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Monte Carlo Criticality Calculations – History & Recent Progress

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INTRODUCTION

Monte Carlo (MC) methods are used routinely today for the detailed analysis of critical experiments and reactors. In this paper, we provide an overview of the historical progression of MC capabilities for criticality calculations. Then, recent progress in MC criticality capabilities and current R&D efforts are noted. As an example of current R&D efforts, we provide some perspective on the fission matrix method as applied to MC criticality calculations. This example serves to illustrate the close connections and synergy among MC methods, computer capabilities, and theoretical work from the 1940-50s on the fundamental theory and mathematics that support today's computational methods. Researchers, especially students, should note that to take full advantage of today's large computers, it is often useful or necessary to delve back into the pioneering work in reactor theory. Often an older method that went largely unused due to computer limitations may be practical and effective in today's computing environment. In addition, new MC capabilities can help to investigate and clarify some of the original theoretical work.

HISTORY OF MONTE CARLO CRITICALITY CALCULATIONS

The history of Monte Carlo (MC) methods for criticality problems is closely linked to that of computers. John von Neumann developed the first computer program for MC calculations of particle transport in 1947 [1] for the ENIAC. In the 1950s [2-5] MC criticality calculations were limited by computer speed and capacity to small critical experiments or simplified systems. The first fully-detailed calculations of reactors began in the 1960s [5,6], and by the 1970s fully-detailed, 3D whole-core MC reactor calculations were routine. The progression in MC capabilities matched the growth in computer speed and capacity. In the pre-2000s, supercomputers were found primarily at national laboratories; today large Linux clusters are widely available, so that universities and industry have access to comparable systems. Due to the cpu-intensive nature of MC codes, they were often some of the first codes to be converted to new computers.

Over the past 60+ years of methods and code development for Monte Carlo, there has been steady progress in all areas: Geometry modeling capabilities began with a dozen or fewer regions, then grew to a few 1000s in the 1970s, 10-100K in the 1990s, and now to millions or more in some codes. The introduction of hierarchical geometry (i.e., embedded geometry, "holes", "universes", etc.) has enabled large models with reusable geometry parts. Physics interaction data as provided by libraries of nuclear cross-sections has likewise grown from nonexistent to the current ENDF/B-VII libraries that can require gigabytes of storage.

Today's supercomputer clusters have a billion or more times the performance and capacity of computers 40 years ago for MC criticality calculations, resulting in: much larger, more detailed calculation models are used; many more calculations are run; and more neutron histories are run in each calculation. As codes and computers evolved, so did the typical results obtained from MC: MC calculations of reactors usually produced only k_{eff} in the 1960s; k_{eff} and detailed assembly power distributions in the 1970s; k_{eff}, detailed 2D whole-core power, and assembly depletion in the 1980s; k_{eff}, detailed 3D whole-core power, 2D core depletion in the 1990s; and k_{eff}, detailed 3D whole-core power, 3D depletion, and reactor design parameters in the 2000s. Going forward in the 2010s, capabilities for total uncertainty quantification are maturing, to analyze the impact of uncertainties in cross-sections, manufacturing tolerances, methodology, etc.

RECENT PROGRESS AND R&D EFFORTS

The most significant recent and current R&D efforts for MC criticality calculations worldwide are focused on: multigroup sensitivity/uncertainty analysis of cross-section uncertainties; hybrid MC and deterministic methods; source convergence diagnostics (e.g., Shannon entropy); adjoint-weighted continuous-energy MC tallies using the iterated fission probability; quantification of bias and uncertainty; depletion methods, including equilibrium Xenon and control searches; stochastic geometry for modeling the random locations of fuel particles in newer reactor fuel systems; multiphysics calculations to provide feedback in MC due to fluid flow, thermal, and mechanical effects; on-the-fly neutron Doppler broadening with temperature; continuous-energy sensitivity/uncertainty analysis; application of the fission matrix for determining higher eigenmodes and

accelerating convergence; and new algorithms to take advantage of the probable heterogeneity and massive multilevel parallelism of computers expected to appear over the next decade.

AN EXAMPLE – THE FISSION MATRIX METHOD

As an example of recent R&D work, we provide some perspective on the fission matrix method as applied to MC criticality calculations. This method is among the oldest methods for MC criticality calculations [2,3], 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. To tally fission matrix components for every fuel pin in a reactor over 100 axial segments would involve $N \sim 8$M regions, with a matrix of size N^2 requiring 512 TB of memory.

Computational Methods

References [7] and [8] provide detailed descriptions of the theory, MC computational techniques, and results obtained in the initial implementation and testing of the fission matrix method in MCNP. 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. The use of a sparse storage scheme, however, has required the development of numerous new MC computational algorithms, such as performing efficient tallies into the sparse matrix, eigensolvers for both the left and right eigenvectors of a general sparse matrix based on power iteration, Hotelling deflation of the solution space for the sparse power iteration to compute higher-mode left and right eigenvectors, etc. The example problems presented in [8] involve realistic, detailed models using continuous-energy physics, e.g., a 2D whole-core PWR, a large fuel assembly storage vault, the ATR reactor, and the 3D "Kord Smith Challenge" problem. Fig. 1 [8] gives an example of the first 16 eigenfunctions for the 2D whole-core PWR model.

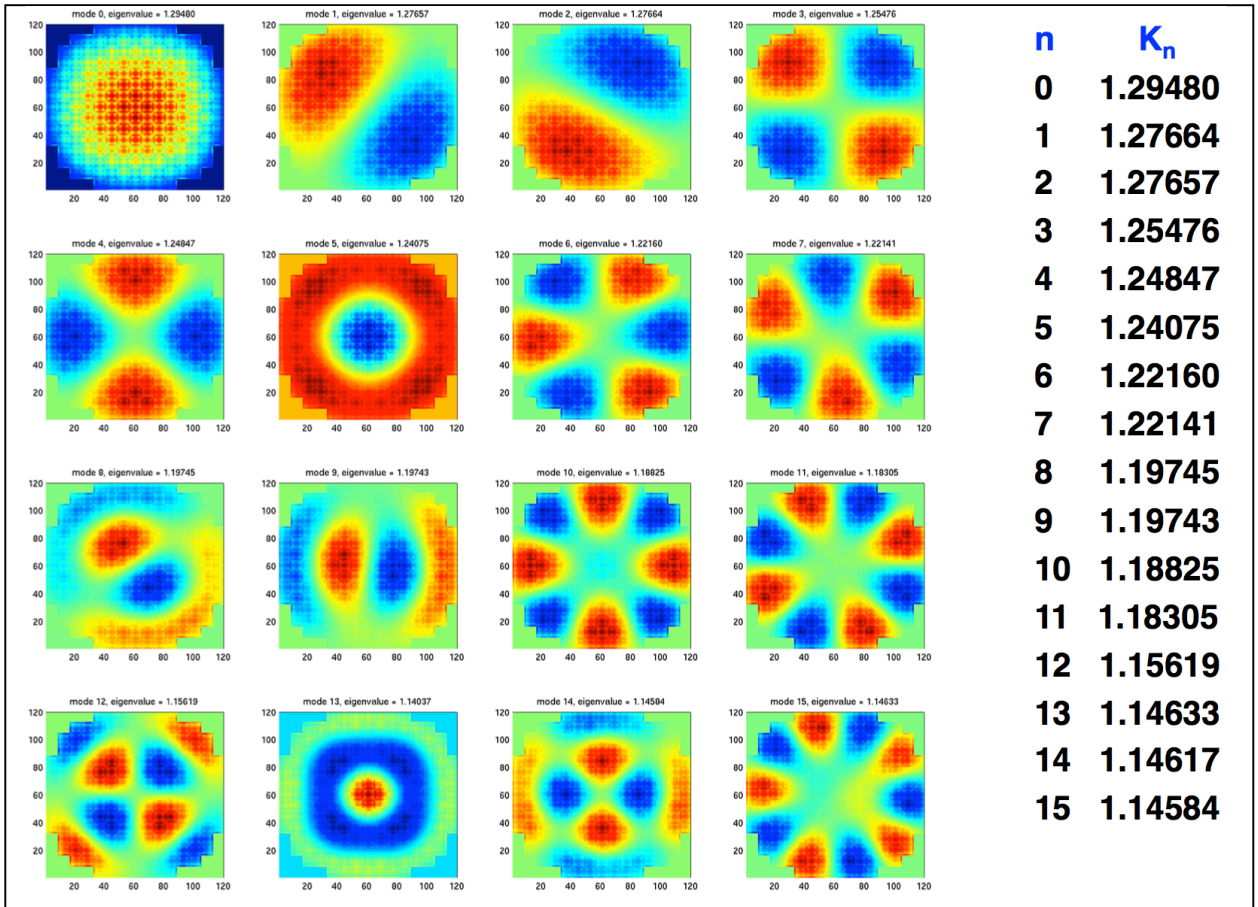

Fig. 1. 2D Whole-core PWR model: First 16 eigenfunctions and eigenvalues for fission neutron source distribution, obtained using a 120x120 tally mesh for the fission matrix (14,400 tally regions, 14,400x14,400 fission matrix). 5M neutrons/cycle, cycles 4-100. Taken from Reference [8].

Applications

The fission matrix is obtained at essentially no cost during the normal simulation for criticality calculations. It can be used to provide estimates of the fundamental mode power distribution, the reactor dominance ratio, the eigenvalue spectrum, and higher mode spatial eigenfunctions. Accurate higher mode eigenfunctions for both the fission source and adjoint fission source have many potential uses in convergence analysis, correction of statistics, reactor stability analysis, perturbation theory, etc. The fundamental mode obtained from the fission matrix can be accurately computed before the actual neutron distribution has converged; it can therefore be used to accelerate the convergence of the power method iterations for the actual neutron distribution.

Relation to Fundamental Reactor Theory

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. This is discussed in detail in [7], and summarized here.

Past theoretical work on the fundamental mathematical basis for k-effective criticality calculations has shown that:

- The transport equation for energy-dependent problems [9] is not self-adjoint; due to neutron slowing down, the kernel for the integral form is not symmetric. Accordingly, eigenfunctions of the k_{eff} form of the transport equation need not form a complete, real, orthogonal set of basis functions. For the energy-dependent k_{eff} form of the transport equation, however, the forward and adjoint fission sources are biorthogonal, and forward and adjoint fluxes are biorthogonal when fission operator weighting is used.

- The fundamental mode eigenvalues and eigenfunctions of the transport equation have been proven to exist, even for the continuous-energy form of the transport equation [10]. The fundamental mode eigenvalue is real and positive, and the fundamental mode eigenfunction is real and non-negative.

- For the 1-speed integral transport equation for the scalar flux assuming isotropic scattering, it has been proven [11] that all of the higher modes exist, with discrete real eigenvalues and real eigenfunctions. The 1-speed integral equation for the scalar flux is self-adjoint due to the symmetry of the kernel in the integral equations. This proof was later extended to include anisotropic scattering [12].

- For the multigroup transport equation and the continuous-energy transport equation, it is conventional practice [9] to assume that higher modes exist, with real eigenvalues and eigenfunctions, even though that has not been proven.

In [7], very fine spatial resolution was used in computing the fission matrix for several realistic problems. The fission matrix is not symmetric (due to the energy dependence in the transport equation). It was shown that, for fine enough spatial resolution, the adjoint fission matrix is simply the transpose of the forward fission matrix. Thus the fission source distribution and its higher modes are *right* eigenvectors of the fission matrix; the adjoint fission source and its higher modes are *left* eigenvectors of the fission matrix. The fission source and its adjoint were proven to be biorthogonal. Numerical evidence for every problem analyzed to date indicates that:

- As the 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. This convergence in spectrum can be used to verify that the resolution is fine-enough to provide accurate solutions.

- 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 is decreased by using more neutrons/cycle, the complex parts become smaller and shift to even higher modes. Such behavior suggests a numerical artifact from the statistical noise in fission matrix tallies.)

- The forward eigenfunctions form a very-nearly othogonal 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 [7] for several realistic problems shows the near-orthogonality of the forward modes. (This is significant, because that is a common assumption in reactor theory.) It is known [13] that even for biorthogonal systems of eigenproblems, the individual sets of forward and adjoint eigenfunctions *may* also be orthogonal among themselves, even though that is not required.

This numerical evidence is highly suggestive, but is not mathematical proof. 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.

SUMMARY & CONCLUSIONS

We have summarized the history and recent progress in MC criticality calculations. As an example, especially for student researchers, recent work on development of fission matrix capabilities was summarized. The intent was to illustrate the synergy among large-scale computer capabilities, advanced numerical schemes, and fundamental theory. Much of the early literature on nuclear engineering is rich in ideas for advanced computation and analysis methods. Many of those ideas could not be realized at the time due to computing limitations, but may be feasible and useful today with advanced computers and improved numerical methods. Understanding the history of theory, mathematics, computer evolution, and code development is a key to making full use of today's large-scale computers.

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