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Fission Matrix Capability for MCNP Monte Carlo

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Abstract:

We describe recent experience and results from implementing a fission matrix capability into the MCNP Monte Carlo code. The fission matrix can be used to provide estimates of the fundamental mode fission distribution, the dominance ratio, the eigenvalue spectrum, and higher mode forward and adjoint eigenfunctions of the fission neutron source distribution. It can also be used to accelerate the convergence of the power method iterations and to provide basis functions for higher-order perturbation theory. The higher-mode fission sources can be used in MCNP to determine higher-mode forward fluxes and tallies, and work is underway to provide higher-mode adjoint-weighted fluxes and tallies. Past difficulties and limitations of the fission matrix approach are overcome with a new sparse representation of the matrix, permitting much larger and more accurate fission matrix representations. The new fission matrix capabilities provide a significant advance in the state-of-the-art for Monte Carlo criticality calculations.

KEYWORDS: ***fission matrix, Monte Carlo, criticality, k-effective, eigenmodes***

I. Introduction

The fission matrix method was introduced into local versions of MCNP [1,2] in 2006 to investigate estimating the dominance ratio for criticality calculations. The method suffered from the same drawback found by others over the last 60 years, that accuracy was severely limited by constraints on memory storage. In 2012, a novel computational approach was tried – using a sparse matrix storage scheme to enable more detailed meshes for the fission matrix estimation. This was first reported in [3], the theory was fully detailed in [4], and numerous realistic examples were presented in [5]. In 2013, significant improvements in the sparse storage methodology were made, along with extensions that enable computing higher mode eigenfunctions for fluxes and reaction rates, rather than just the fission neutron source. In addition, detailed studies using the fission matrix have provided insight into the theoretical basis for criticality calculations. This paper will summarize the work reported in [3-5] and discuss the recent work [6,7] accomplished during early 2013.

II. Background

Monte Carlo criticality calculations for k_{eff} and the fission distribution are carried out iteratively with MCNP using the power method, where batches of neutrons are simulated for a single generation. Since production Monte Carlo codes restrict neutron statistical weights to be non-negative, higher eigenmodes cannot be evaluated directly from the Monte Carlo neutron simulation. The fission matrix approach was proposed in the earliest works on Monte Carlo criticality calculations [8-10] and has been tried by many researchers over the years.

1. Basis of the Fission Matrix Approach

The fission matrix equations were derived in [4], without approximation, from the k-eigenvalue form of the neutron transport equation. The derivation leads to the equations

$$S_J = \int_{\vec{r}\in V_J} d\vec{r} \iint dE'\, d\hat{\Omega}'\, \nu\Sigma_F(\vec{r},E')\Psi(\vec{r},E',\hat{\Omega}'),$$

$$F_{I,J} = \int_{\vec{r}\in V_I} d\vec{r} \int_{\vec{r}_0\in V_J} d\vec{r}_0 \frac{S(\vec{r}_0)}{S_J} \iint dE\, d\hat{\Omega}\, \nu\Sigma_F(\vec{r},E) \iint dE_0\, d\hat{\Omega}_0\, \chi(E_0,\hat{\Omega}_0) G(\vec{r},E,\hat{\Omega};\, \vec{r}_0,E_0,\hat{\Omega}_0)$$

$$S_I = \tfrac{1}{K} \cdot \sum_{J=1}^{N} F_{I,J} \cdot S_J \qquad (1)$$

The kernel $F_{I,J}$ is equal to the number of fission neutrons born in region I due to one average fission neutron starting in region J, and is called the *fission matrix*. Essentially, the fission matrix is a spatially discretized Green's function for the next generation fission neutron source, and Eq. (1) is the k_{eff} form of Peierl's equation. The fundamental mode eigenvalue of this matrix is identical to the k_{eff} eigenvalue, and the fundamental mode eigenvector is the regionwise fission neutron source distribution.

It is important to note that the fission matrix elements can be estimated during inactive batches in the iteration process. As discussed in [4], if a very fine spatial mesh is used for estimating the fission matrix elements, then the $F_{I,J}$ in Eq. (1) are insensitive to $S(r_0)/S_J$. Examining the eigenvalue spectrum of the fission matrix as the mesh is refined provides a practical means of assessing the validity of the fission matrix. The adjoint fission matrix was also derived rigorously in [4], and it was shown that for sufficiently fine meshes, the adjoint fission matrix is simply the transpose of the forward matrix.

2. Initial Implementation

Fission matrix elements can be estimated at essentially no extra cost during the normal Monte Carlo simulation using only the locations of fission neutron sources at the start and end of each batch, without incurring any overhead during the neutron random walks. This approach eliminates overhead from MPI message passing of fission matrix tallies, since the fission matrix can be computed on the master node using the existing "fission bank".

The principal limitation on accuracy has always been the size of the regions for each fission matrix element. Typically, a regular 3D spatial mesh with $N = N_x$ x N_y x N_z elements is used, giving an *NxN* fission matrix, with N^2 entries. A 100x100x100 spatial mesh would give rise to a 10^6x10^6 fission matrix 8,000 GB in size, which could not be stored on today's computers. To overcome the memory limitation, a sparse representation was used in [3-5] for the fission matrix, with a compact banded structure. Neutron sites beyond a few nearest neighbor regions were tallied in the nearest band region. This approximation, inadequate for complex geometries, was removed in the present work [6,7].

III. Sparse Storage for Fission Matrix

Development of the fission matrix method in MCNP is in progress, with an anticipated release during 2014. 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. If the fission matrix elements are tallied for a regular 3D spatial mesh with $N = N_x$ x N_y x N_z mesh cells, then a fission neutron starting from mesh cell $[i,j,k]_S$ that creates a next-generation fission neutron in mesh cell $[i,j,k]_T$ would be tallied in the fission matrix tally bin $F(I,J)$, where $J=i_S+(j_S-1)N_x+(k_S-1)N_xN_y$ and $I=i_T+(j_T-1)N_x+(k_T-1)N_xN_y$. Only the nonzero $F(I,J)$ entries are stored. In the compressed-row scheme illustrated in Figure 1, the $L(I)$ array entries point to the start of a list of J indices and corresponding nonzero $F(I,J)$ tallies. To look up the tally for $F(I,J)$, it is necessary to search the J array from location $L(I)$ through $L(I+1)-1$ for the desired J (if it exists), and then retrieve the corresponding F tally. If the $F(I,J)$ entry is not already stored, then it must be inserted during the tallying. The size of the J and F arrays thus increases as more neutrons are simulated.

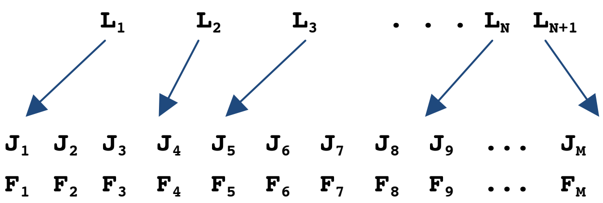

Figure 1. Compressed Row Storage

If M is the total number of nonzero $F(I,J)$ tally entries, then the L array has $N+1$ entries, and the J and F arrays each have M entries. In practice, $M<<N^2$, resulting in very large reductions in the memory storage for the $F(I,J)$ tallies. Figure 2 shows a typical structure of the fission matrix for a 2D PWR problem. The white portions of the plot correspond to zero $F(I,J)$ entries that are not stored in the compressed-row storage scheme

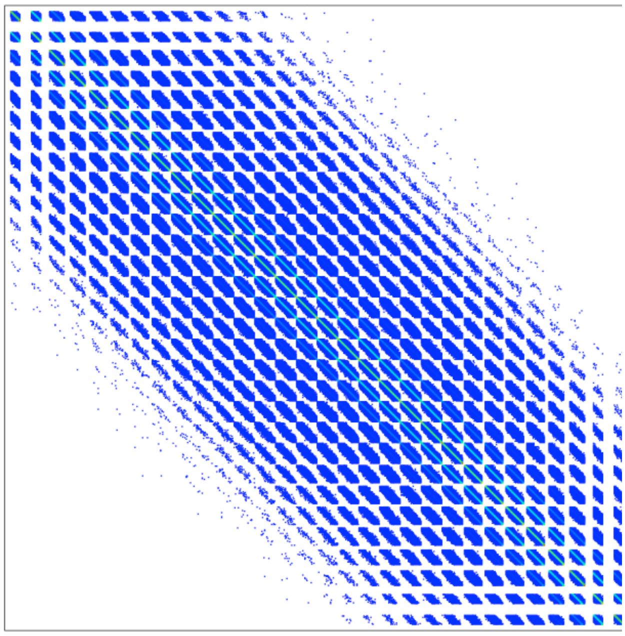

Figure 2. Fission matrix structure for 2D PWR

The use of a sparse storage scheme has required the development of numerous new Monte Carlo computational algorithms, such as performing efficient tallies into the sparse matrix, eigensolvers for both the left and right eigenvectors of a general sparse nonsymmetric 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. Very highly optimized coding was developed to perform the tallies in an efficient manner, so that the fission matrix tallies typically require less than 1 second at the end of each batch in the Monte Carlo simulation.

In practice, MCNP simulations are run using a very fine spatial mesh for the fission matrix tallies, typically 1000x1000 mesh cells for 2D problems or 1000x1000x1000 mesh cells for 3D problems. After the MCNP runs have finished, the fission matrix tallies are aggregated into a more compact matrix, by combining a moderate number of entries for neighboring spatial mesh cells. This aggregation results in reduced statistical uncertainties in the fission matrix elements. In addition, by aggregating the matrix several times and finding the eigenvalue spectrum each time, it is straightforward to assess the degree of spatial mesh detail that is necessary for a converged spectrum.

III. Higher Eigenmodes for the Fission Source

The fission matrix capability was implemented in a local version of MCNP with the sparse matrix tally scheme. Testing was performed on a variety of different reactor applications. The results described below were obtained for a 2D whole-core PWR model with ENDF/B-VII.0 continuous-energy nuclear data [4,5]. The fission matrix was accumulated during standard KCODE calculations. Tallies for the fission matrix were made only for the 4th and successive batches in order to reduce discretization error arising from the arbitrary initial distribution. The total MCNP running time was increased by less than 1% due to the extra operations required for tallying the fission matrix.

After completion of the MCNP run, higher-mode eigenvalues and eigenfunctions for the fission neutron source were determined from the fission matrix. Four different methods for determining the higher modes were tried, to check on the correctness of the higher-mode solutions: standard power iteration with Hotelling deflation, a direct nonsymmetric eigensolver (for smaller fission matrices), an iterative solver using the implicitly restarted Arnoldi method (IRAM), and the nonsymmetric eigensolver available in Matlab. The IRAM solver was fastest for general use [7] and is well suited to sparse matrix problems. It requires only the multiplication of the sparse matrix times a vector, and does not require storage of the full matrix. Power iteration was robust but slow. The direct solver and Matlab solver require storage of the full fission matrix, hence can only be used for problems with a small fission matrix (i.e., very coarse spatial resolution).

Figure 3 shows the eigenvalue spectrum of the fission matrix. For this example, MCNP was run with a 120x120x1 spatial mesh for the fission matrix tallies. Only the first 195 of the set of 14,400 eigenvalues are shown in Figure 3.

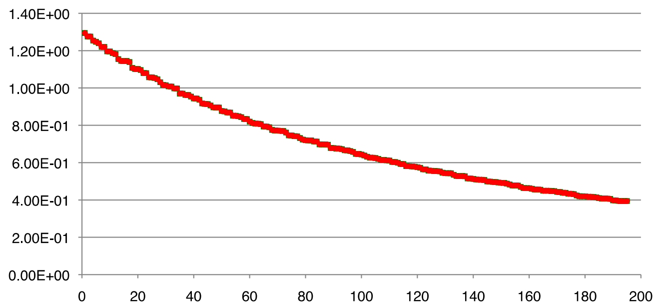

Figure 3. First 192 eigenvalues for 2D PWR problem, using a 120x120 spatial mesh for fission matrix tallies.

Figure 4 shows the fundamental eigenmode (i.e., the fission neutron source distribution) and 9 higher eigenmodes for the 60x60x1 mesh case. These plots are especially interesting, since the higher eigenmodes cannot normally be obtained directly from a Monte Carlo calculation.

IV. Higher Eigenmodes for the Flux

Using the higher eigenmodes for the fission neutron source, MCNP calculations can be performed in a fixed-source manner to determine the higher-mode neutron fluxes and any desired reaction rates. To determine the mode n flux, the mode n eigenfunction of the fission matrix is used as the fixed source. As both flux and fission source modes can be positive or negative for n>0, a flag is used internally in MCNP to mark the sign of a neutron's weight. That is, source neutrons are started according to the magnitude of the higher mode source and are flagged as either positive or negative. Source points are sampled in an analog manner from the loaded fission source mode, and starting locations are resampled until fissionable material is found. The NONU card is used to treat fission as absorption. Positive neutron weights are used in the transport simulation, but tallies may be added or subtracted according to the neutron flag. A concern here is that for greater positive/negative oscillation in the source as mode number rises, there will be more score cancellation in tallies. This may lead to larger tally variances than is manageable. This issue is examined below.

To test the forward flux calculations, a fission matrix was generated for the 2D PWR problem using a 50x50 spatial mesh, 500 batches (skipping the initial 2), and 500k neutrons/batch. Then the first 30 eigenmodes of the fission matrix were found. Each of these 30 eigenmodes for the fission neutron source was then used as the source for fixed source calculations to determine fluxes. The 30 fixed source calculations each used only 500k neutron histories. Figures 5 and 6 give results for the flux and relative uncertainties. Each of these fixed source flux calculations required only about 1 minute of MCNP time using 8 threads. Group 1 flux modes are very similar to the fission source modes, and the

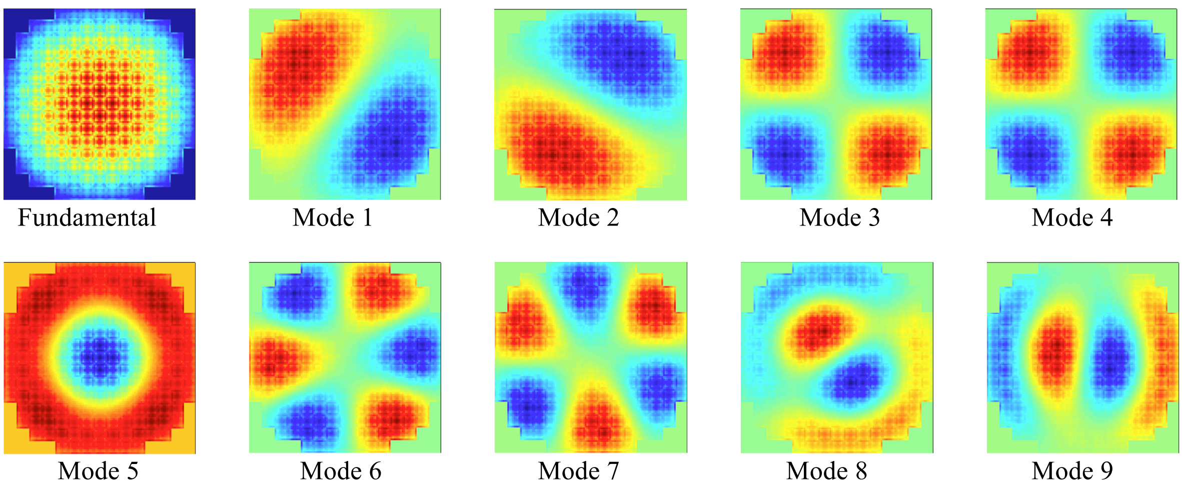

Figure 4. Fundamental and higher eigenmodes for 2D PWR model obtained from a fission matrix using a 60x60x1 spatial mesh.

most notable feature of the group 2 flux modes are the new peaks in the peripheral water moderator. The relative

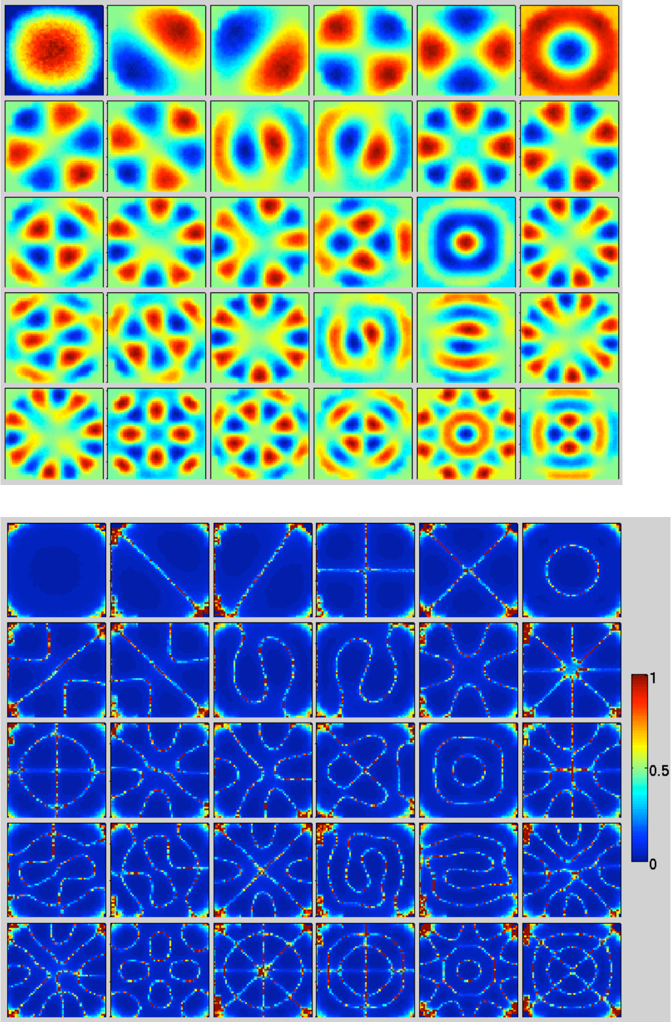

Figure 5. First 30 forward flux modes (top) of 2D PWR and relative uncertainties (bottom), Group 1 (0.625 eV – 20 MeV).

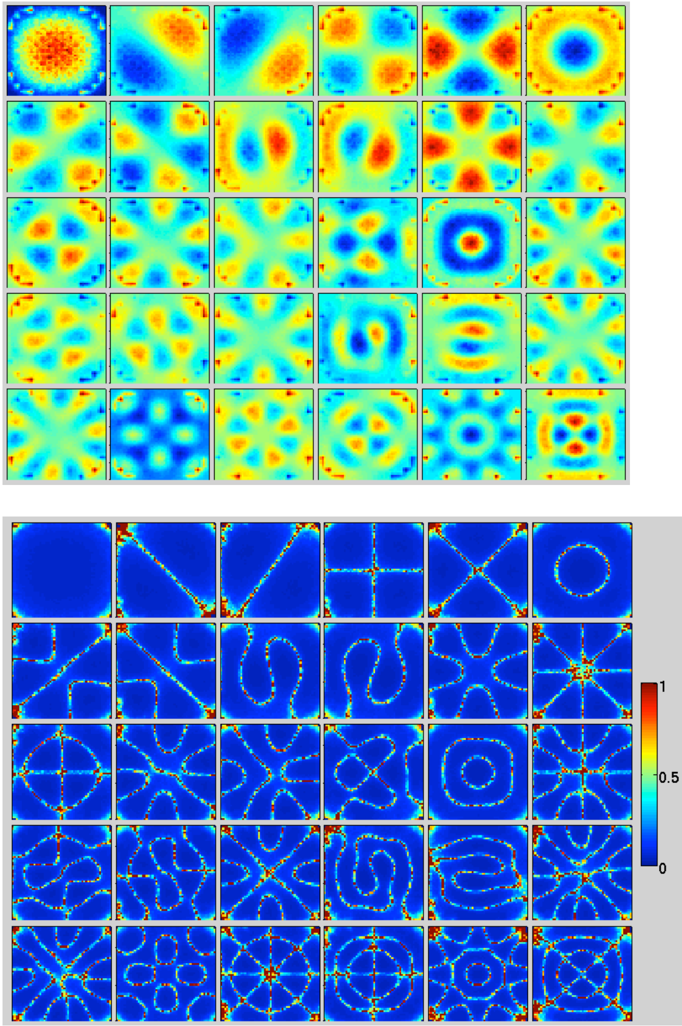

Figure 6. First 30 forward flux modes (top) of 2D PWR, and relative uncertainties (bottom), Group 2 (0 - 0.625 eV).

uncertainty plots give a reassuring result – the high relative uncertainties are localized near the inflection lines. Uncertainties are manageable where the functions are significantly nonzero, notwithstanding the cancellation of tallies.

V. Investigations into Fundamental Reactor Theory

The fission matrix method can be used to investigate and understand some unanswered questions on the fundamental theoretical basis for continuous-energy Monte Carlo criticality calculations. This is discussed in detail in [4] and summarized here. Some new results are also presented.

1. Eigenvalue Spectrum

It is known from past theoretical work [11] on the fundamental mathematical basis for k-effective criticality calculations that: (1) The fundamental mode eigenvalues and eigenfunctions of the continuous-energy form of the transport equation have been proven to exist [12]. The fundamental mode eigenvalue is real and positive, and the fundamental mode eigenfunction is real and non-negative. (2) For the 1-speed integral transport equation for the scalar flux, it has been proven [13,14] that all of the higher modes exist, with discrete real eigenvalues and real eigenfunctions.

For the multigroup transport equation and the continuous-energy k-effective transport equation, it is conventional practice [11] to assume that higher modes exist, with real eigenvalues and eigenfunctions, even though that has not been proven. To investigate this assumption, the complete eigenvalue spectrum of the fission matrix has been determined for the 2D PWR problem. In [4], a 120x120 spatial mesh was used for the fission matrix tally elements, giving 14,400 eigenvalues. In this work, we use a 30x30 spatial mesh to simplify the reporting of results, giving 772 eigenvalues. (128 spatial regions contain no fissionable material, hence are null columns and rows in the fission matrix. These are excluded from the eigenvalue calculations.) Figure 7 gives the complete set of 772 eigenvalues, including both real and imaginary parts. Figure

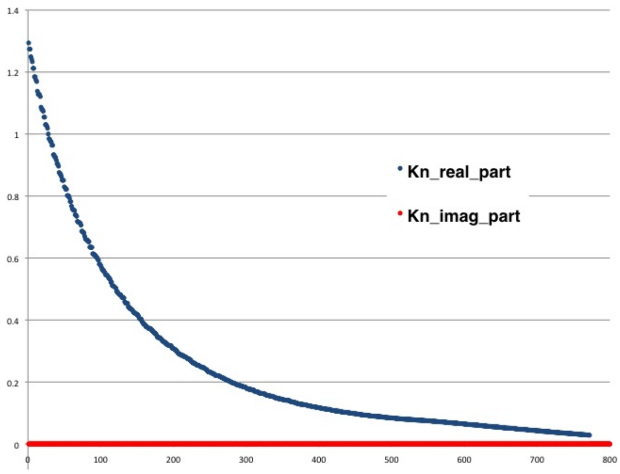

Figure 7. Real and Imaginary parts of the 772 eigenvalues for the 2D PWR problem, using a 30x30 spatial mesh for fission matrix tallies.

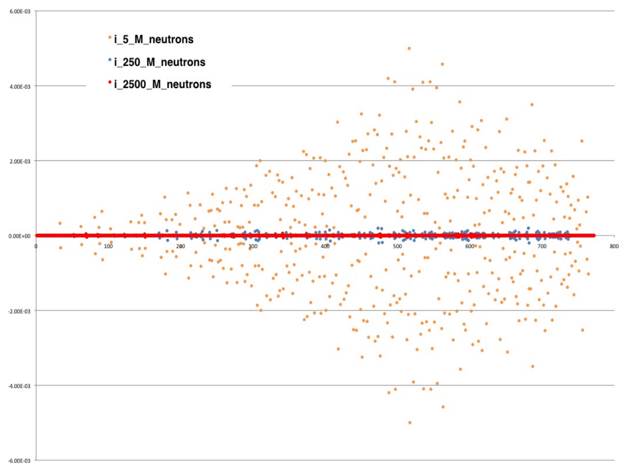

Figure 8. Detail for imaginary parts of 2D PWR eigenvalues, after 5M, 250M, and 2500M neutrons. (vertical scale: $-6x10^{-3}$ to $+6x10^{-3}$)

8 shows detail for the imaginary parts of the eigenvalues after runs with 5M, 250M, and 2500M neutrons. It can be seen from Figure 8 that as more neutrons are followed, the imaginary parts of the eigenvalues become very much smaller. Because the fission matrix is nonsymmetric and each of the matrix elements has associated statistical uncertainty, the numerical solutions can give rise to imaginary components. However, both the magnitude and frequency of occurrence of the imaginary parts diminish greatly as more neutrons are run to reduce statistical uncertainties. This behavior provides strong evidence (but not proof) that all of the eigenvalues are discrete and real-valued.

2. Spectrum Convergence with Mesh Refinement

Figure 9 shows the detailed convergence with mesh refinement of the first 10 eigenvalues for the 2D PWR model. The number of mesh regions for fission matrix tallies is increased (i.e., finer resolution) from 5x5 to 10x10, 15x15, 30x30, 60x60, and finally 120x120. The 15x15 case corresponds to one mesh cell per fuel assembly. For this problem, it appears that the 120x120 mesh provides satisfactory convergence for the 10 modes shown. These mesh refinement studies demonstrate that the eigenvalue spectrum converges smoothly to a stationary discrete distribution. Further mesh refinement will not change the spectrum of lower eigenvalues, indicating that the fission matrix results have converged to the limiting values of the fully-continuous form of the transport equation.

3. Biorthogonality & Orthogonality of Modes

For the energy-dependent k_{eff} form of the transport equation, the forward and adjoint fission sources are biorthogonal [11], and forward and adjoint fluxes are biorthogonal when fission operator weighting is used. For the 2D PWR example problem with a 30x30 spatial mesh used for fission matrix tallies, Figure 10 (left) shows inner products of forward and adjoint fission source modes for all 772^2 combinations. The inner products are strongly diagonally dominant and near zero for off-diagonal terms. This supports the biorthogonality, with minor deviations due to the statistical uncertainty of fission matrix elements and hence solutions. Figure 10 (right) shows the inner products of different forward modes with other forward modes for all 772^2 combinations. The appearance is similar to the left plot, and indicates that the forward modes are nearly orthogonal among themselves. While the orthogonality of forward modes alone is not proven, this assumption is often made for reactor analysis. The results shown in Figure 10 indicate that this is a reasonable assumption.

VI. Work in Progress

We are investigating the use of the fission matrix to

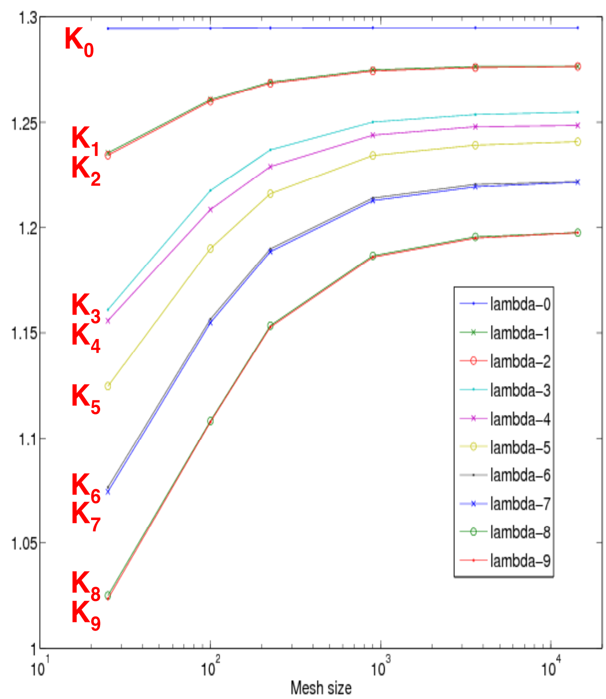

Figure 9. Convergence of the first 10 eigenvalues for whole-core 2D PWR model as *N* is increased (*N* = spatial mesh cells for fission matrix tallies).

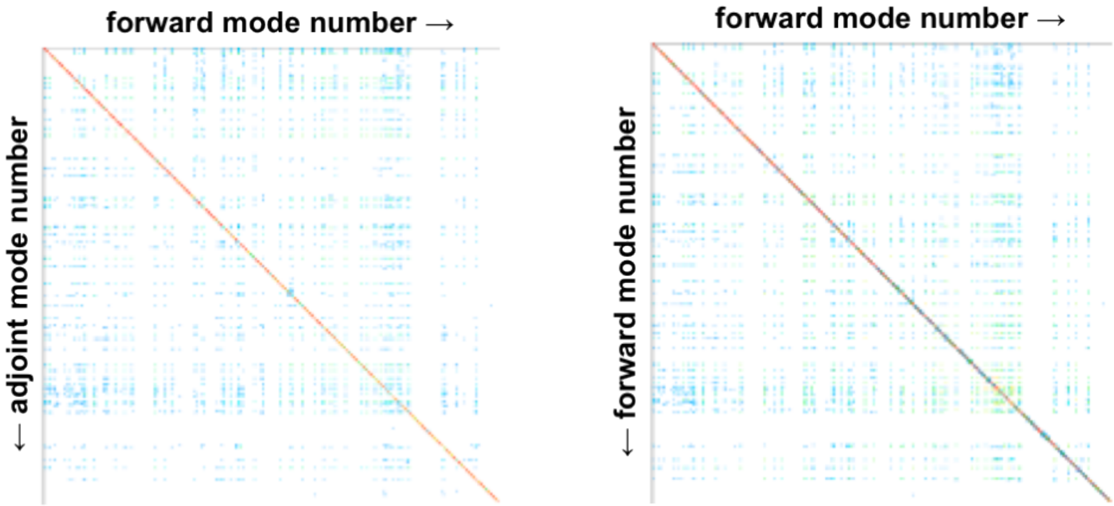

Figure 10. Biorthogonality of forward and adjoint fission source modes (left), and orthogonality of forward modes (right). Plotted points are inner products of modes. (scales: red - near 1.0, blue ≤ 0.1)

accelerate the power method convergence of Monte Carlo criticality calculations. In a hybrid high-order/low-order scheme, the actual Monte Carlo simulation of neutron histories would be the high-order method to be accelerated using a low-order solution obtained from the fission matrix. Only the fundamental mode solution from the fission matrix is needed, so that higher-mode solutions are not necessary during the Monte Carlo simulation. It is likely that coarser fission matrix resolution will be used initially, with refinement as fission matrix uncertainties are reduced with more neutrons. Because the fission matrix can be determined accurately with only a few batches during the inactive portion of the calculation, the fundamental eigenmode can be used to bias the fission neutron source, forcing the source distribution based on Monte Carlo histories to converge more quickly. Initial testing of this method is encouraging, and further study and development are in progress.

The higher modes obtained from the fission matrix are useful in explaining, evaluating, and predicting convergence of the Monte Carlo source distribution. Convergence can be predicted for various choices of the initial guess for the fission source [6]. In addition, the number of iterations needed to transition from a base-case fundamental mode to a perturbed fundamental mode can be predicted [7]. This capability may be useful in determining the number of iterations required for stable multiphysics calculations.

Higher-mode adjoint flux weighting, necessary for higher order perturbation calculations, is another application of higher modes. This weighting is possible by incorporating the fission matrix forward and adjoint source modes with the iterated fission probability method.

VII. Conclusions

New developments and recent progress in the implementation and testing of a fission matrix capability in MCNP were discussed. The method can be used to obtain interesting and valuable information for criticality problems, including the higher mode forward and adjoint eigenvalues and eigenfunctions of the fission neutron source. A new sparse matrix storage scheme removes previous limitations of the fission matrix approach, permitting accurate solutions to large, detailed 2D and 3D reactor problems.

The fission matrix approach is well founded in theory, does not significantly increase the cost of standard Monte Carlo criticality calculations, and does not significantly increase code complexity. Accuracy of the method improves as the spatial tally mesh is refined. The fission matrix can be used to study fundamental properties of the continuous-energy k-effective transport equation. From these studies, common assumptions can be confirmed, such as a real-valued set of eigenvalues and near-orthogonality of the forward eigenfunctions.

Recent extensions to the method include the determination of higher modes for the forward flux, and the calculation of coupling coefficients between base and perturbed cases. Work is in progress to combine the fission matrix and iterated fission probability methods to provide higher-mode adjoint-weighted quantities and higher-order perturbation theory.

A high-order / low-order acceleration matrix that is strictly Monte Carlo based is under development and appears promising. This scheme would provide total consistency between the continuous-energy Monte Carlo simulation and the associated fission matrix. The simplicity and robustness of the method should provide a distinct advantage over other acceleration schemes.

Acknowledgment

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