in k_{eff} and the source distribution. If the batch size is too small, the final results of k_{eff} and the source distribution may have large departures from the true values. The undersampling phenomenon depends on the number of neutrons per cycle, and cannot be remedied by increasing the number of cycles. Although MC code users can observe the undersampling phenomenon by performing independent runs with increasing batch sizes, it is important in practice to diagnose undersampling in a direct manner. Ueki (2005) has proposed criterions for undersampling diagnostics based on information theory. The third problem is underestimation of the variance on k_{eff} and tallies. This is caused by the correlation of fission source between cycles, and is not reduced by running more cycles or more neutrons per cycle. The underestimation is specifically significant in the reactor systems which have a large dominance ratio. In order to determine or to reduce the variance biases, several methods have been developed by Gelbard and Prael (1990), Ueki and Nease (2006), Shim (2009) and other researchers.

It is noted that only a few methods are proposed to diagnose undersampling, whereas most methods either diagnose only convergence or variance bias. This work focuses on the undersampling problem in MC criticality calculations. A novel method based on the fission matrix is proposed for undersampling diagnostics. The proposed method has been implemented in the RMC Monte Carlo code (Wang et al., 2011; She et al., 2013). Numerical results are presented for the well-known "*k*-effective of the world" problem

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(Whitesides, 1971) and the full-core MC performance benchmark (Hoogenboom et al., 2011). It is shown that the fission matrix method is reliable and convenient for undersampling diagnostics. Also, the mesh effect on the fission matrix method is discussed.

2. Power iteration and undersampling

The transport equation can be written as

$$(L + C - S)\Psi = \frac{1}{k_{eff}}F\Psi, \tag{1}$$

where the operators L, C, S, and F represent the leakage term, scatter-in term, collision term, and fission term, respectively. Eq. (1) can be solved numerically using the standard power iteration method:

$$\Psi^{(n+1)} = \frac{1}{k_{eff}^{(n)}}F\Psi^{(n)}, \quad n = 0, 1, \cdots \tag{2}$$

In the MC power iteration process, the neutrons generated by fission during the previous cycle are taken as the source distribution of the subsequent cycle. Before beginning the subsequent cycle, the source distribution needs to be normalized at the end of the previous cycle to keep the batch size constant. However, this renormalization has been proved to introduce a bias in both k_{eff} and the source distribution, known as the undersampling problem (Kiedrowski and Brown, 2009; Shim and Kim, 2009). The expected bias in k_{eff}, Δk, has been shown to be (Brissenden and Garlick, 1986).

$$\Delta k \propto \sigma_k^2 \propto \frac{1}{M}, \tag{3}$$

where σ_k^2 is the apparent variance in k (computed assuming uncorrelated values of k for each cycle), and M is the number of particles per cycle (i.e. the batch size). The biases in k_{eff} and local tally results are inversely proportionate to the batch size, M, but are independent of the number of cycles, N. That is to say, unless sufficient neutron histories in each individual cycle are simulated, the biases will always exist regardless the number of cycles. This could be explained that the source distribution cannot be steadily sampled if the number of neutrons per cycle is insufficient. Considering the existence of undersampling, MC code users should be always cautioned that the results can be still biased even though they have simulated a large number of active neutron histories and obtained apparently small variance.

The undersampling phenomenon can be examined by making trial runs with increasing batch sizes, such as $M = 500$, $M = 1000$, $M = 10{,}000$, until the biases tend to be negligible. In practice, however, it is useful to directly diagnose the undersampling effect after a single criticality simulation. This issue is especially important from the view of criticality safety because the undersampling problem underestimates the k_{eff} value.

3. Fission matrix and undersampling diagnostics

The eigenvalue mode transport equation is given in the form of

$$Hs = ks, \tag{4}$$

where s is the fission source distribution, k is the multiplication factor, and H is the operator representing the fission neutron production during the transport. Fission matrix, F, approximates the operator H by dividing the whole system into individual regions. The fission matrix element (F_{ij}) represents the probability that a fission neutron born in a region j causes a birth of a fission neutron in a region i:

$$F_{ij} = \frac{\int_{V_i} dr \int_{V_j} dr' f(r' \to r) s_0(r')}{\int_{V_j} dr' s_0(r')}, \tag{5}$$

where the fission kernel, $f(r' \to r)$, represents the probability that a neutron born at r' causes a birth of a fission neutron at r. According to Eq. (5), the elements of the fission matrix can be evaluated at essentially no extra cost during the normal Monte Carlo simulation.

The fission matrix method has shown its potential to accelerate the fission source convergence (Dufek and Gudowski, 2009) and it is recently implemented into MCNP6 (Carney et al., 2012). but it was seldom applied to the undersampling problem. In the present work, what we are interested in is to investigate the capability of fission matrix on undersampling diagnostics. Different from the fission matrix for accelerating source convergence, here the fission matrix for undersampling diagnostic is cumulatively estimated through all active neutron histories. In principle, each individual fissionable region should be sufficiently sampled during the whole active cycles, but it is not necessary to assure a steadily source distribution in each cycle. As such, the fission matrix is not sensitive to the neutron population per cycle, and it can estimate k_{eff} and source distribution even in the case of undersampling.

The fission matrix method for undersampling diagnostics is implemented as follows.

- Firstly, given a mesh covering all fissionable regions, the fission matrix is cumulatively estimated during all active cycles. Note that the fission matrix for undersampling diagnostics is tallied in a different way from that for accelerating source convergence. The latter is usually tallied during each inactive cycle.
- Secondly, k_{eff} and the fission source distribution are deterministically solved by Eq. (4) using the standard power method. The solver has been implemented in the RMC code.
- Thirdly, the k_{eff} and source distributions obtained by the power iteration and fission matrix are compared to diagnose undersampling.

Two diagnostic criterions are proposed for practice. The first criterion is used to diagnose the bias in k_{eff}:

$$\Delta k = k^{\mathrm{FM}} - k^{\mathrm{MC}} < \varepsilon$$

$$\varepsilon = \begin{cases} 3\sigma_k & \text{acceptable} \\ \sigma_k & \text{desirable} \end{cases} \tag{6}$$

where k^{FM} is the eigenvalue calculated from the fission matrix; k^{MC} and σ_k is the k_{eff} mean and standard variance calculated from the MC power iteration, respectively. Noting that the apparent variance is usually lower than the true variance because of the cycle correlation, we use the apparent standard deviation in Eq. (6) for conservation. The first criterion is an easy-to-use and also the principal criterion for undersampling diagnostics.

The second criterion is to diagnose the bias in fission source distribution by using the relative entropy (Ueki, 2005),

$$D(s^{\mathrm{MC}}|s^{\mathrm{FM}}) = -\sum_j s^{\mathrm{MC}}(j)\log_2\frac{s^{\mathrm{MC}}(j)}{s^{\mathrm{FM}}(j)} < \varepsilon$$

$$\varepsilon = \begin{cases} 10^{-4} & \text{acceptable} \\ 10^{-5} & \text{desirable} \end{cases} \tag{7}$$

where s^{FM} is the normalized eigenvector calculated from the fission matrix, s^{MC} is the normalized average source distribution in the MC power iteration, and j is the mesh index of spatial region. Attention should be paid to the dependence of the relative entropy on the mesh discretization. Generally speaking, all entropy-based methods more or less rely on the mesh discretization. It is speculated that the diagnostic method using Shannon entropy and relative entropy proposed by Ueki should also have such problem. From the general view of statistics, relative entropy below 10^{-5} usually means