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Optimal neutron population growth in accelerated Monte Carlo criticality calculations

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ABSTRACT

We present a source convergence acceleration method for Monte Carlo criticality calculations. The method gradually increases the neutron population size over the successive inactive as well as active criticality cycles. This helps to iterate the fission source faster at the beginning of the simulation where the source may contain large errors coming from the initial cycle; and, as the neutron population size grows over the cycles, the bias in the source gets reduced. Unlike previously suggested acceleration methods that aim at optimisation of the neutron population size, the new method does not have any significant computing overhead, and moreover it can be easily implemented into existing Monte Carlo criticality codes. The effectiveness of the method is demonstrated on a number of PWR full-core criticality calculations using a modified SERPENT 2 code.

1. Introduction

One of the reasons for high computing cost of Monte Carlo criticality calculations is the computing cost of inactive cycles. This cost corresponds to computing time used for converging the initial guess of the fission source distribution to the fundamental mode of the system. Since the inactive cycles are not used for improving the statistics of the results, these cycles increase the overall computing cost of the Monte Carlo criticality calculations. Various approaches, such as Wielandt's method (Yamamoto and Miyoshi, 2004), the fission matrix-based methods (Kitada and Takeda, 2001), or the hybrid CMFD/Monte Carlo methods (Lee et al., 2010), were proposed for accelerating the fission source convergence thus reducing the required number of inactive cycles. However, reducing the number of inactive cycles alone may not necessarily improve the efficiency of Monte Carlo criticality calculations as the methods may add to the computing cost of a single cycle.

Selecting a small neutron population size (the number of neutrons simulated per cycle) could lower the computing cost of inactive cycles; however, a considerable bias could be introduced in the fission source this way. Brissenden and Garlick (1986) explained that the bias of order $O(1/m)$, where m is the population size, is present in the fission source due to normalisation of the source at each cycle. While the initial error and the statistical error decay over the simulation cycles, the bias does not decay and eventually may dominate the total error. Therefore, a large neutron population size is commonly preferred to assure that the results are not affected by the source bias (Brown et al., 2010). On the other hand, a large population size increases the computing time of a single cycle, thus limiting the number of cycles which can be simulated in a certain computing time. Therefore, the selection of the neutron population size represents an efficiency optimisation problem (Tuttelberg and Dufek, 2015).

Dufek and Tuttelberg (2016) identified that efficiency of Monte Carlo criticality simulations can be improved by gradually increasing the neutron population size over the successive cycles, and proposed an on-the-fly neutron population control method. In this strategy, the starting population size is relatively small, allowing for fast decay of the initial error over the iterations (in terms of computing time). The population size is then gradually increased, reducing the source bias.

In the above method, the population size is set so that the bias is in proportion to an estimate of the total relative error in the cumulative fission source (a source combined over the cycles). The error estimation is performed using the fundamental-mode eigenvector of a fission matrix. While the method was shown to increase the simulation efficiency, tallying the fission matrix and computing the fundamental mode eigenvector introduces computing overhead which may reduce the efficiency gain, especially in case of large systems.

The necessity of computing the eigenvector of the fission matrix may limit the application of the method to problems in which the matrix and its eigenvector can be easily obtained. In this paper, we

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therefore suggest a method for neutron population control that does not require the fission matrix eigenvector for estimating the total error in the fission source. We show that the total error can, for this purpose, be approximated by the statistical error alone, which can be estimated without the fission matrix. The computing overhead associated with tallying the fission matrix and computing the eigenvector can be then eliminated.

We explain the method in Section 2. We demonstrate the improvement in computing efficiency on a number of full-core PWR test calculations in Section 3. Section 4 summarises our conclusions.

2. Method

The total error in the Monte Carlo fission source can be decomposed into three components: a contribution originating from the initial cycle, a statistical error and an error caused by a bias in the fission source. The error in the source sampled in the initial cycle propagates into sources in the successive cycles, and while this error decays over the cycles, it may constitute a significant part of the total error in systems with large dominance ratios (Ueki et al., 2003). The statistical error of order $O(1/\sqrt{m})$ is introduced into the fission source at each cycle since the fission source is sampled at a finite number, m, of sites. The systematic bias of order $O(1/m)$ is caused by normalisation of the fission source to the required population size at each cycle (Brissenden and Garlick, 1986).

The study of the source convergence is complicated by the fact that the statistical (random) error of order $O(1/\sqrt{m})$ is always present in the fission source. For this reason we choose to monitor the source convergence via the so-called cumulative fission source, i.e. the source combined over all cycles. The statistical error that is introduced into the simulation via random sampling procedures decreases in the cumulative fission source over the cycles as random errors cancel out each other with better statistics. Hence, the statistical error in the cumulative fission source is $O(1/\sqrt{h})$, where h is the number of all neutron histories. Note that this relates only to statistical error that is newly introduced at each cycle.

The error in the cumulative fission source also closely relates to the error in actual tallied results, such as the power distribution or the effective multiplication factor since these are also collected over multiple cycles. A figure-of-merit of a calculation based on the cost of the calculation and the error in the cumulative fission source can therefore be also taken as a good measure the efficiency of the simulation.

As both the statistical error and the error originating from the initial fission source decay in the cumulative fission source over simulation cycles, the source bias may start dominating the total error after a certain number of cycles. The neutron population size is fixed over the cycles in standard Monte Carlo calculations, so the source bias (which is inversely proportional to the neutron population size) remains constant over the cycles as well. The source bias may therefore become large compared to other errors and dominate the total error at some point in the simulation; consequently, simulating more cycles cannot improve the results. Therefore, a large population size is commonly recommended for Monte Carlo criticality calculations (Brown et al., 2010).

Although a large neutron population size is desirable for lowering the bias, it may negatively affect the simulation efficiency. Simulation of a large neutron population size requires a proportionally large computing cost per cycle. The number of cycles that can be performed within a certain computing time may then be insufficient for ensuring a converged fission source, which could result in a poor simulation efficiency. Nevertheless, simulations with a small neutron population size may not necessarily do any better. While a small neutron population size may allow for many cycles within the same computing time, the source bias associated with the small population size may corrupt the results, thus causing poor simulation efficiency as well.

The computing efficiency hence depends on the selection of the neutron population size, which represents an optimisation problem: a small population size is desirable for reducing the computing time per cycle, while a large population size is desirable for reducing the source bias. Tuttelberg and Dufek (2015) proposed a population size optimisation procedure for standard Monte Carlo criticality calculations. At the beginning of the simulation, the method optimises the population size for the computing time allocated for the whole simulation and the population size then remains constant over all cycles.

Dufek and Tuttelberg (2016) further suggested a method that gradually increases the neutron population size over successive simulation cycles. The authors argued that at any cycle in the simulation, the neutron population size should be kept small enough for efficient source iteration, while at the same time large enough for limiting the source bias. Since the initial and the statistical errors dominate the total error at the beginning of a simulation, a large initial population size is unnecessary for assuring a small value of the source bias; as the errors decay in the successive cycles, the population size is increased, reducing the source bias.

For practical implementation of the above approach, Dufek and Tuttelberg (2016) proposed splitting the simulation into several stages, estimating the total error in the cumulative fission source at each stage, and selecting such a population size that its associated bias is in a certain proportion to the estimated error in the cumulative source. The error estimation is performed using the fundamental-mode eigenvector of a fission matrix. The fission matrix is tallied during the simulation, and the fundamental-mode eigenvector of the matrix is computed at each simulation stage. This constitutes additional computing overhead, which may prevent efficient application of the method to large-scale problems, where a fine mesh resolution for the fission matrix may be required. Then, the computing overhead associated with the on-the-fly error estimation may reduce the overall efficiency gain.

Here, we suggest a modification to the above method, removing the necessity for computing the fission matrix. We suggest selecting the population size so that the associated source bias remains in a certain proportion to the statistical error in the cumulative fission source. Our choice is motivated by the fact that the statistical error represents the largest contribution to the total error in the cumulative fission source when the fission source is being optimally iterated. This is demonstrated in Section 3.

The statistical error in the cumulative fission source, ε_s, can be approximated at the beginning of cycle i as

$$\varepsilon_s^{(i)} \cong \frac{a}{\sqrt{h_i}}, \tag{1}$$

where a is a system-dependent constant, which formally denotes the magnitude of the statistical error for a given system, and h_i is the total number of neutron histories simulated prior to cycle i. The approximation is based on the order of the statistical error in the cumulative fission source, which is $O(1/\sqrt{h})$.

The fission source bias in cycle i, $\beta^{(i)}$, can be approximated as

$$\beta^{(i)} \cong \frac{b}{m_i}, \tag{2}$$

where b is a system-dependent constant, which formally denotes the magnitude of the source bias for a given system. The approximation is based on the fact that the fission source bias is $O(1/m)$.