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Fission Matrix Capability For MCNP

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ABSTRACT

This paper describes the initial experience and results from implementing a fission matrix capability into the MCNP Monte Carlo code. 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 dominance ratio, the eigenvalue spectrum, and higher mode spatial eigenfunctions. It can also be used to accelerate the source convergence of the power method iterations. 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. Numerous examples are presented.

Key Words: Monte Carlo, neutron transport, k-effective, eigenvalues

1 INTRODUCTION

Continuous-energy Monte Carlo codes such as MCNP [1] simulate neutron behavior using the best available nuclear data, accurate physics models, and detailed geometry models. Reactor criticality calculations for k_{eff} and the power distribution are carried out iteratively, using the power method, where batches of neutrons are simulated for a single generation. The fission matrix approach was proposed in the earliest works on Monte Carlo criticality calculations [2-4] and has been tried by many researchers over the years. The present work takes advantage of the very large computer memories available today and a new sparse matrix representation to overcome past difficulties. A recent paper [5] describes the theoretical basis for this fission matrix capability.

2 FISSION MATRIX METHOD

2.1 Fission Matrix Equations

As derived in [5], if the physical problem is segmented into *N* spatial regions, and the k-effective form of the integral transport equation is integrated over the volumes of each initial region *J*, with $\vec{r}_0 \in V_J$, and final region *I,* with $\vec{r} \in V_I$, then the following equations are obtained:

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

where

$$F_{I,J} = \int_{\vec{r}\in V_I} d\vec{r} \int_{\vec{r}_0\in V_J} d\vec{r}_0 \frac{S(\vec{r}_0)}{S_J} \cdot H(\vec{r}_0 \to \vec{r}), \qquad S_J = \int_{\vec{r}'\in V_J} S(\vec{r}')\,d\vec{r}' \tag{2}$$

S_J is the fission neutron source in region *J*, and H is an energy- and angle-averaged Green's function. The matrix element $F_{I,J}$ is equal to the number of next-generation fission neutrons born in region *I* due to one average fission neutron starting in region *J*. The matrix $\bar{F}$ is called the *fission matrix*. The fundamental mode eigenvalue of this matrix is formally identical to k-effective, and the fundamental mode eigenfunction is the regionwise fission neutron source distribution. In matrix-vector form, Eq. (1) is

$$\vec{S} = \tfrac{1}{K} \cdot \bar{F} \cdot \vec{S} \tag{3}$$

where $\vec{S}$ is a vector of length *N* giving the single-generation production of neutrons in each region from fission, and $\bar{F}$ is a full matrix of size *N*x*N*. Higher eigenmodes of Eq. (3) can be determined according to:

$$\begin{aligned} &\vec{S}_n = \tfrac{1}{K_n} \cdot \bar{F} \cdot \vec{S}_n \qquad n = 0,1,\ldots N \\ &k_0 > |k_1| > |k_2| > \ldots > |k_N| \end{aligned} \tag{4}$$

where the subscript *n* refers to the mode, with *n*=0 the fundamental mode. For a problem with *N* regions in the mesh for the fission matrix, $\bar{F}$ is an *N*x*N* matrix with *N* discrete eigenvalues. Because $\bar{F}$ is a nonsymmetric matrix, the eigenvalues and eigenvectors may be complex, although the evidence presented in [5] suggests that they are real-valued. The fundamental mode must be strictly real and nonnegative.

2.2 Monte Carlo Estimation of the Fission Matrix

In this section, we describe the choices implemented in MCNP6 for the initial proof-of-principle testing of the fission matrix method, including the region shapes and size, the initial source guess, the tallying procedure, the iteration strategy, and parallel computing issues.

2.2.1 Regions for fission matrix tallies

The choice of region shapes and sizes for determining the fission matrix is arbitrary, as long as all fissionable regions in the physical problem are covered. For the initial testing in MCNP6, we have chosen to use a simple, uniform, 3D, Cartesian mesh, with different numbers of mesh intervals permitted in the x-, y-, and z-directions. The mesh overlays the detailed Monte Carlo geometry for the physical problem and must encompass all fissionable regions in the problem. The choice of mesh for tallying the fission matrix does not affect the ordinary Monte Carlo tracking in any manner. Future development will include more general meshes.

2.2.2 Initial source guess

While the initial guess for the fission neutron source distribution is arbitrary for criticality calculations, the use of a uniform volumetric source in fissionable regions of the problem is the most prudent choice. This ensures that tallies of fission matrix elements will be made for all fissionable regions in the initial stages of the power iteration process used in MCNP. Future development will automate this and include stratified sampling techniques.

2.2.3 Tallying the fission matrix elements

Tallies for fission matrix elements can be made using only the locations of fission neutron sources at the start and end of each batch, without incurring any overhead during the random walk simulation of the neutrons – simply remember the region a fission neutron was born in (*J*), determine the region a next-generation fission neutron is produced in (*I*), and tally the *(I,J)*-th element of the fission matrix. For Monte Carlo codes that use a fixed number of starting source neutrons for every cycle, the region tallies are simply incremented by 1 for each neutron; for MCNP with a varying number of neutrons starting each cycle, the tallies need to be incremented by M_0/M, where M_0 is the number of neutrons starting the initial cycle, and M is the number that started the current cycle. Before solving the fission matrix equations, the tallies need to be normalized by dividing each *(I,J)*-th element by the total number of starters in region *J*.

If a coarse mesh is used to define the spatial regions, then the fission matrix tallies cannot be made until after the fission source distribution has converged, since the spatial weighting functions in Eq. (2) correspond to the stationary source distribution. However, if a fine enough mesh is used such that

$$\frac{S(\vec{r}_0)}{S_J/V_J} \approx 1 \quad \text{for} \;\; \vec{r}_0 \in V_J \tag{5}$$

then Eq. (2) becomes independent of the spatial weighting functions, and valid tallies can be made even before the source distribution converges [5].

2.2.4 Tally updates and iteration strategy

During a standard k-effective calculation, at the end of each cycle the $F_{I,J}$ estimators are updated by tallying the fission neutron weight using the starting and ending mesh region numbers for each point in fission bank. If the mesh is fine enough that Eq. (5) is valid, the tallies may be accumulated over cycles even during the inactive cycles, prior to convergence of the fission source distribution. In practice, we have chosen to begin the fission matrix tallies at the 4th iteration cycle, and to accumulate the tallies over all subsequent cycles. Single-cycle estimates of the fission matrix are never used.

At any desired cycle, the eigenvalues and eigenvectors of the fission matrix may be found by simple power iteration. If higher modes are desired, then Hotelling deflation or direct solvers may be used. In practical application, the fission matrix tallies are accumulated for all problem iterations, and then the fission matrix eigenvalues and eigenvectors are determined only after the Monte Carlo calculation completes. If it is desired to obtain the fission matrix solution during the Monte Carlo calculation, to potentially use it to accelerate the overall source convergence, then the fundamental mode eigenvector could be determined at the end of any cycle.

2.3 Sparse Fission Matrix Representation

The principal limitation on the accuracy of the fission matrix approach is, and always has been, the size of the regions for each fission matrix element. Typically, a regular 3D spatial mesh with $N = N_I \times N_J \times N_K$ elements is used, giving an NxN fission matrix, with N^2 entries. A 100x100x100 spatial mesh would give rise to a fission matrix with 10^{12} elements, which could not be stored even on today's computers.

To overcome this limitation, we are using a sparse matrix storage scheme. Clearly, not every region in a large 3D problem is tightly coupled to every other region; fission neutrons induce most further fissions in neighboring regions, and few or none in distant regions. To investigate this, we examined the structure of the fission matrix for a typical 2D PWR problem. **Fig. 1** shows the structure of the fission matrix for the 15x15x1 mesh case, where each mesh element corresponds to an assembly-sized region. We have chosen to use the compressed-row sparse matrix storage scheme for the fission matrix in order to reduce the memory storage requirements by one or more orders of magnitude. By doing so, even a fission matrix with 10^{12} elements can be run on an office computer.

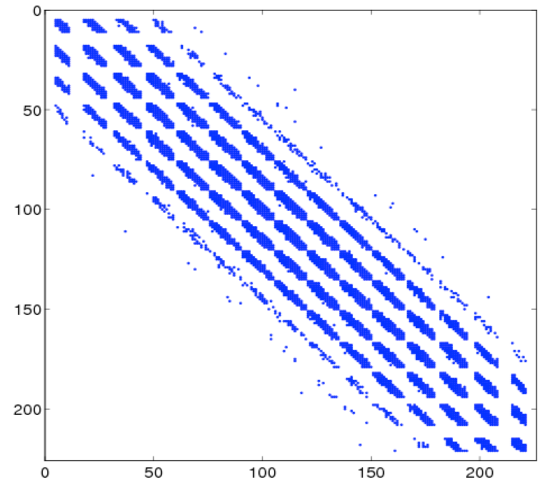


Fig. 1. Fission matrix structure for a 2D whole-core PWR model, for a 15 x 15 x 1 spatial mesh. Matrix dimensions are 225 x 225. Points in blue are non-zero elements of the fission matrix.

3 EXAMPLES OF HIGHER MODE ANALYSIS USING THE FISSION MATRIX

In this section we provide examples for problems where MCNP was used to compute a fission matrix, and then higher eigenvalues and eigenfunctions of the fission neutron source distribution are obtained from the fission matrix. All MCNP calculations were performed with continuous-energy collision physics using ENDF/B-VII.0 cross-section data [6].

3.1 2D Whole-core PWR

A 2D whole-core PWR model is shown in **Fig. 2** (previously used in [7], based on [8]). The fission matrix was accumulated during standard KCODE calculations with 500K

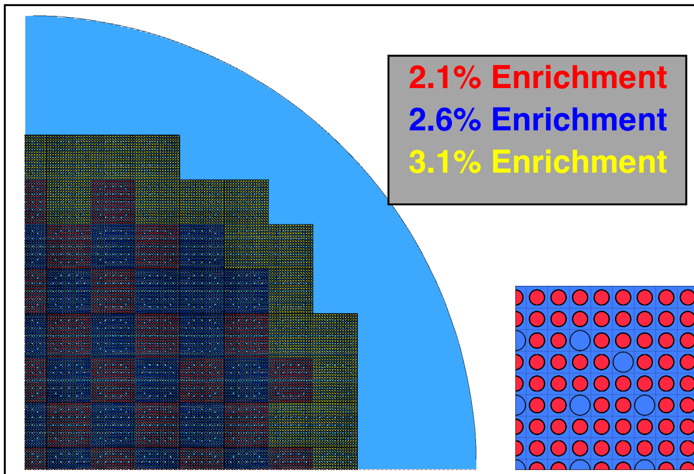
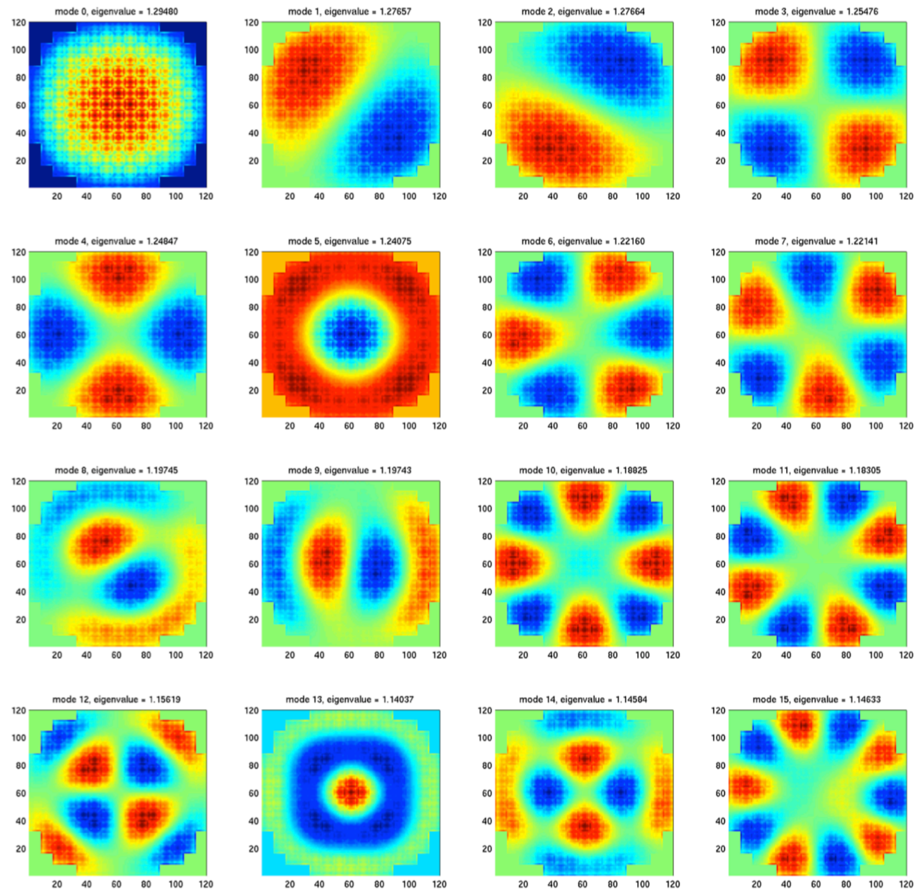


Fig. 2. 2D quarter-core PWR model, with detail shown for the center 1/4-assembly. For the current work, a whole-core model was used.



n	K_n
0	1.29480
1	1.27664
2	1.27657
3	1.25476
4	1.24847
5	1.24075
6	1.22160
7	1.22141
8	1.19745
9	1.19743
10	1.18825
11	1.18305
12	1.15619
13	1.14633
14	1.14617
15	1.14584

Fig. 3. 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.

neutrons/cycle. Tallies for the fission matrix elements were made only for the 4th and successive cycles. k_{eff}, the fundamental mode eigenfunction, and the dominance ratio from the fission matrix were determined via an iterative method. Higher-mode eigenvalues and eigenfunctions for the fission matrix were determined using Matlab. As discussed in [5], a convergence study of the eigenvalue spectrum with mesh refinement was used to determine that the 120x120 mesh provided sufficient resolution to produce accurate eigenvalues and eigenfunctions.

Fig. 3 shows the fundamental eigenmode (i.e., the fission neutron source distribution) and 15 higher eigenmodes for the 120x120x1 mesh case. These plots are especially interesting, since the higher eigenmodes cannot normally be obtained directly from a Monte Carlo calculation. For this calculation, the spatial mesh included 14,400 regions, and the fission matrix size was 14,400x14,400. During the calculation, the dominance ratio k_1/k_0 was obtained every cycle, and all 14,400 eigenvalues and eigenfunctions were obtained after the MCNP calculation using Matlab.

3.2 Fuel Storage Vault

This is Benchmark Problem 1 from the OECD/NEA Source Convergence Benchmarks [9]. The problem contains 36 large, loosely coupled spent fuel assemblies in water surrounded by concrete reflector. A sole assembly has concrete reflector on two sides, as opposed to one or zero for the others. Consequently, this single assembly is by far the most reactive, with a total fission rate over a factor of 10,000 greater than the least reactive assembly. Conventional Monte Carlo requires around 2000 cycles for fission source convergence with a flat initial guess.

Fig. 4 shows the convergence behavior of the standard MCNP and fission matrix results. The fission matrix is tallied for cycles 3-200, with a batch size of 1 M. The spatial mesh is 96x12x10, corresponding in the x-y plane to sixteen mesh regions for every assembly. By cycle 30, the fission matrix gives a reasonably converged fundamental eigenvector. Thus we see the potential for excellent source convergence acceleration with the fission matrix.

Fig. 5 shows the first 8 eigenfunctions for the fuel storage vault problem, and **Table I** gives the corresponding eigenvalues.

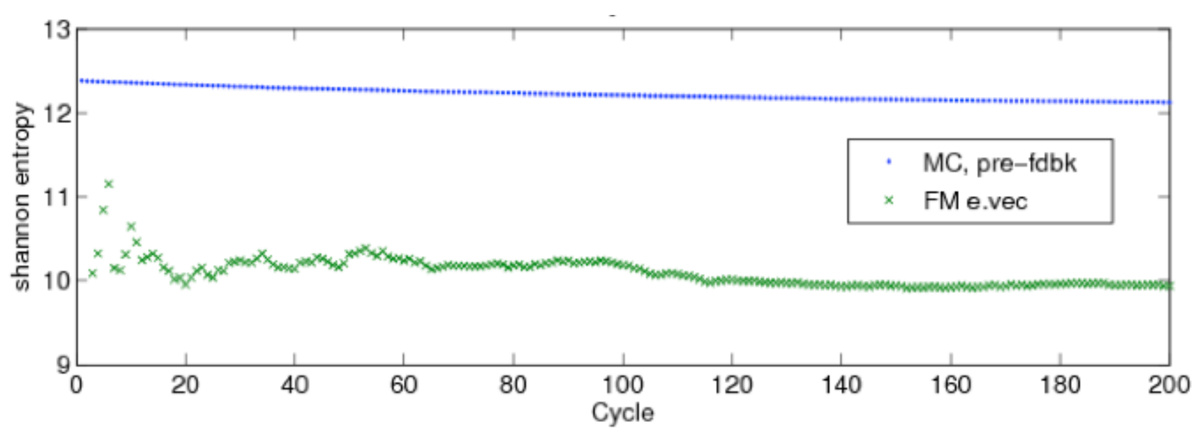


Fig. 4. Vault model: Shannon entropy to diagnose source convergence for standard MCNP (blue) and the fission matrix approach (green). After about 2,000 cycles, the standard MCNP value decreases to match the fission matrix value obtained at 30 cycles.

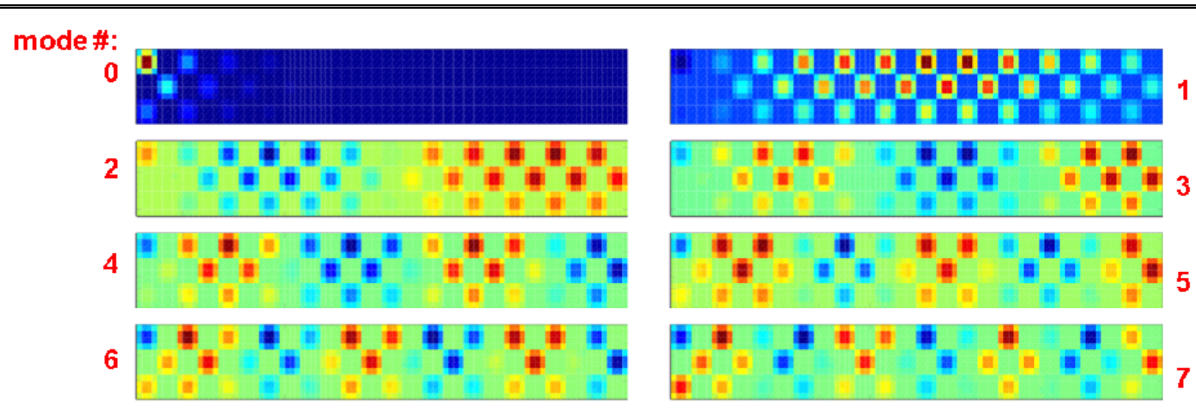


Fig. 5. Vault model: First 8 eigenmodes, with a 96x12x10 spatial mesh. Fission matrix tallied cycles 4-200, batch size of 1 M.

Table I. First 8 eigenvalues for the fuel storage vault problem with a 96x12x10 spatial mesh.

n	k_n
0	0.88947
1	0.88653
2	0.88600
3	0.88533
4	0.88399
5	0.88275
6	0.88112
7	0.87945

3.3 Advanced Test Reactor

The final problem examined is the Advance Test Reactor (ATR) at Idaho National Laboratory [10]. Used primarily for the study of radiation effects, this core has a complex serpentine-shape fuel arrangement that does not easily adhere to a Cartesian mesh. There are 40 curved fuel assemblies with 93% enriched uranium aluminide powder fuel; each wraps 45 degrees. Each assembly has 19 plates of thickness 0.2 cm; the actual thickness of the fuel within each plate is 0.05 cm.

Fig. 6 shows the first 16 eigenfunctions for the ATR model, using a 100x100x1 spatial mesh for fission matrix tallies. The fission matrix tallies were made for cycles 2-200, with 1M neutrons/cycle. **Table II** gives the first 16 eigenvalues for the ATR problem.

Table II. First 16 eigenvalues for the ATR, with a 100x100x1 mesh.

n	k_n		n	k_n
0	0.99490		8	0.47004
1	0.85630		9	0.46173
2	0.84612		10	0.45794
3	0.78265		11	0.41144
4	0.64564		12	0.32865
5	0.55461		13	0.29454
6	0.55207		14	0.28401
7	0.53659		15	0.28327

4 SUMMARY AND CONCLUSIONS

We have described the initial experience and results from implementing a fission matrix capability into the MCNP Monte Carlo code. 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. It can also be used to accelerate the convergence of the power method iterations. Past difficulties and limitations of the fission matrix approach are

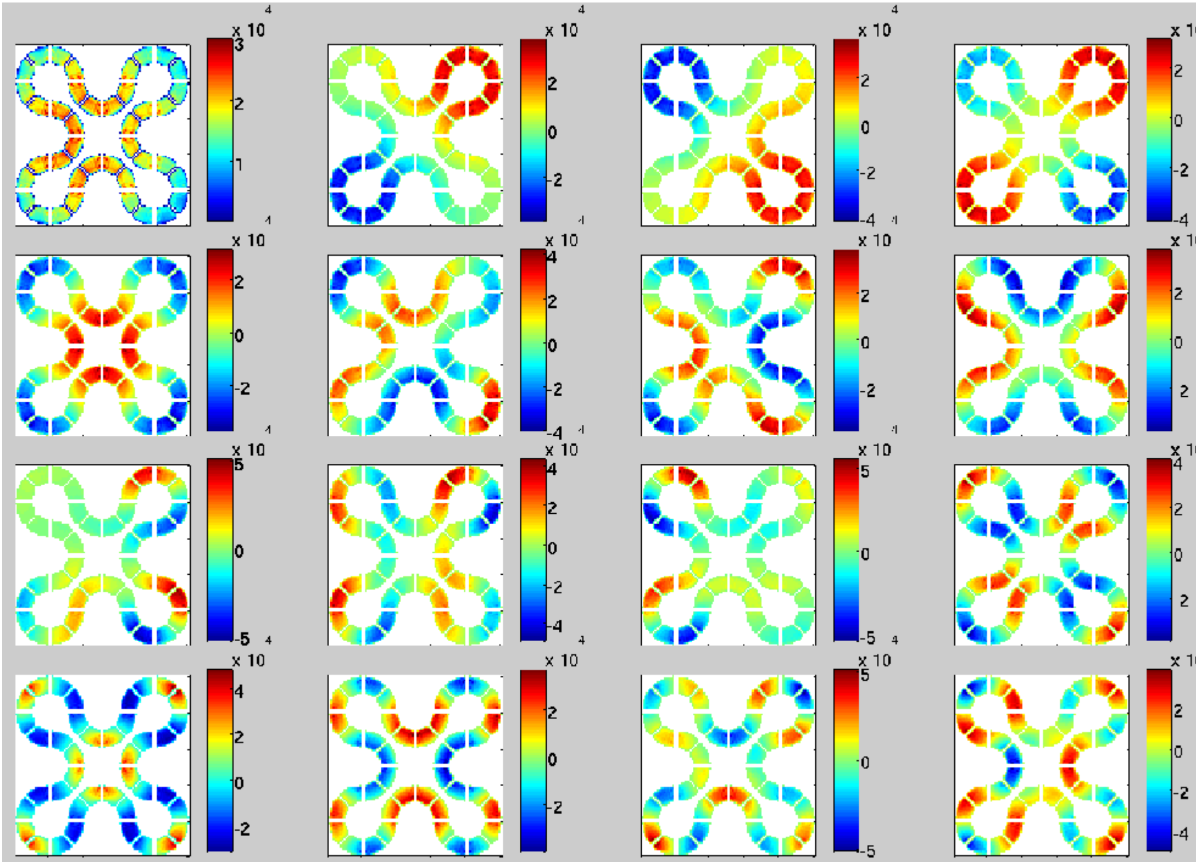


Fig. 6. ATR model: First 16 eigenfunctions for the fission neutron source distribution, obtained from the fission matrix.

overcome for many problems with a new sparse representation of the matrix, permitting much larger and more accurate fission matrix representations.

We are investigating the use of the fission matrix to accelerate the power method convergence of Monte Carlo criticality calculations. Because the fission matrix can be determined accurately with only a few cycles 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.

5 ACKNOWLEDGMENTS

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