Monte Carlo Fission Matrix Acceleration Method with Adaptive Mesh (postprint)

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Abstract

In large-scale, loosely coupled systems, Monte Carlo criticality calculation always suffers from slow fission source convergence resulting from the high dominance ratio. The fission matrix acceleration method has shown its potential to accelerate the convergence of the fission source in many numerical simulations. In practice, however, instability of this method may be caused by imbalanced precisions of elements of the fission matrix. Hence, an improved method, in which the space mesh used to compute the fission matrix is defined adaptively based on the fission bank in each cycle, is introduced. The proposed method ensures balanced precisions of elements of the fission matrix, so is more stable than the existing fission matrix method.

Full Text

Preamble

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Monte Carlo Fission Matrix Acceleration Method with Adaptive Mesh

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In large-scale, loosely coupled systems, Monte Carlo criticality calculations suffer from slow fission source convergence due to high dominance ratios. The fission matrix acceleration method has demonstrated potential for accelerating fis-

sion source convergence in numerous numerical simulations. However, practical applications may encounter instability caused by imbalanced precision among elements of the fission matrix. This paper introduces an improved method where the spatial mesh for computing the fission matrix is defined adaptively based on the fission bank in each cycle. The proposed method ensures balanced precision across fission matrix elements, thereby achieving greater stability than conventional fission matrix methods.

Keywords: Monte Carlo, Criticality, Fission matrix, Adaptive

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Introduction

The Monte Carlo (MC) method is widely employed to compute the multiplication factor and fundamental mode eigenfunction of critical systems in reactor physics. The power iteration method serves as the primary technique for criticality calculations in most Monte Carlo codes. However, this approach suffers from slow fission source convergence in large, loosely coupled systems, requiring numerous inactive cycles before active cycles can begin. This slow convergence leads to unacceptable computational costs, particularly for whole-core analysis of commercial reactors.

Various acceleration methods have been proposed to address this issue. The super-history method [1] and Wielandt' s method [2] reduce the dominance ratio by modifying the power iteration scheme, thereby decreasing the number of inactive cycles needed for fission source convergence. However, these methods increase computational expense during each inactive cycle. The functional method [3] and the coarse-mesh finite difference accelerating Monte Carlo method [4] utilize standard Monte Carlo techniques to estimate nonlinear functionals, which are then employed in low-order functional Monte Carlo (FMC) equations and coarse-mesh finite difference (CMFD) equations to obtain eigenvalues and discrete representations of the eigenfunction. The modified power iteration method [5] can accelerate convergence and calculate the second eigenpair, though no examples demonstrate its effectiveness for continuous-energy problems.

Compared to these approaches, the fission matrix acceleration (FM) method [6] offers greater intuitiveness. When the system is spatially discretized, the fission matrix can be tallied during each Monte Carlo simulation cycle. The FM method adjusts fission neutron weights according to the fundamental mode eigenvector of the fission matrix at each cycle, showing potential for accelerating fission source convergence in many numerical simulations. However, instability issues limit its practical application. The conventional FM method constructs a fixed spatial mesh before iteration begins and uses this mesh to tally the fission matrix in each cycle. Since elements correspond to zones with varying source intensities, they are tallied with different sample sizes, leading to varying precisions. After several cycles, fission source intensities may become very small

in some zones, resulting in large statistical errors in the corresponding columns of the fission matrix. This imbalanced precision can cause FM method instability.

The semi-fixed-source FM method [7] recently addressed this instability by sampling all fission matrix elements with an equal number of particles to improve efficiency. However, this approach increases computational cost significantly, particularly when the actual fission source is severely imbalanced, as it requires sampling many more particles than the conventional method. This paper proposes defining the spatial mesh for computing the fission matrix adaptively based on the fission bank in each cycle. This approach ensures balanced precision of fission matrix elements without increasing the number of sampled particles. While "accumulation" [8] can improve fission matrix precision, it cannot balance precision across matrix elements.

II. Fission Matrix Method with Adaptive Mesh

A. Fission Matrix Method

The primary objective of criticality calculations is to find the fundamental mode solution of the eigenvalue equation [7]:

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

where k is the eigenvalue, $s(\mathbf{r}, E)$ is the corresponding fission source distribution function, and

$$Hs(\mathbf{r}, E) = \int_0^\infty \int dE' d\mathbf{r}' f(\mathbf{r}', E' \to \mathbf{r}, E) s(\mathbf{r}', E')$$

in which $f(\mathbf{r}', E' \to \mathbf{r}, E)$ is the fission kernel representing the expected number of first-generation fission neutrons produced per unit volume at $\mathbf{r}$ per unit energy at E from a fission neutron born at $\mathbf{r}'$ with energy E'. Fission neutrons are assumed to emit isotropically (this assumption simplifies the formulation but is not necessary for Monte Carlo simulation).

The standard power method solves problem (1) in most Monte Carlo codes. An initial fission source distribution, either guessed or obtained from other calculations, is iteratively recalculated until convergence is achieved. Cycles performed before obtaining a converged fission source are called inactive cycles, while subsequent cycles are active cycles used for tallying final results.

When the system is spatially discretized, the actual fission source distribution satisfies:

$$\mathbf{HS} = k\mathbf{S}$$

where **S** indicates a fission source distribution vector whose elements represent the fraction of fission source in each zone, k is the multiplication factor, and the fission matrix **H** is defined as:

$$H_{i,j} = \frac{\int_0^\infty \int dE d\mathbf{r} \int_0^\infty \int dE' d\mathbf{r}' f(\mathbf{r}', E' \to \mathbf{r}, E) s(\mathbf{r}', E')}{\int_0^\infty \int dE' d\mathbf{r}' s(\mathbf{r}', E')}$$

The "cycle fission matrix" [9] can be constructed in each cycle as:

$$H_{i,j}^{(n)} = \frac{\int_0^\infty \int dE d\mathbf{r} \int_0^\infty \int dE' d\mathbf{r}' f(\mathbf{r}', E' \to \mathbf{r}, E) s^{(n-1)}(\mathbf{r}', E')}{\int_0^\infty \int dE' d\mathbf{r}' s^{(n-1)}(\mathbf{r}', E')}$$

Since the fission source distribution evaluated from the fission matrix converges more rapidly than in ordinary Monte Carlo simulations [7], fission source convergence can be accelerated by adjusting fission neutron weights according to the fundamental mode eigenvector of $\mathbf{H}^{(n)}$ in each cycle. If the m-th fission neutron is produced in region i, its weight w_m is corrected to:

$$w'_m = w_m \frac{(S_f^{(n)})_i}{(S_f^{(n)})_i}$$

where $S_f^{(n)}$ is the fundamental eigenvector of $\mathbf{H}^{(n)}$, and $(S_f^{(n)})_i$ is the relative source intensity at zone i obtained from an ordinary MC simulation (normalized to the same magnitude as $S_f^{(n)}$). In practice, fission matrix acceleration is applied only during inactive cycles, and it is recommended that several inactive cycles without weight correction be performed before active cycles begin to eliminate bias from region-averaged correction factors.

B. Adaptive Mesh

In Monte Carlo simulations, the number of histories sampled in each zone depends on the source intensity. When a fixed mesh is used for computing the fission matrix throughout all FM method cycles, fission source intensities may become very small in some zones after several cycles, resulting in fewer sampled histories in those zones. This leads to imbalanced precision among fission matrix elements and causes FM method instability. To improve efficiency and overcome instability, this paper proposes an adaptive mesh approach:

1. Define a relatively fine mesh consisting of many zones.
2. At the beginning of each cycle, construct a coarse mesh by combining zones from the fine mesh according to the source distribution, making source intensities roughly equal across different coarse mesh zones. Each coarse mesh zone may contain several fine mesh zones, and different cycles may have different numbers of coarse mesh zones.

3. Calculate the fission matrix based on the coarse mesh during each cycle, allowing the order of fission matrices to vary between cycles.
4. Count first-generation fission neutrons in each fine mesh zone and construct the fission bank for the next cycle.
5. After each cycle, adjust neutron weights in the fission bank according to the fundamental eigenvector of the fission matrix.

Step (2) is the key to this method. Implementation is straightforward for one-dimensional models. For a fine mesh containing N zones defined by $I_i = [x_{i-1}, x_i]$, the source intensity of zone I_i is Δs_i according to the fission source bank from the previous cycle. To construct a coarse mesh with approximately K zones ($K \ll N$), each coarse mesh zone should have source intensity of about $t = \frac{\sum_{i=1}^{N} \Delta s_i}{K}$. We first select k_1 satisfying:

$$\left| \sum_{i=1}^{k_1} \Delta S_i - t \right| = \min_{1 \le k \le N} \left| \sum_{i=1}^{k} \Delta S_i - t \right|$$

Let $\bigcup_{i=1}^{k_1} I_i$ be the first coarse mesh zone, then find k_2 satisfying:

$$\left| \sum_{i=k_1+1}^{k_2} \Delta S_i - t \right| = \min_{k_1+1 \le k \le N} \left| \sum_{i=k_1+1}^{k} \Delta S_i - t \right|$$

Let $\bigcup_{i=k_1+1}^{k_2} I_i$ be the second coarse mesh zone, and continue similarly. If the intensity of the last coarse mesh zone is less than a specified value (e.g., $t/2$), the final two coarse mesh zones are combined. Since this method cannot make intensities exactly equal to t, the number of zones in coarse meshes may differ slightly from K.

III. Numerical Results

We consider a one-dimensional problem featuring large heterogeneous fissile regions surrounded by a thin reflector. Neutrons are assumed to scatter isotropically, with physical data provided in .

Monte Carlo simulations were performed with 500,000 histories per cycle. The initial fission source distribution is spatially uniform. The FM method discretizes the fissile regions into 10 zones, while the fine mesh for the adaptive fission matrix acceleration method (ADFM) equally discretizes the 30 cm fissile region into 300 zones. The number of coarse mesh zones constructed for ADFM is also approximately 10, though it may vary slightly across cycles.

[Figure 1: see original paper] shows the number of fission neutrons in each zone for the initial source, cycle 5, and cycle 20 when using a fixed mesh. The figure reveals that the number of fission neutrons becomes highly imbalanced

after several cycles, which would result in severely imbalanced precision among fission matrix elements since only histories originating from zone j contribute to tallies of elements H_{ij}.

[Figure 2: see original paper] illustrates the coarse meshes for the ADFM method at different cycles. The ADFM mesh matches the FM mesh at the first cycle, but becomes noticeably different in subsequent cycles. After performing 100 cycles separately with the FM and ADFM methods, the Shannon entropy evolution is shown in [Figure 3: see original paper] (calculated using the fine mesh). The reference value is taken as the average Shannon entropy over cycles 3001 to 5000 from standard Monte Carlo power iteration (PI).

presents the cycle numbers when Shannon entropy first crosses the reference after terminating weight correction by FM and ADFM at different cycles (standard PI first crosses the reference at cycle 851). The results demonstrate that ADFM is more efficient and stable than the conventional FM method.

[Figure 5: see original paper] compares eigenfunctions estimated during cycles 50 to 100 by the FM method, ADFM method, and standard power iteration, with the eigenfunction from cycles 3001 to 3050 of standard PI serving as reference.

As shown in [Figure 3: see original paper], both FM and ADFM methods cause Shannon entropy to cross the reference more rapidly than standard PI, but the FM method exhibits much stronger oscillations than ADFM. In some cases, many cycles may be required to eliminate these oscillations after terminating weight correction with the FM method. For example, [Figure 4: see original paper] shows the Shannon entropy evolution when weight correction terminates at cycle 48.

IV. Discussion

Source distribution convergence can be diagnosed by checking whether Shannon entropy crosses the reference value [11]. Numerical results ([Figure 3: see original paper] and [Figure 4: see original paper]) show that both FM and ADFM methods enable rapid crossing of the reference by Shannon entropy, suggesting similar convergence rates. However, the FM method exhibits excessive oscillations in this model, requiring additional cycles without weight correction before active cycles to eliminate these oscillations. Terminating weight correction at different cycles with the FM method produces varying effects, sometimes requiring many cycles for Shannon entropy to cross the reference again, with the number of extra cycles potentially comparable to that needed by standard PI. In contrast, ADFM consistently requires far fewer cycles than standard PI to achieve reference crossing after terminating weight correction (), making it more efficient and stable.

The additional time required for ADFM compared to FM is negligible in the tested one-dimensional model, and the same is expected for two- or three-dimensional problems. The primary extra cost of ADFM involves calculating

fission source intensity in each fine mesh zone. When using ADFM, a regular fine mesh can be defined (the union of fine mesh zones must contain the fissile regions but need not coincide exactly with them). Locating fission neutrons in the fission source bank and counting their numbers (which represents fission source intensity) in each fine mesh zone is straightforward.

The FM method has been implemented in the MCNP code for two- and three-dimensional continuous-energy problems [12]. The only difference between ADFM and FM lies in mesh construction. Although ADFM is tested here on a one-dimensional multi-group problem for simplicity, its application to continuous-energy problems presents no difficulty.

Extending ADFM to two- and three-dimensional problems is also straightforward, though coarse mesh construction must be performed carefully for complex systems to ensure efficiency. Weight corrections in both FM and ADFM methods can only accelerate fission source balance between different zones, not local fission source balance within each zone. In ADFM, since source intensities are roughly equal across coarse mesh zones, local balance in large zones is less critical due to their low source densities. For one-dimensional problems, local fission source balance in small zones is easily achieved. However, for two- or three-dimensional problems, small zone area or volume does not guarantee rapid local fission source balance, as a zone may have a large dimension in one direction (e.g., a long, narrow rectangle). For ADFM to be efficient, coarse mesh zones must satisfy an additional requirement: no single direction' s scale should be much larger than the others.

V. Conclusion

The fission matrix acceleration method has demonstrated potential for accelerating fission source convergence in numerous numerical simulations. However, practical instability may arise from imbalanced precision among fission matrix elements. This paper proposes defining the spatial mesh for computing the fission matrix adaptively based on the fission bank in each cycle. This approach ensures balanced precision across fission matrix elements, resulting in greater stability. Although ADFM is tested here on a one-dimensional multi-group problem for simplicity, it can be readily applied to two- or three-dimensional continuous-energy problems with properly constructed adaptive meshes.

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Note: Figure translations are in progress. See original paper for figures.