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Monte Carlo Criticality Problems & The Fission Matrix

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1. Introduction

We provide some perspective on the fission matrix method as applied to Monte Carlo (MC) criticality calculations. This method is among the oldest methods for MC criticality calculations [1,2], and has been proposed and tried by many researchers over the past 60 years. The past efforts were successful only for very small problems due to computer memory limitations and the N^2 nature of the method. Some of the most interesting aspects of the fission matrix method pertain to the understanding and resolution of unanswered questions on the fundamental theoretical basis for continuous-energy MC criticality calculations.

2. Fission Matrix Method

References [3] and [4] provide detailed descriptions of the theory, computational techniques, and results obtained in the initial implementation of the method in MCNP. In [3], we derive the forward and adjoint fission matrix equations, without approximation, from the k-eigenvalue form of the neutron transport equation. Fission matrix elements are estimated at essentially no extra cost during the normal MC simulation using only the locations of fission neutron sources at the start and end of each batch, without incurring any overhead during the random walks. The key computational advance is the use of a sparse, compressed-row storage scheme for the fission matrix tallies. With this scheme, no approximations are made; the sparsity is general, not banded, and all tallies are rigorously recorded. Eigensolvers for both the left and right eigenvectors of a general sparse matrix are based on power iteration, with Hotelling deflation for producing higher modes. The example problems in [4] are realistic, detailed models using continuous-energy physics – a 2D PWR, a large fuel storage vault, the ATR reactor, and a 3D reactor. Fig. 1 [4] shows the first 10 eigenfunctions for the 2D PWR model.

The fission matrix can provide estimates of the fundamental mode distribution, the dominance ratio, the eigenvalue spectrum, and higher mode eigenfunctions. Accurate higher modes for the fission source and adjoint have many potential uses in convergence analysis, stability analysis, perturbation theory, etc. The fundamental mode from the fission matrix can be accurately computed before the actual neutron distribution has converged; it can therefore be used to accelerate convergence of the power iterations for the actual neutron distribution.

3. Relation to Fundamental Reactor Theory

The k_{eff} form of the transport equation for energy-dependent problems [5] is not self-adjoint; due to neutron slowing down, the kernel for the integral operator is not symmetric. Accordingly, eigenfunctions need not form a complete, real, orthogonal set of basis functions. The forward and adjoint fission sources are biorthogonal. The fundamental mode eigenvalues and eigenfunctions have been proven to exist, even for continuous-energy transport [6]. The fundamental mode eigenvalue is real and positive, and the fundamental mode eigenfunction is real and non-negative. For 1-speed transport with isotropic scattering, it has been proven [7] that all of the higher modes exist, with discrete real eigenvalues and real eigenfunctions. The 1-speed equation for the scalar flux is self-adjoint due to the symmetry of the integral operator kernel. This proof was later extended to include

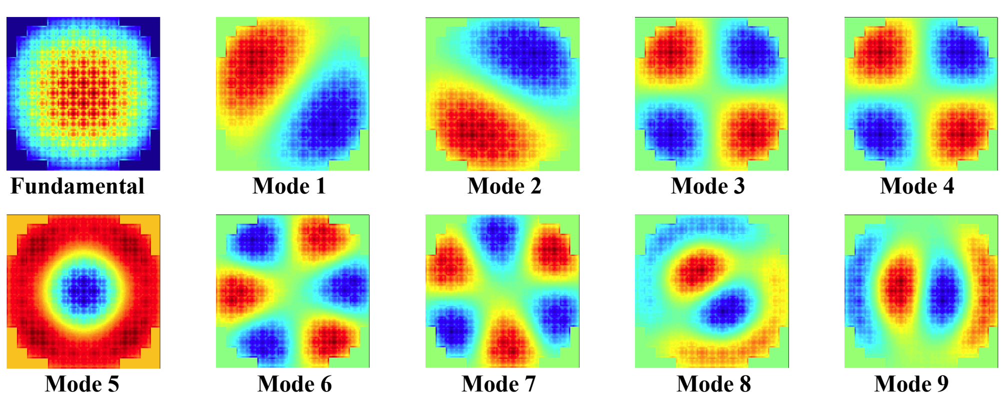

Fig. 1. First 10 eigenmodes for PWR obtained from a fission matrix using a 120x120x1 spatial mesh.

anisotropic scattering [8]. For multigroup and continuous-energy transport, it is conventional practice to assume that higher modes exist, with real eigenvalues and eigenfunctions, even though that has not been proven.

In [3,4], very fine spatial resolution was used in computing the fission matrix for realistic problems. It was shown that, for fine enough spatial resolution, the adjoint fission matrix is simply the transpose of the forward fission matrix, so that the fission source distribution and its higher modes are *right* eigenvectors, while the adjoint and its higher modes are *left* eigenvectors. The fission source and its adjoint were proven to be biorthogonal. Numerical evidence for every problem analyzed to date indicates that:

- As spatial resolution is refined, the eigenvalue spectrum of the fission matrix converges smoothly. For *N* spatial regions and an *NxN* fission matrix, there are *N* eigenvalues. As *N* is increased, the lowest modes converge smoothly. See Fig. 2 for an example.
- The eigenvalues are discrete and real. (This is debatable, since some complex eigenvalues appear for some of the highest modes. However, as *N* is increased and statistical noise decreased by using more neutrons, the complex parts become smaller and shift to even higher modes.)
- The forward eigenfunctions form a very-nearly orthogonal set. Theory dictates that the forward and adjoint solutions are biorthogonal, and that the forward modes alone need not be orthogonal to each other. The numerical evidence in [3,4] for several realistic problems shows the near-orthogonality of the forward modes. See Fig. 3 for an example.

4. Conclusions

Further study is ongoing into the above and additional aspects of the fundamental theoretical basis of the k_{eff} form of the transport equation. The accuracy of the fission matrix method using continuous-energy and very fine spatial resolution – made possible by the new sparse storage algorithms – provides a valuable new tool for both theoretical and practical studies of critical systems.

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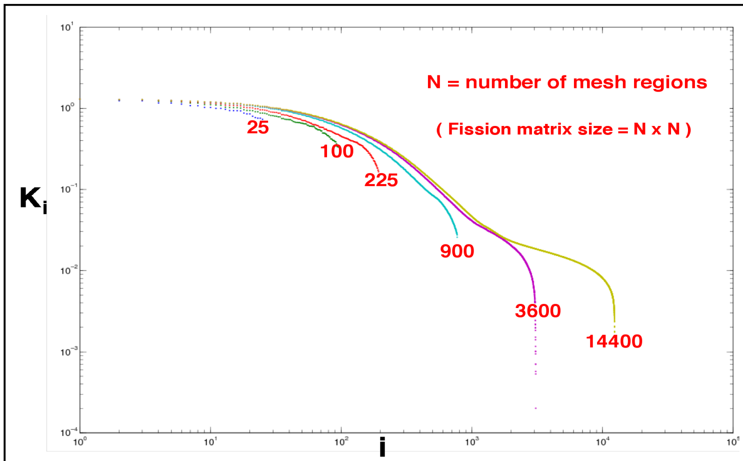

Fig. 2. Eigenvalue spectrum for PWR model. Real part of K_i is shown for various fission matrix spatial meshes.

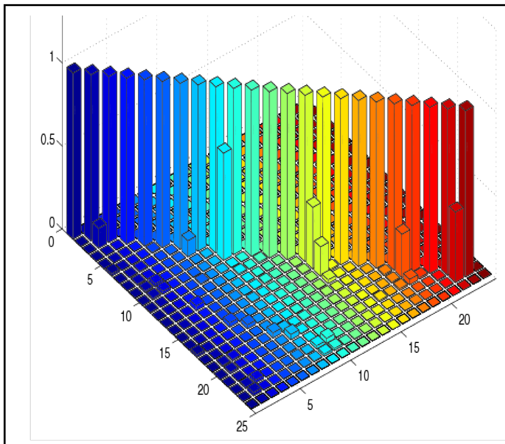

Fig. 3. Inner products of first 25 forward mode eigenfunctions for 2D PWR.