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Title: Fission Matrix Capability for MCNP Monte Carlo

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Fission Matrix Capability for MCNP Monte Carlo

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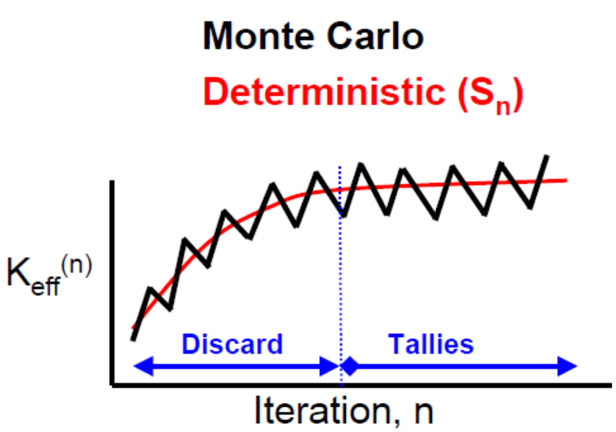
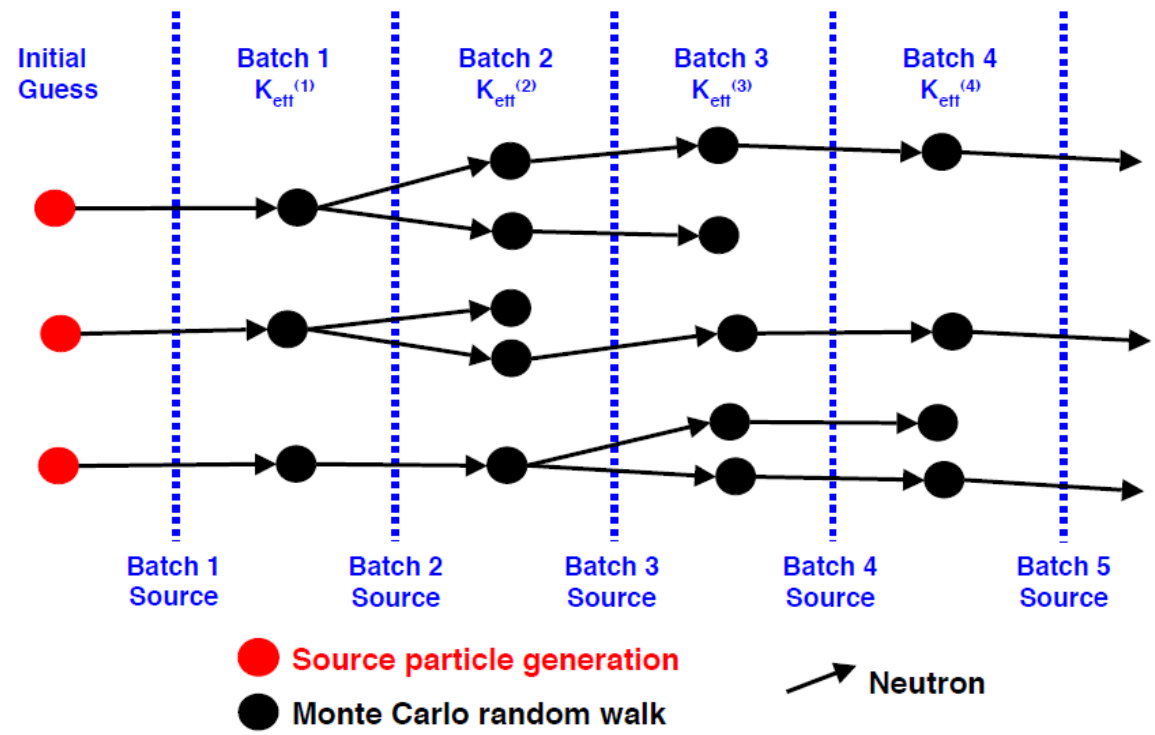
We describe the initial experience and results from implementing a fission matrix capability into the MCNP Monte Carlo code. The fission matrix is obtained at essentially no cost during the normal simulation for criticality calculations. It can be used to provide estimates of the fundamental mode fission distribution, the dominance ratio, the eigenvalue spectrum, and higher mode spatial eigenfunctions. It can also be used to accelerate the convergence of the power method iterations and to provide basis functions for higher-order perturbation theory. 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.

Monte Carlo K-effective Calculation

1. Start with fission source & eigenvalue **guess**
2. **Repeat until converged**:
   - **Simulate neutrons, save fission sites for next cycle**
   - **Calculate k-eff, renormalize source**
3. Continue iterating & tally quantities of interest





Fission Matrix - Theory

- **Transport equation, k-eigenvalue form**

$$M \cdot \Psi(\vec{r},E,\hat{\Omega}) = \tfrac{1}{K} \cdot \frac{\chi(E)}{4\pi} \cdot S(\vec{r}),$$

$$M \cdot \Psi(\vec{r},E,\hat{\Omega}) = \hat{\Omega} \cdot \nabla\Psi(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}) - \iint dE'\, d\hat{\Omega}' \Sigma_S(\vec{r},E' \to E,\hat{\Omega}' \to \hat{\Omega})\Psi(\vec{r},E',\hat{\Omega}'),$$

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

- **Define Green's function & integral transport equation**

$$M \cdot G(\vec{r}_0,E_0,\hat{\Omega}_0 \to \vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0) \cdot \delta(E-E_0) \cdot \delta(\hat{\Omega}-\hat{\Omega}_0),$$

$$\Psi(\vec{r},E,\hat{\Omega}) = \tfrac{1}{K} \cdot \iiint d\vec{r}_0\, dE_0\, d\hat{\Omega}_0\, \frac{\chi(E_0)}{4\pi} \cdot S(\vec{r}_0) \cdot G(\vec{r}_0,E_0,\hat{\Omega}_0 \to \vec{r},E,\hat{\Omega})$$

- **Multiply by $\nu\Sigma_F$, integrate over E, Ω, & initial regions (r_0) & final regions (r)**

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

$$F_{I,J} = \int_{\vec{r} \in V_I} d\vec{r} \int_{\vec{r}_0 \in V_J} d\vec{r}_0\, \frac{S(\vec{r}_0)}{S_J} \cdot \int\iiint dE\, d\hat{\Omega}\, dE_0\, d\hat{\Omega}_0 \cdot \nu\Sigma_F(\vec{r},E) \cdot \frac{\chi(E_0)}{4\pi} \cdot G(\vec{r}_0,E_0,\hat{\Omega}_0 \to \vec{r},E,\hat{\Omega})$$

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

Exact equations for integral source S_I, N = # spatial regions, F is NxN matrix

Fission Matrix - Theory

- $F_{I,J}$ = next-generation fission neutrons produced in region I, for each fission neutron starting in region J (J→I)

- In the equation for F,
  - $S(r_0)/S_J$ is a local weighting function within region J
  - **As V_J → 0:**
    - $S(r_0)/S_J$ → 1
    - **Discretization errors → 0**
    - **Can accumulate tallies of $F_{I,J}$ even if not converged**

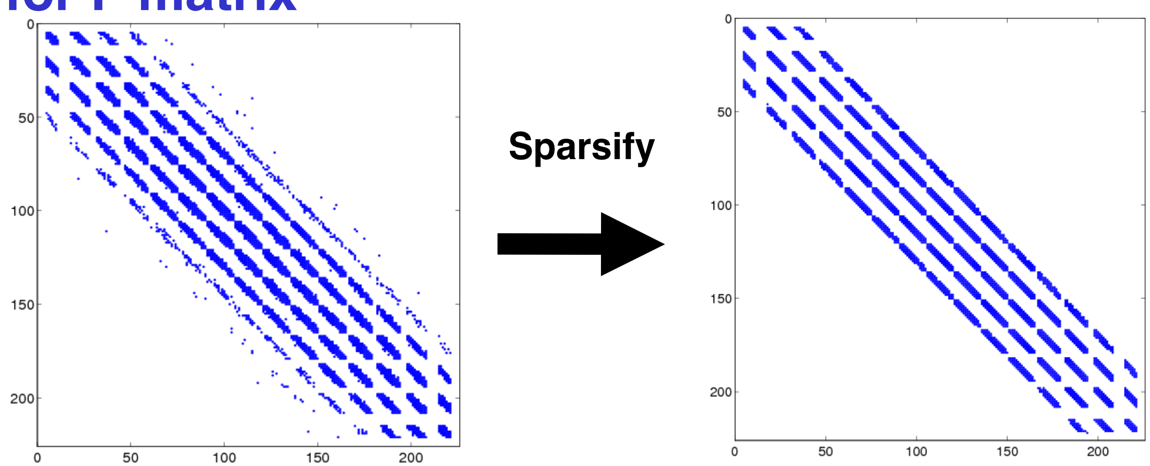
- $F_{I,J}$ tallies:
  - Previous F-matrix work: tally during neutron random walks
  - **Present F-matrix work: tally only point-to-point, using fission-bank in master proc (~free)**
    - Eliminates excessive communications for parallel
    - Provides more consistency, $F_{I,J}$ nonzero only in elements with actual sites
    - Analog-like treatment, better for preserving overall balance

Fission Matrix – Sparse Structure

- **For a spatial mesh with N regions, F matrix is N x N**
  - 100x100x100 mesh → F is 10^6 x 10^6, **8 TB** memory
  - In the past, memory storage was always the major limitation for F matrix

- **Sparse storage for F matrix**

3D reactor with
15x15 spatial mesh,
225x225 F matrix



  - Don't store zero elements
  - **Nearest-neighbor scheme** to only store "most" contributions
  - In practice, ~ 99.5% of sites is sufficient
  - **Reduces F matrix storage,** **9 GB** for 100x100x100 mesh
  - For now, matrix bandwidth is determined empirically to preserve physics, could readily be automated for future production

A Brief Review of Transport Theory

- **K-eigenvalue form of transport equation**

$$M \cdot \Psi(\vec{r},E,\hat{\Omega}) = \tfrac{1}{K} \cdot \frac{\chi(E)}{4\pi} \cdot S(\vec{r}),$$

  - 60 years ago it was proven that:
    - **A single, non-negative, real, fundamental eigenfunction & eigenvalue exist**
  - 50 years ago it was proven that:
    - **If energy dependence is ignored (1-speed or 1-group), then a complete set of self-adjoint, real eigenfunctions & discrete eigenvalues exist**
  - Nothing else has been proven on structure & properties for energy-dependent form of transport equation
- **It is always assumed that higher-mode solutions exist**
  - Due to energy dependence, higher modes are **not** orthogonal
  - **Energy-dependent transport equation is bi-orthognal**, forward & adjoint modes are orthogonal
- **In the present work based on the Fission Matrix:**
  - **We provide empirical evidence that higher modes <u>exist</u>, are <u>real</u>, have <u>discrete</u> eigenvalues, and are very <u>nearly self-adjoint</u>** **(for reactor-like problems)**
  - **Approach is similar to Birkhoff's original proof for fundamental mode**
  - **This has never been done before using continuous-energy Monte Carlo**

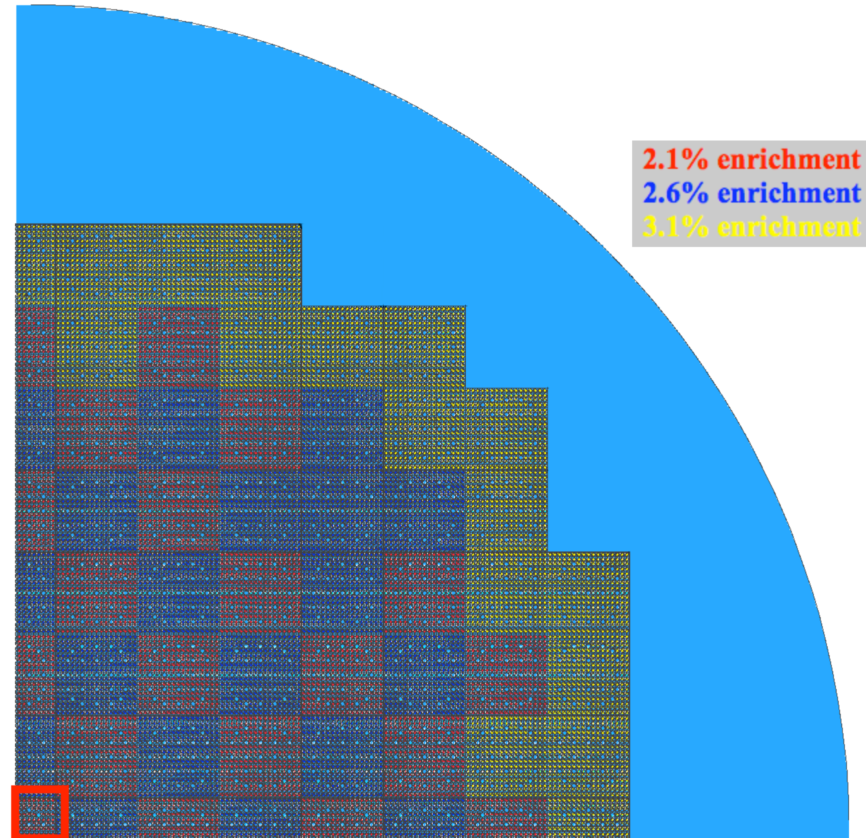
Whole-core 2D PWR

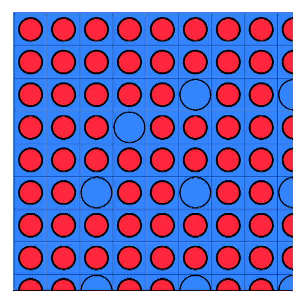
Eigenvalue spectrum
Spatial Eigenmodes

Whole-core 2D PWR Model

2D PWR (Nakagawa & Mori model)

- **48 1/4 fuel assemblies:**
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes for control rods or detectors
- **Each assembly:**
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- **Dominance ratio ~ .98**





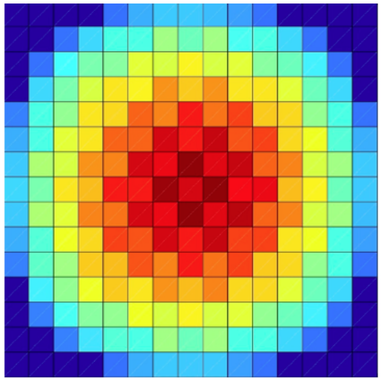
- **Calculations used whole-core model, symmetric quarter-core shown at right**
- **ENDF/B-VII data, continuous-energy**
- **Tally fission rates in each quarter-assembly**

PWR – Eigenvalue Spectrum & Fundamental Mode

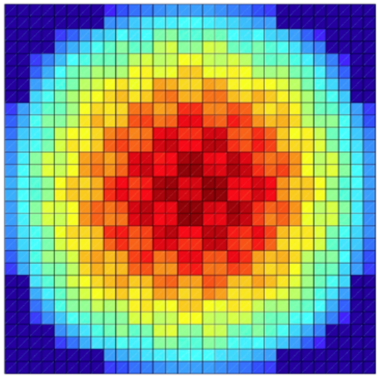
500 k neutrons / cycle

fission matrix tallies for cycles 4-55

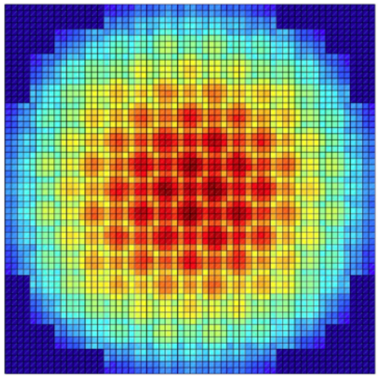
Local distance ≥ 2 assembly widths



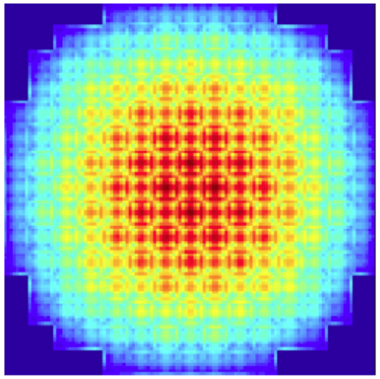
15 x 15 mesh



30 x 30 mesh



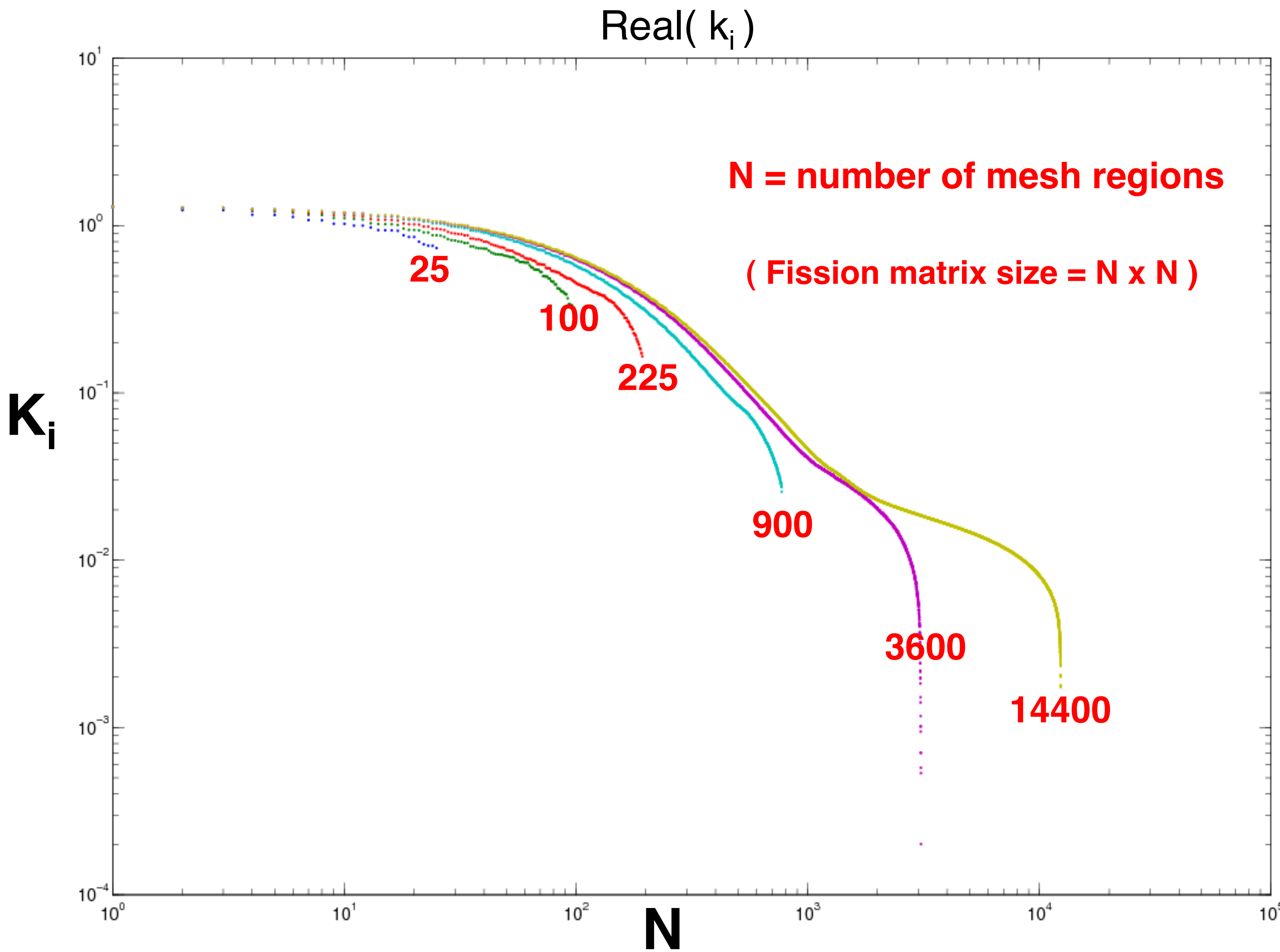
60 x 60 mesh



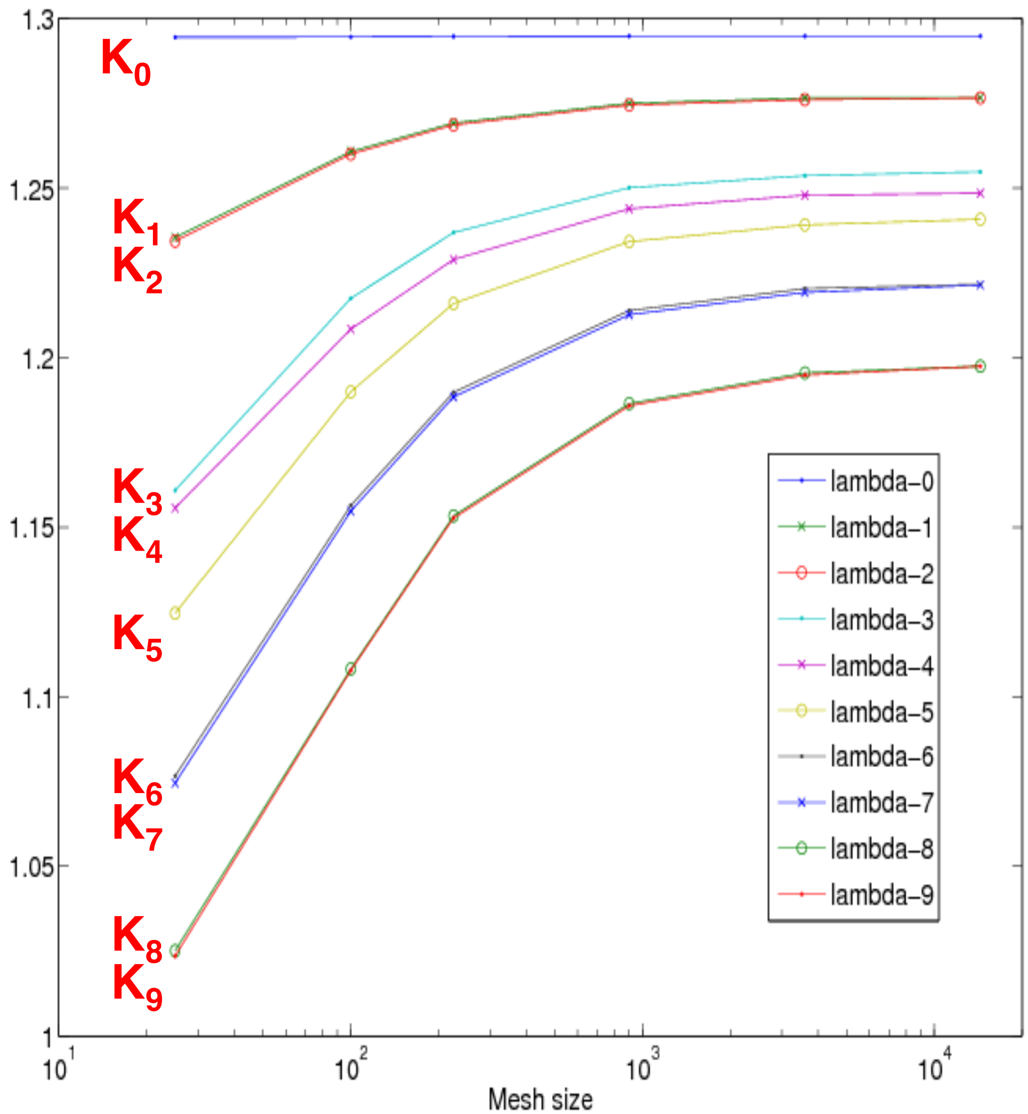
120 x 120 mesh

- Fission matrix computed during MCNP k-effective inactive cycles
- Fundamental eigenmode of the fission matrix for a 2D whole-core PWR model, for various spatial meshes used to tally the fission matrix

Eigenvalue Spectra with Varying Meshes



Spectrum Convergence from Mesh Refinement



# Mesh Regions			K_0
5x5	=	25	1.29444
10x10	=	100	1.29453
15x15	=	225	1.29469
30x30	=	900	1.29477
60x60	=	3600	1.29479
120x120	=	14400	1.29480

For fine-enough spatial mesh, eigenvalue spectrum converges

120 by 120 Spectrum, Varying Neutrons/cycle

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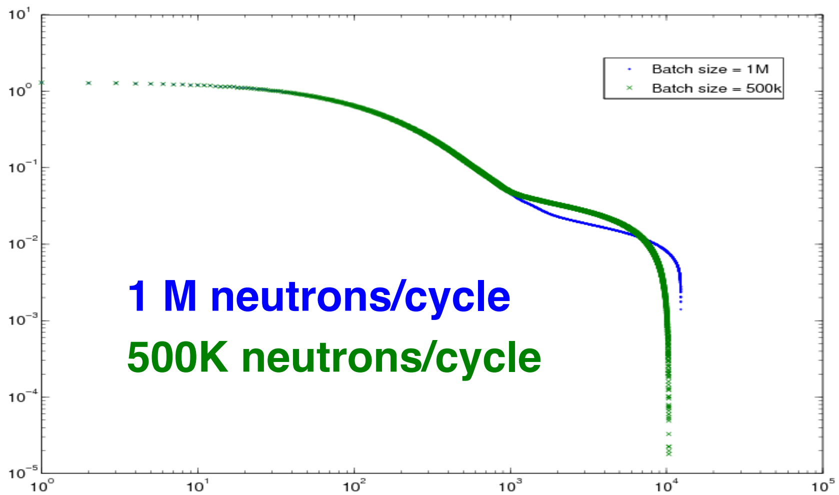
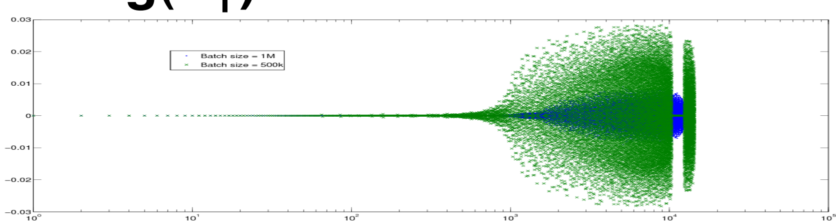
Real(k_i):



Imag(k_i):



The appearance of complex eigenvalues appears to be strictly an artifact of Monte Carlo statistical noise

When more neutrons/cycle are used to decrease statistical noise, complex components diminish or vanish

The first few 100s or 1000s of discrete eigenvalues are real, and presumably all would be with sufficiently large neutrons/cycle

PWR – Eigenmodes for 120x120x1 Spatial Mesh

mcnp
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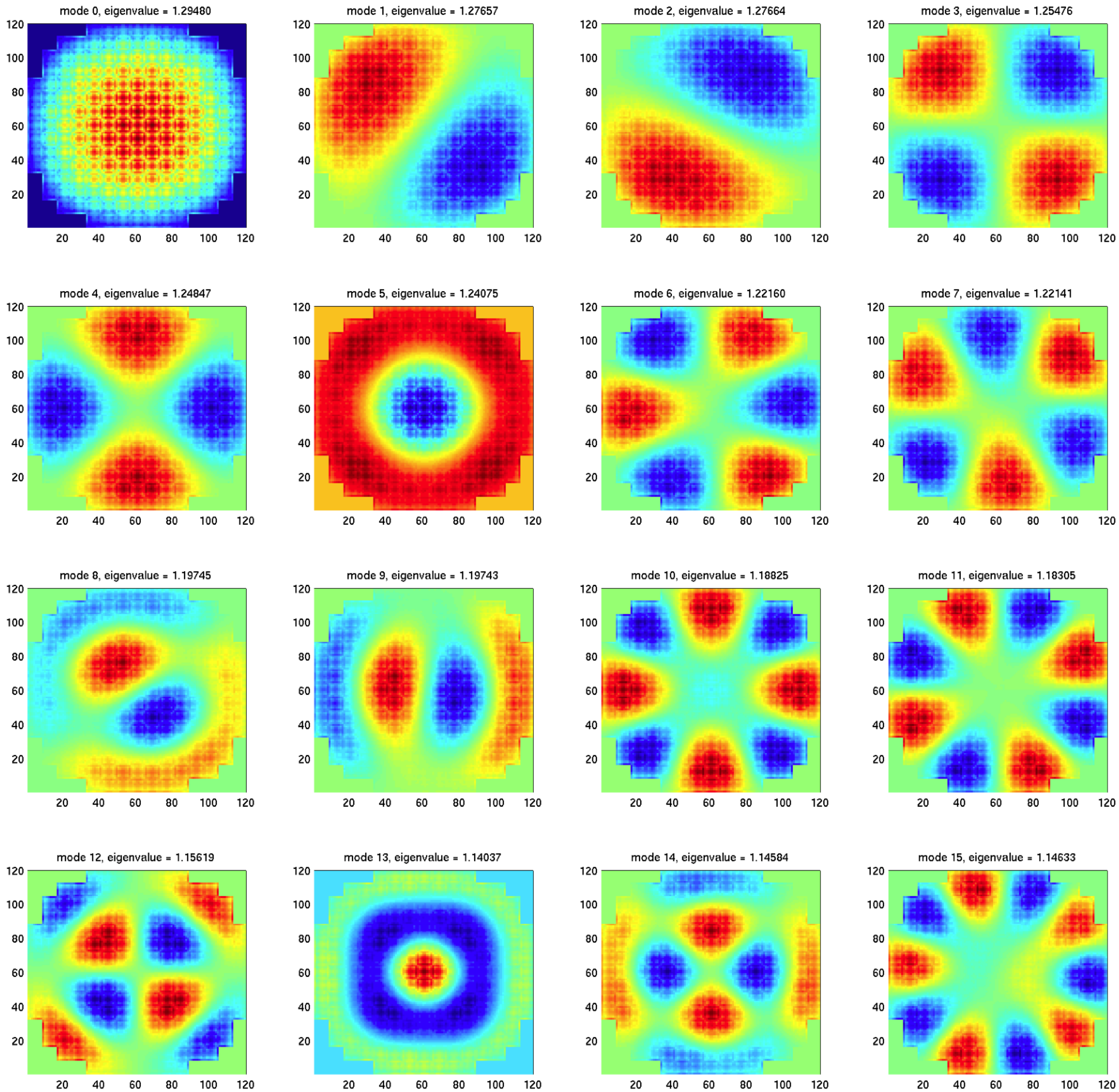

n	K_n
0	1.29480
1	1.27664
2	1.27657
3	1.25476
4	1.24847
5	1.24075
6	1.22160
7	1.22141
8	1.19745
9	1.19743
10	1.18825
11	1.18305
12	1.15619
13	1.14633
14	1.14617
15	1.14584

PWR – First 100 Eigenmodes for 120x120x1 Spatial Mesh

mcnp
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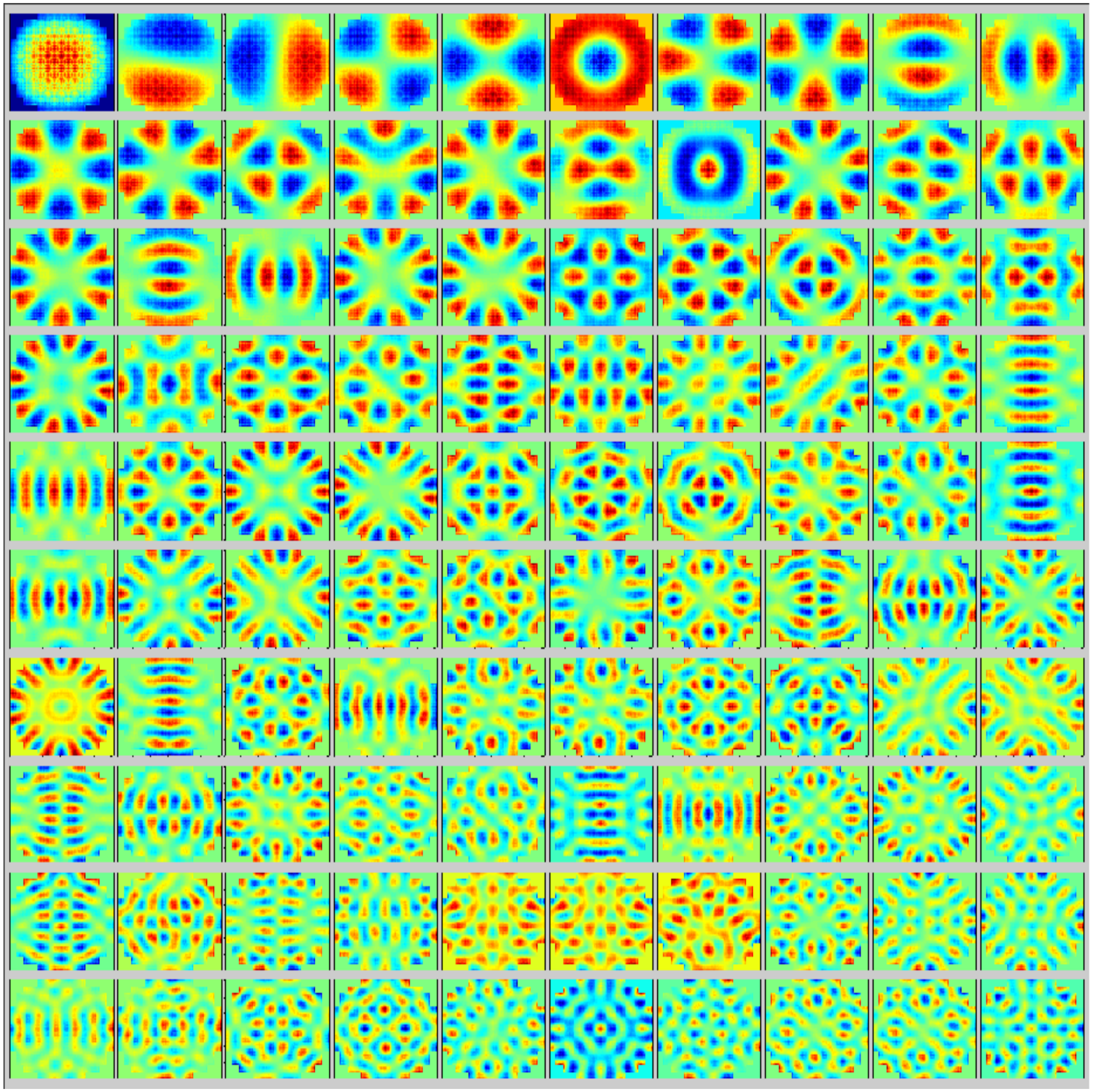
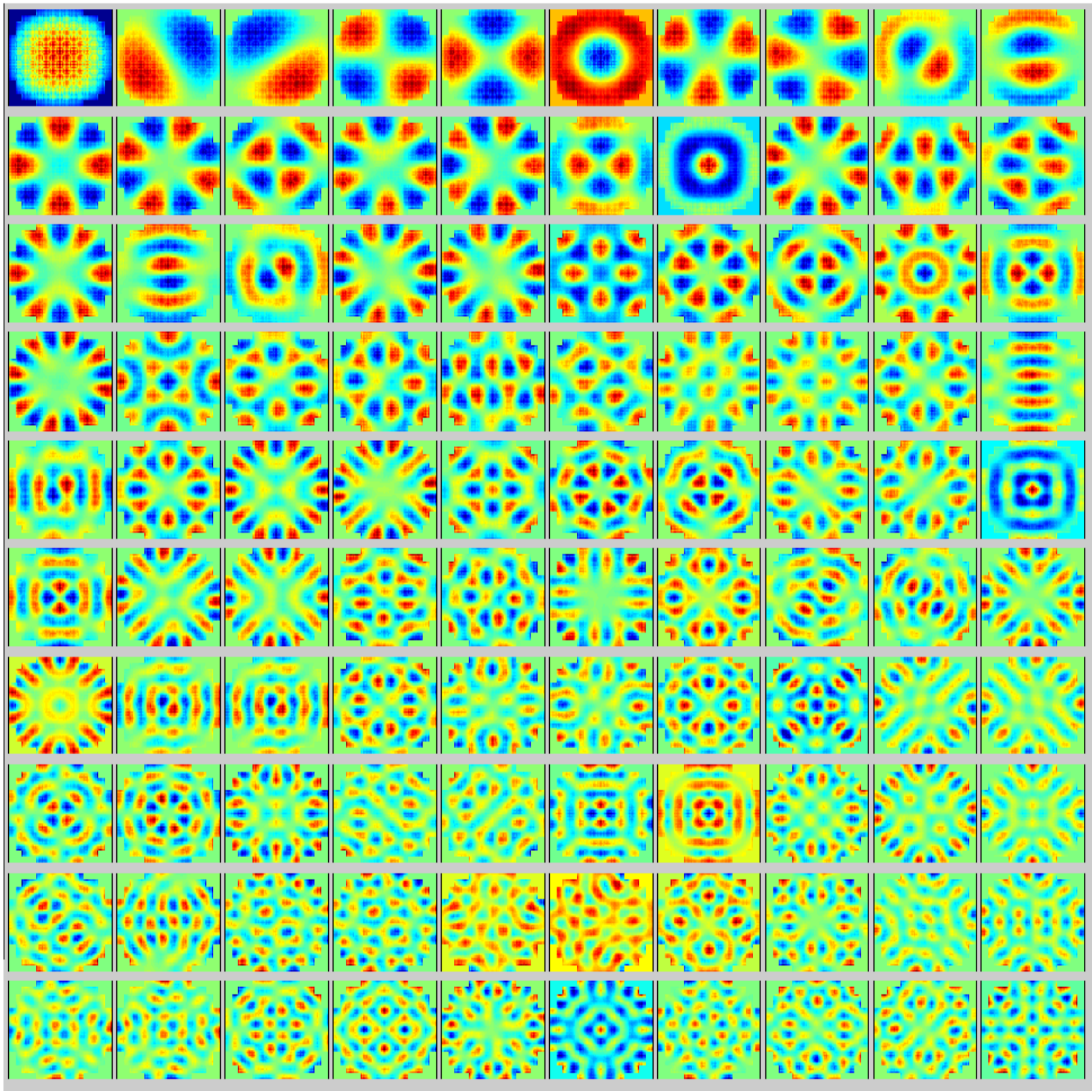
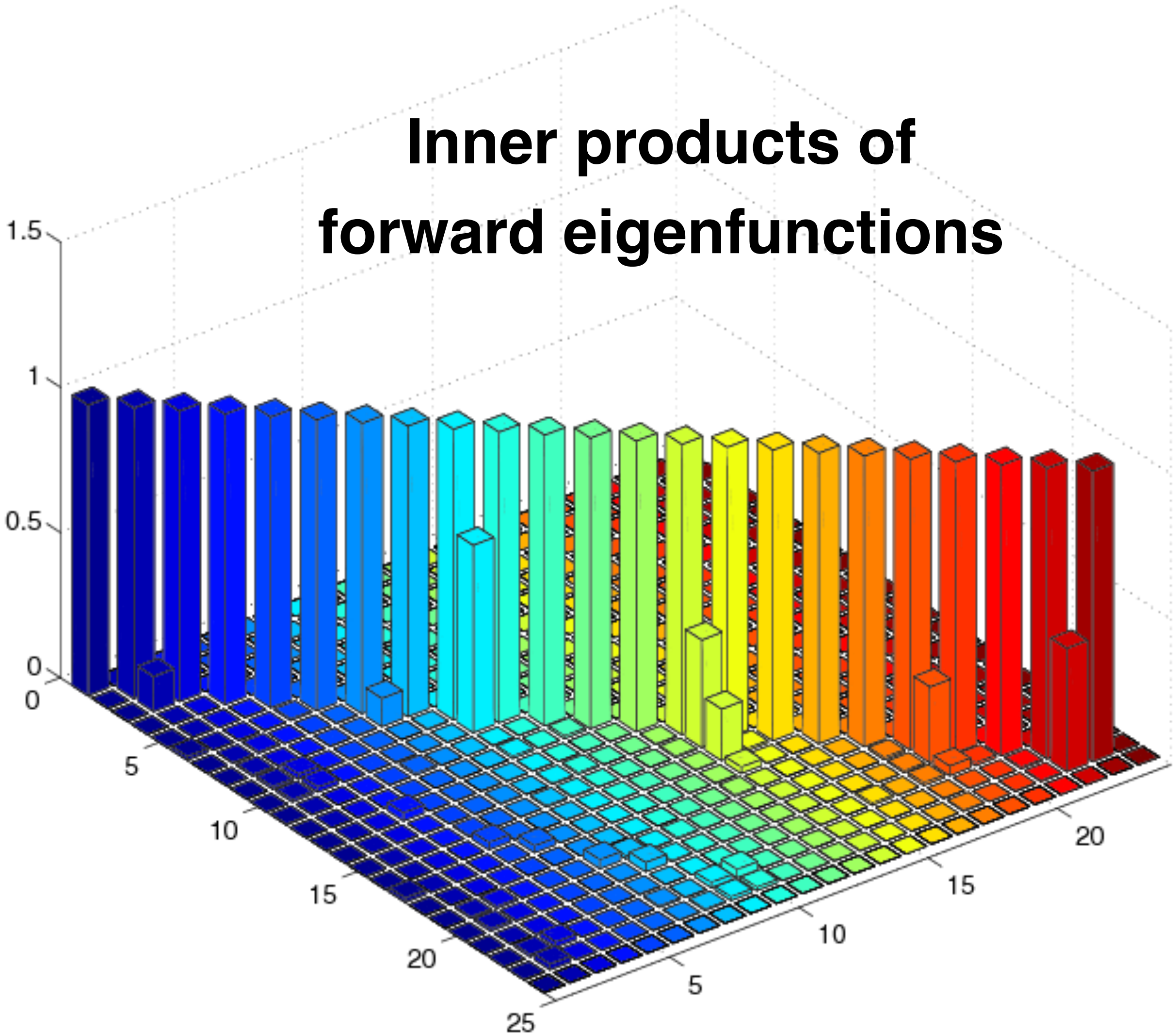


PWR – First 100 Eigenmodes, with More Neutrons



PWR – Inner Products of Forward Eigenmodes



$$\int d\vec{r}\, \psi_n(\vec{r})\psi_m(\vec{r})$$
$$= \delta_{nm} \;\; if \;\; fission\, kernel$$
$$is\ self\ adjoint/symmetric$$

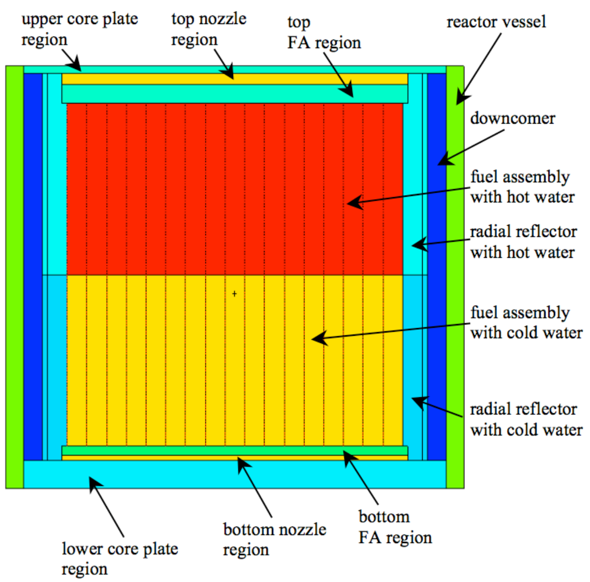
Strictly, eigenfunctions of the transport equation are bi-orthogonal.

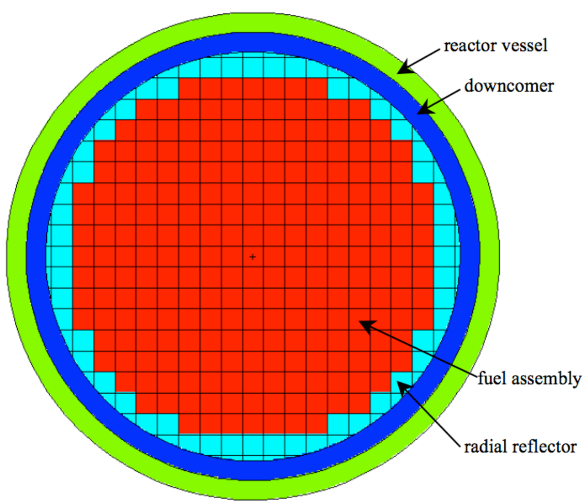
As shown above, **forward eigenfunctions are very nearly orthogonal**.

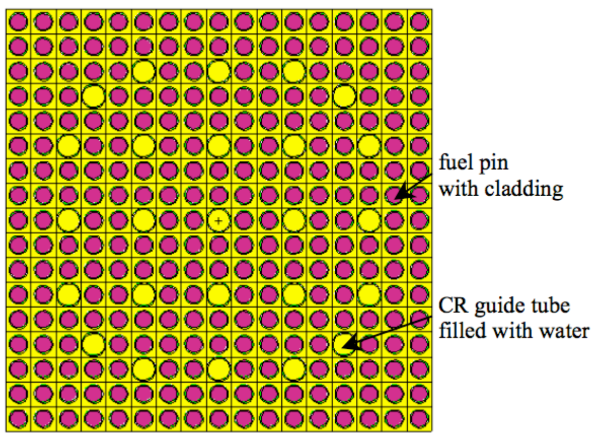
Kord Smith
Challenge Problem
-
3D Whole-Core PWR

Full core, 3D benchmark for assessing MC computer performance

- Specified by Hoogenboom & Martin for OECD/NEA (2010)
- LWR model: 241 assemblies, 264 fuel pins/assembly
- Fuel contains 17 actinides + 16 fission products; borated water
- Detailed 3D MCNP model
  - Mesh tallies for pin powers, (63,624 pins) x (100 axial) = 6.3M pin powers
  - Runs easily on deskside computer (Mac Pro, 2 quad-core, 8 GB memory)







Standard MCNP & the "Kord Smith Challenge"

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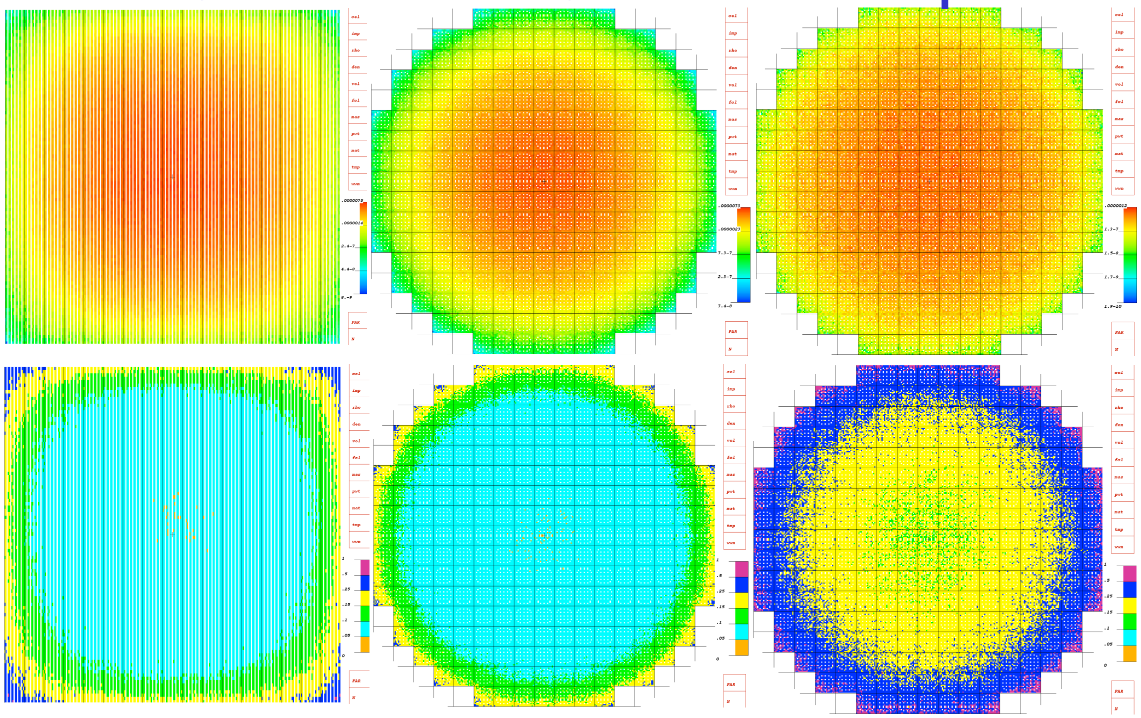
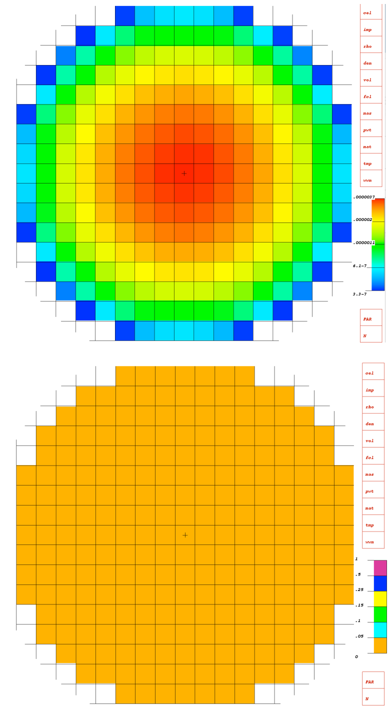
Pin Powers & Std.Dev

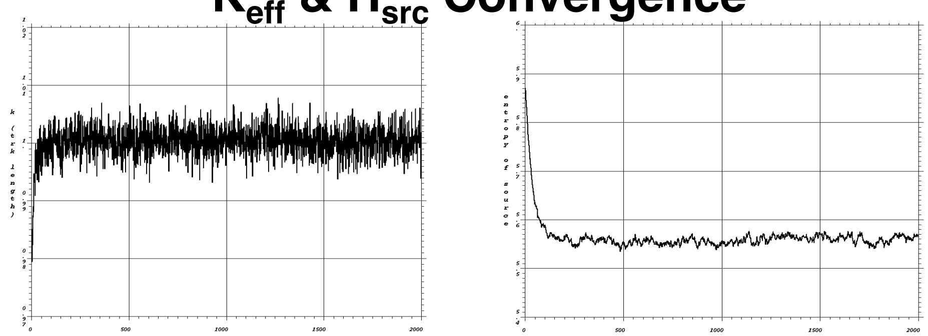
Axial Mid Top



Assembly Power & Std.Dev



K_{eff} & H_{src} Convergence

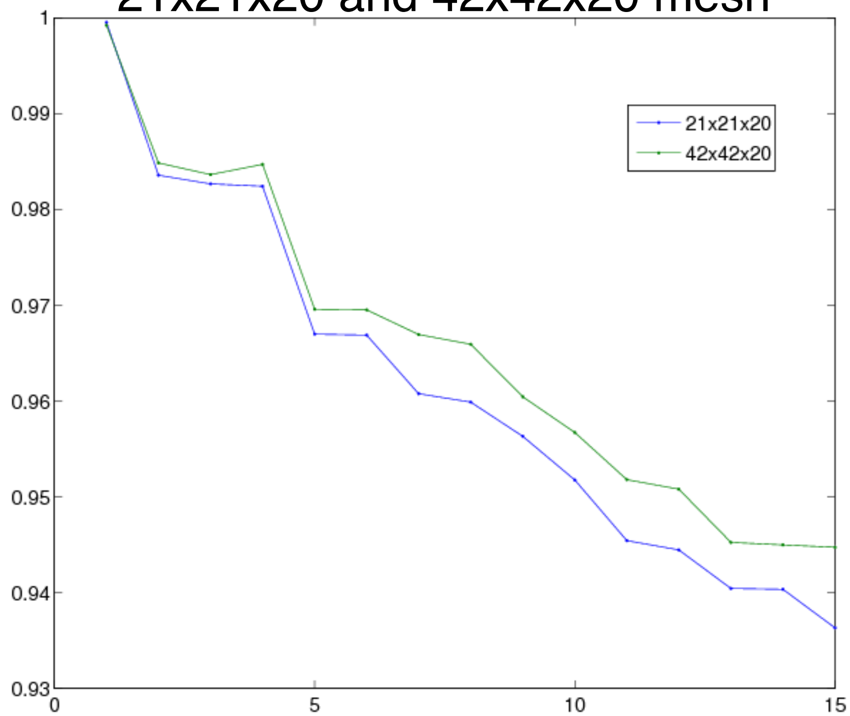


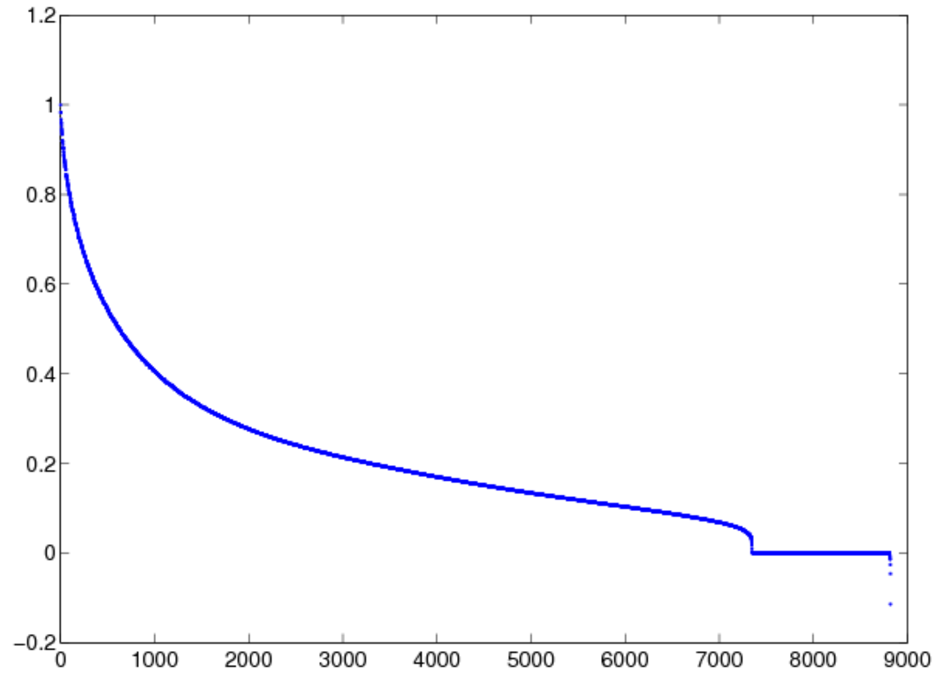
200M neutrons

Mac Pro, 8 cpu

Kord Smith Challenge Eigenvalue Spectrum

First 15 eigenvalues for
21x21x20 and 42x42x20 mesh





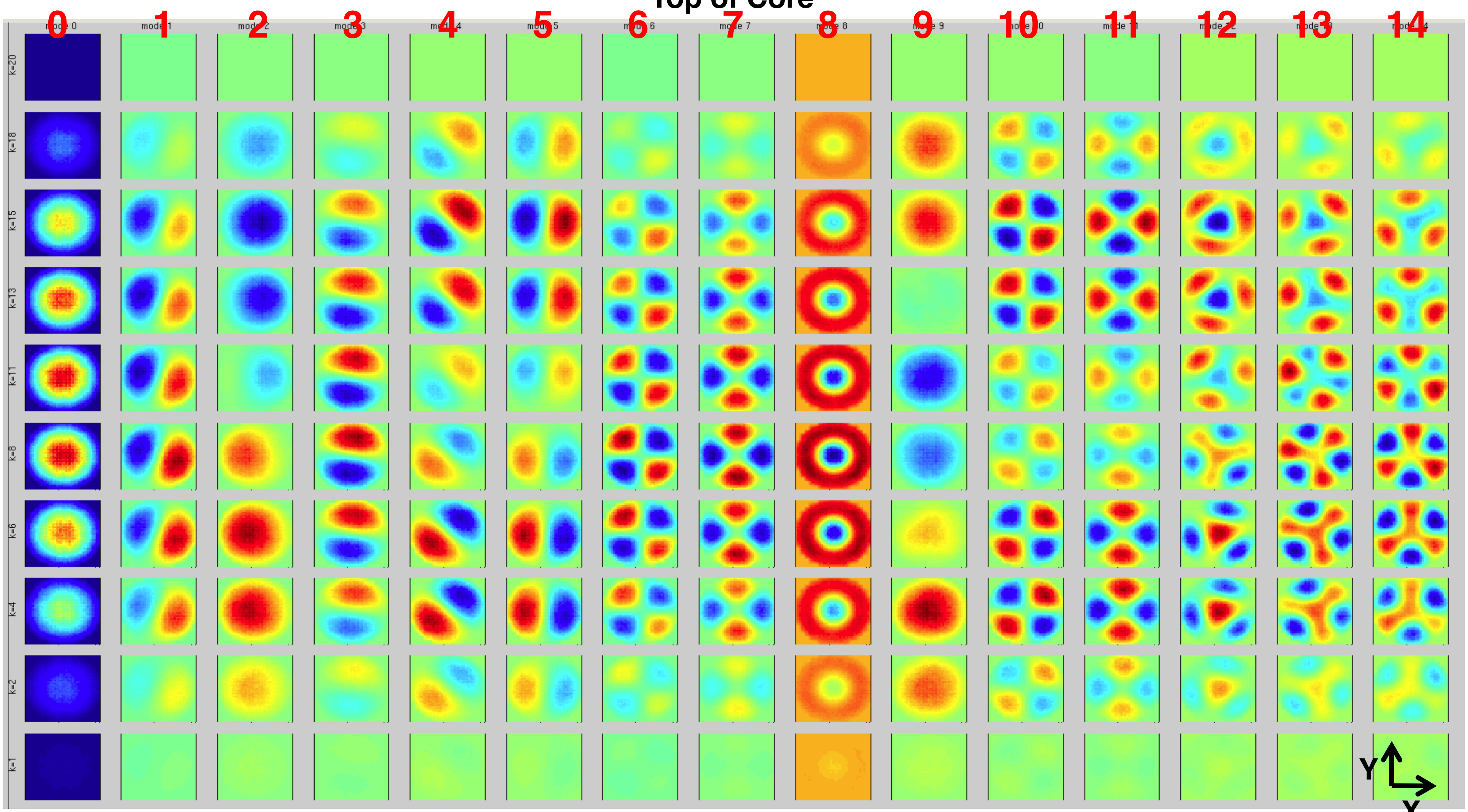
21x21x20 mesh entire Real(spectrum)

Eigenfunctions from Fission Matrix

XY plots of eigenfunctions at various Z elevations, 55 cycles with 1 M neutrons/cycle

42x42x20 spatial mesh, 35280x4913 fission matrix

Top of Core



Bottom of Core

Eigenvalues & Inner Products of Eigenfunctions

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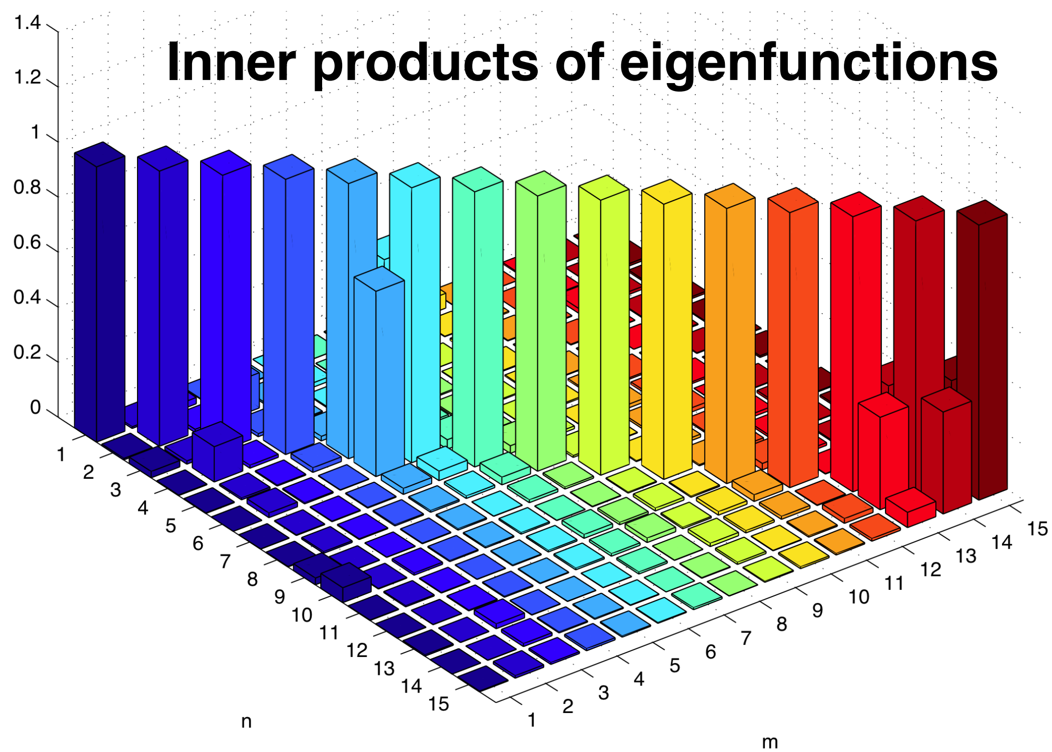
42x42x20 spatial mesh, 35280x4913 fission matrix

55 cycles, 1 M neutrons/cycle

fission matrix tallies for cycles 4-55

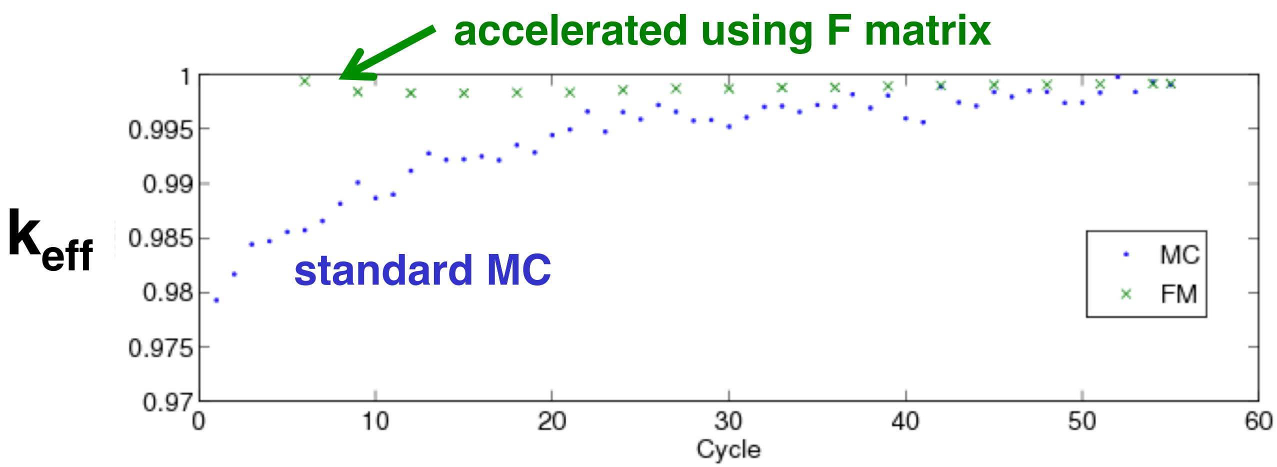
n	K_n
0	0.99919
1	0.98483
2	0.98362
3	0.98469
4	0.96956
5	0.96950
6	0.96693
7	0.96591
8	0.96043
9	0.95671
10	0.95178
11	0.95078
12	0.94524
13	0.94497
14	0.94472

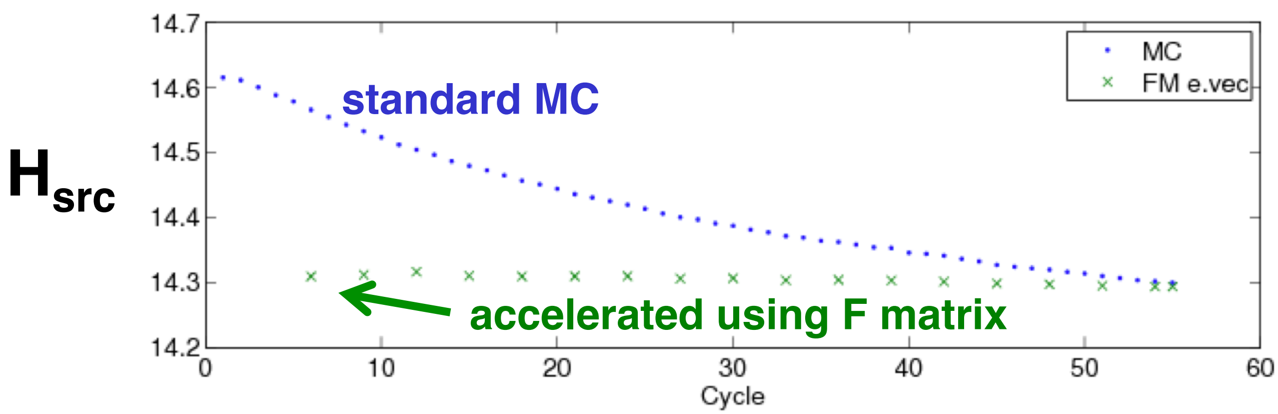


Convergence Acceleration Using Fission Matrix

- **Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles**

- **Very impressive convergence improvement**





Spent Fuel Storage Vault

(idealized benchmark)

Loosely-Coupled Problem

Fuel Vault Problem

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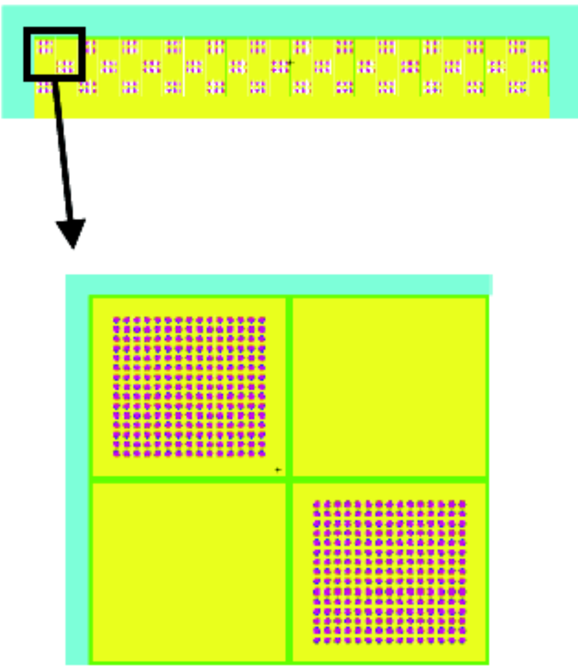
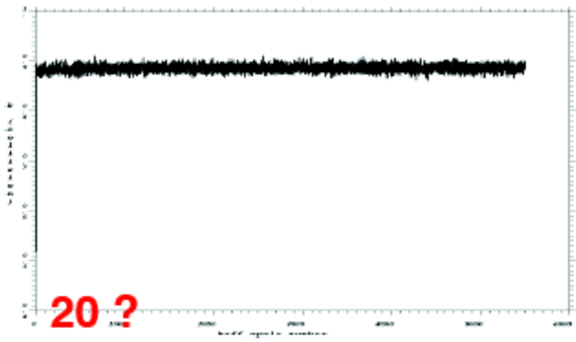
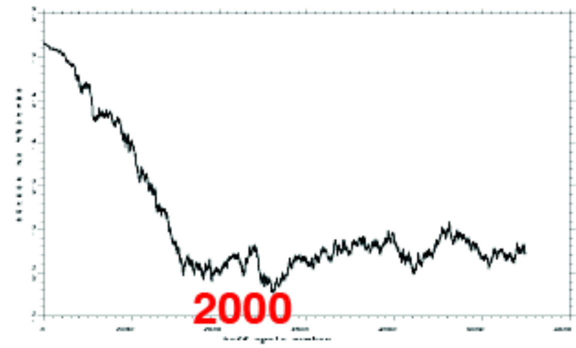
Fuel Storage Vault



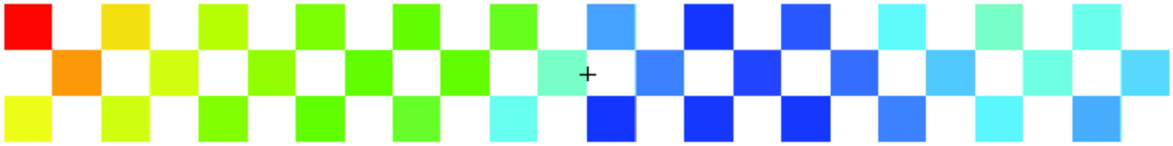
K vs cycle



H_{src} vs cycle



Assembly Heating Distribution

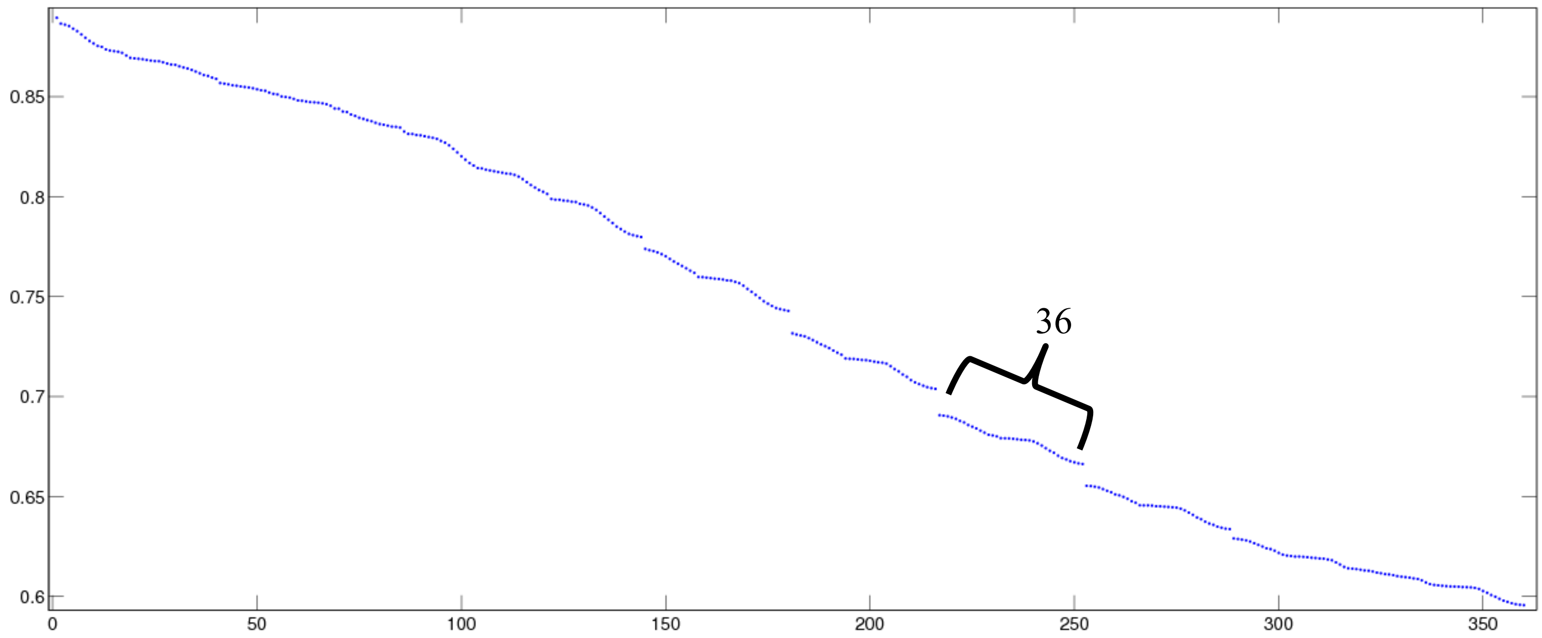


For this calculation,

- **Should discard ~20 cycles if calculating Keff only**
- **Should discard ~2000 cycles if calculating heating distribution**

Eigenvalue Spectrum for Fuel Vault Problem- First 360

Real(k_i), i = 1,2,..360



36 semi-coupled assemblies -> Mini-groups of 36 in size

XY Eigenmodes of Fuel Vault Problem, 96 by 12 by 10

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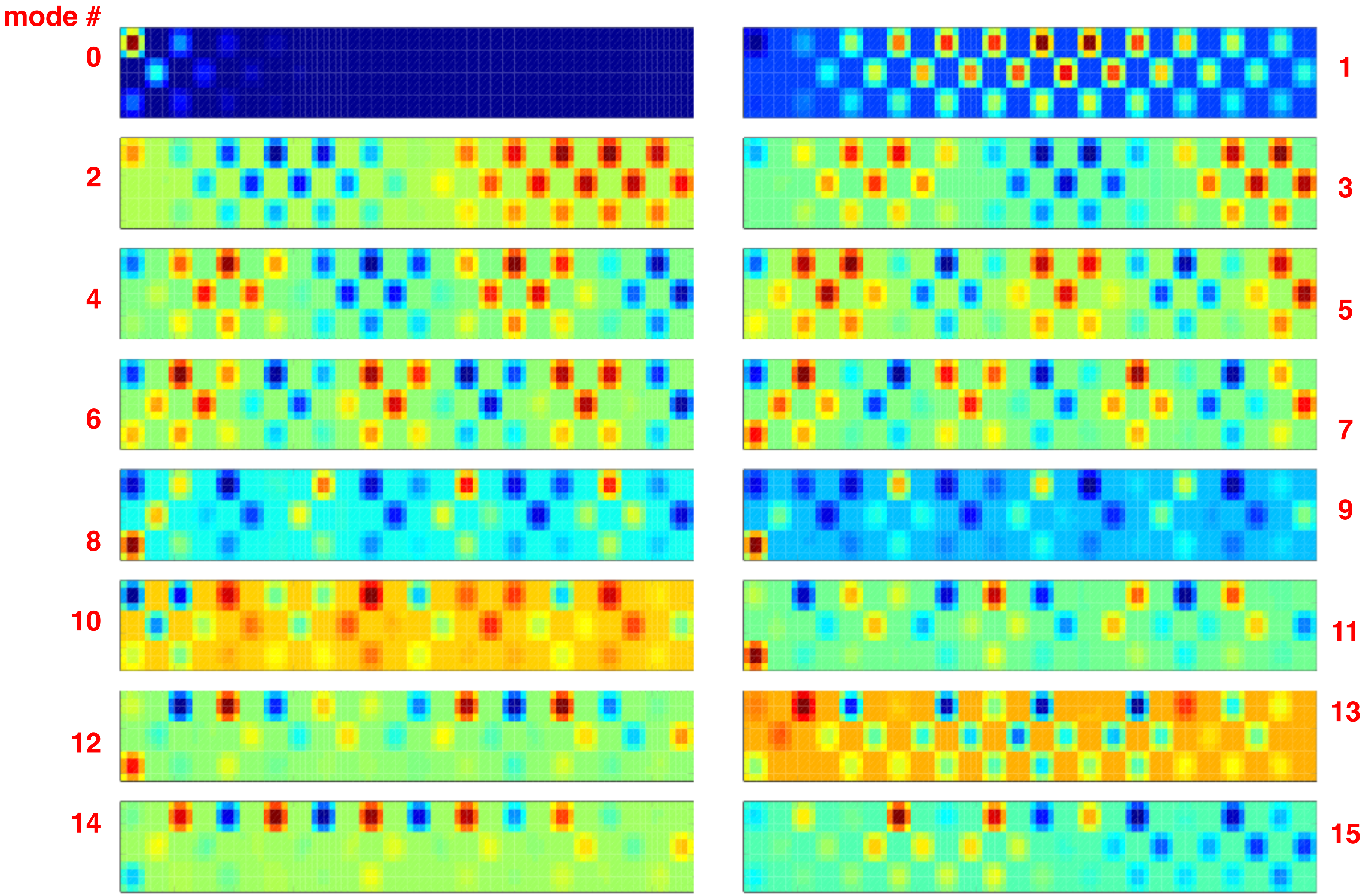

XY planes mid-height. Axial shape is sine, #10,13,15 have change in sign in z

Fuel Vault Problem Convergence Acceleration- 200 cycles

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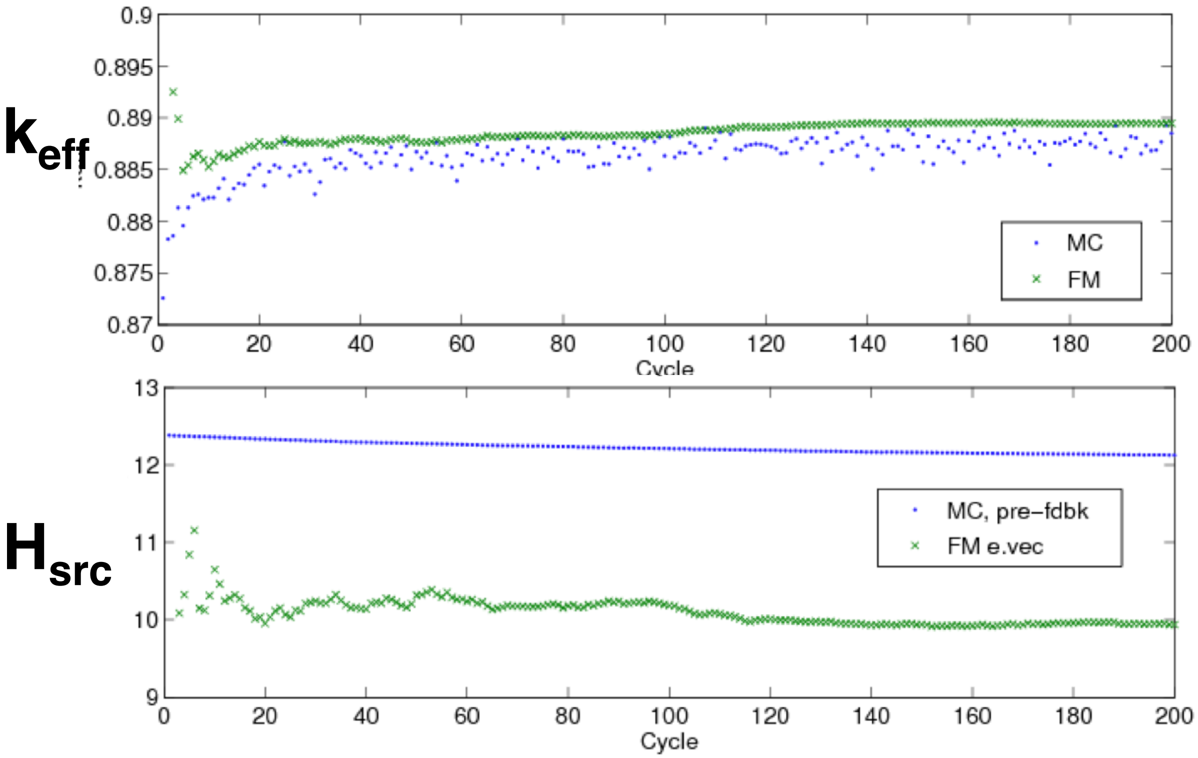
It takes ~2,000 cycles for standard MC to converge for this problem,

Using the fission matrix for source convergence acceleration, only ~20 cycles are needed



standard MC
accelerated using F matrix

Standard MC decreases slowly, converges to same value as F matrix after ~2,000 cycles

Advanced Test Reactor

Idaho National Laboratory

Advanced Test Reactor

"Serpentine Arrangement of Highly Enrichment Water-Moderated Uranium-Aluminide Fuel Plates Reflected by Beryllium"

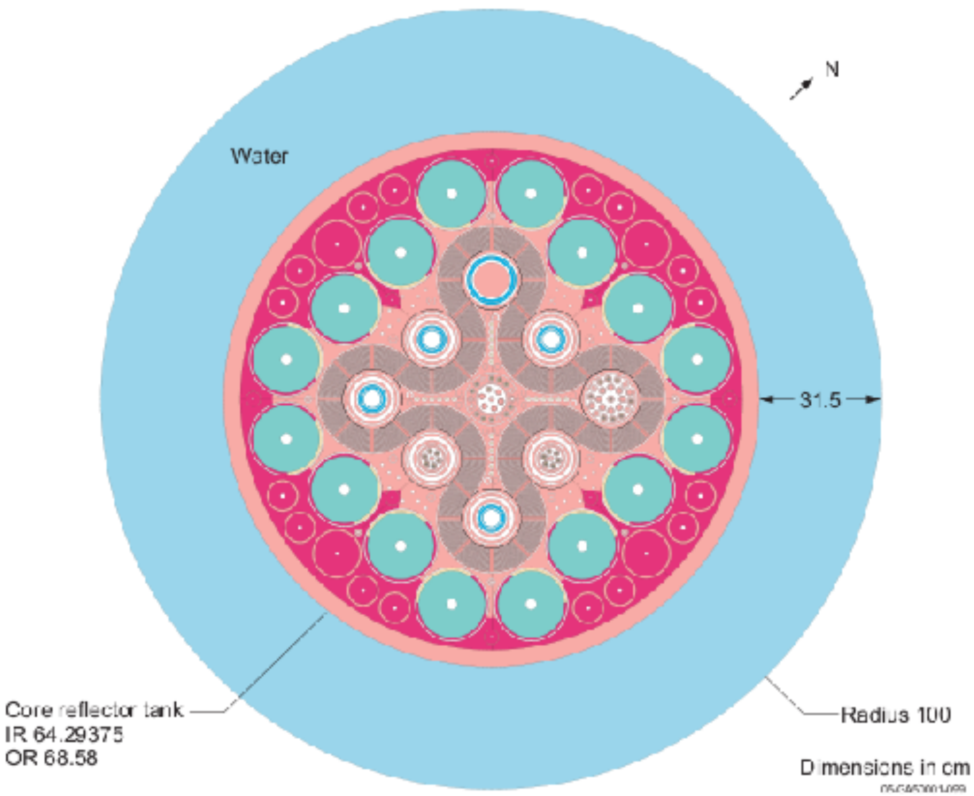
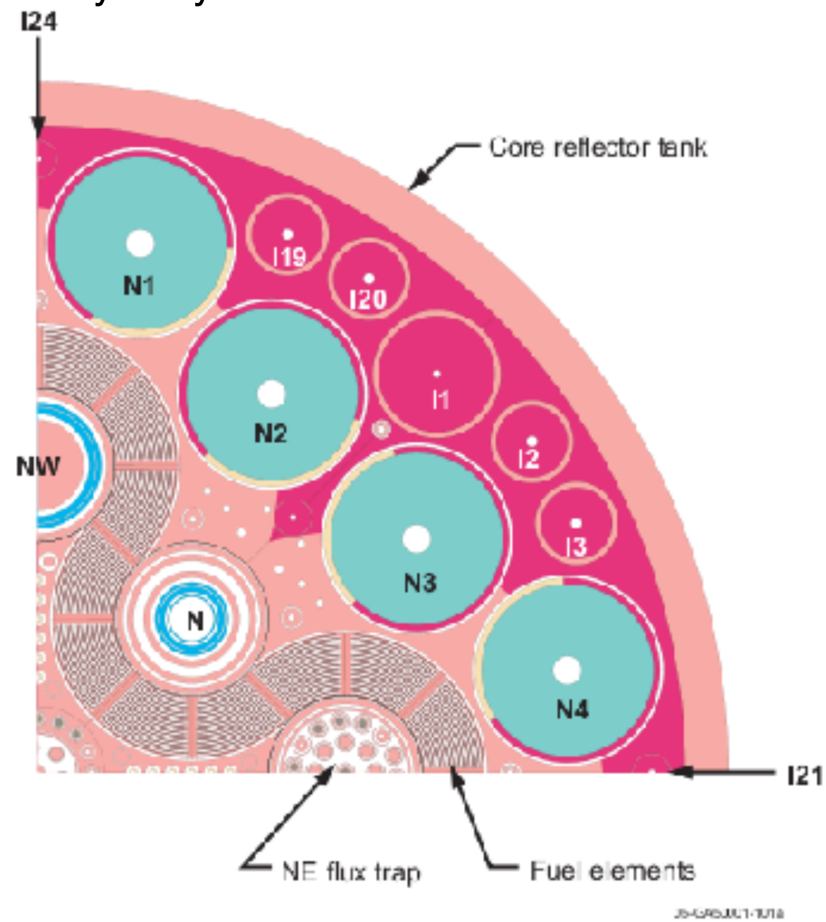


Figure 20. An XY View at x=0,y=0 of the Benchmark Model.

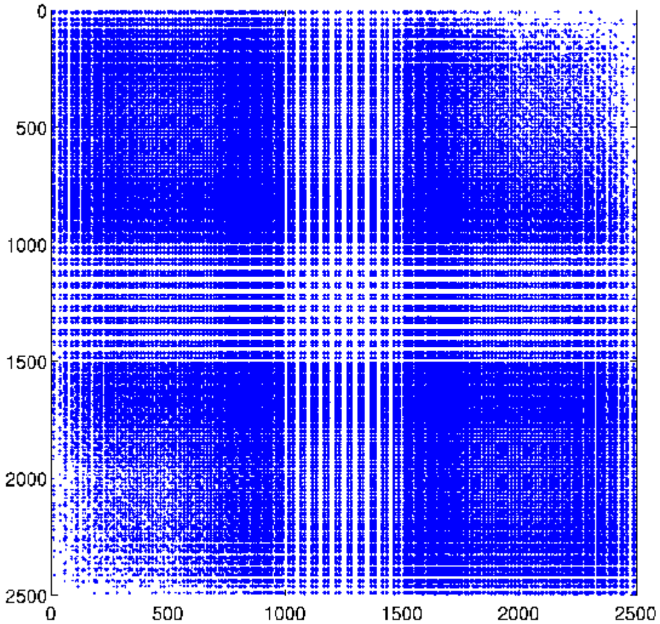


S. S. Kim, B. G. Schnitztler, et. al., "Serpentine Arrangement of Highly Enrichment Water-Moderated Uranium-Aluminide Fuel Plates Reflected by Beryllium", HEU-MET-THERM-022, Idaho National Laboratory (September 2005).

ATR - Fission Matrix Structure

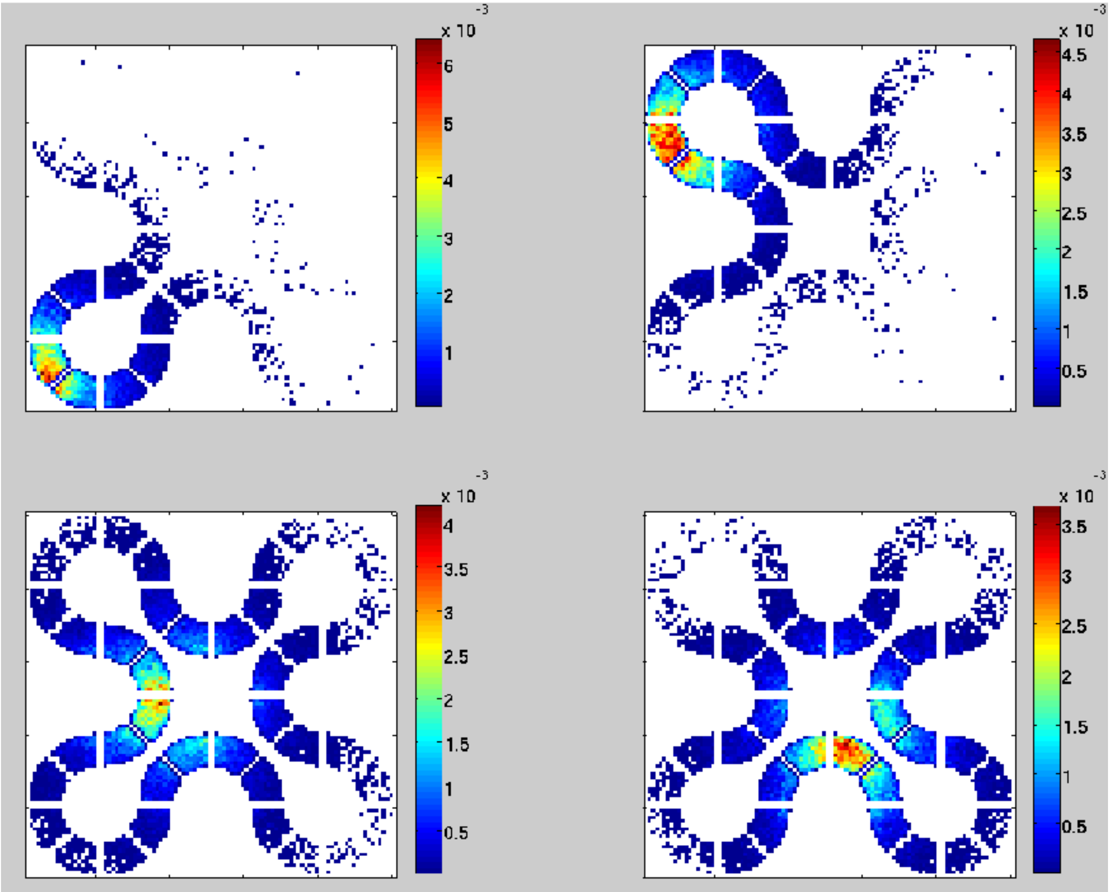
Matrix structure

(50x50 spatial mesh)



Can't use sparse storage

Four matrix columns (100x100 spatial mesh)



ATR - Fundamental Eigenvector, Eigenvalues

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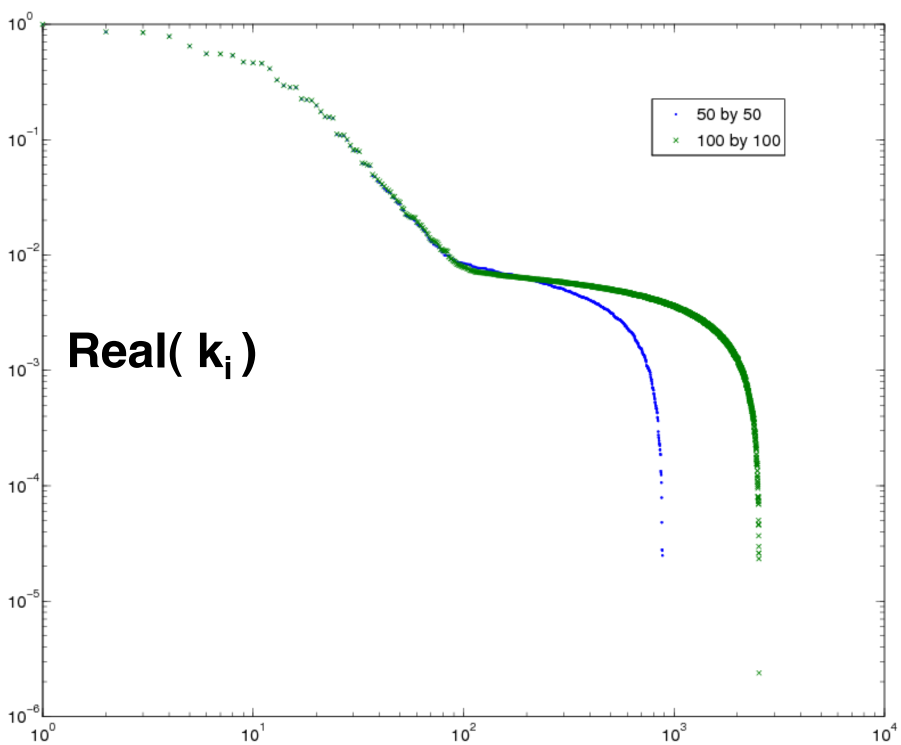

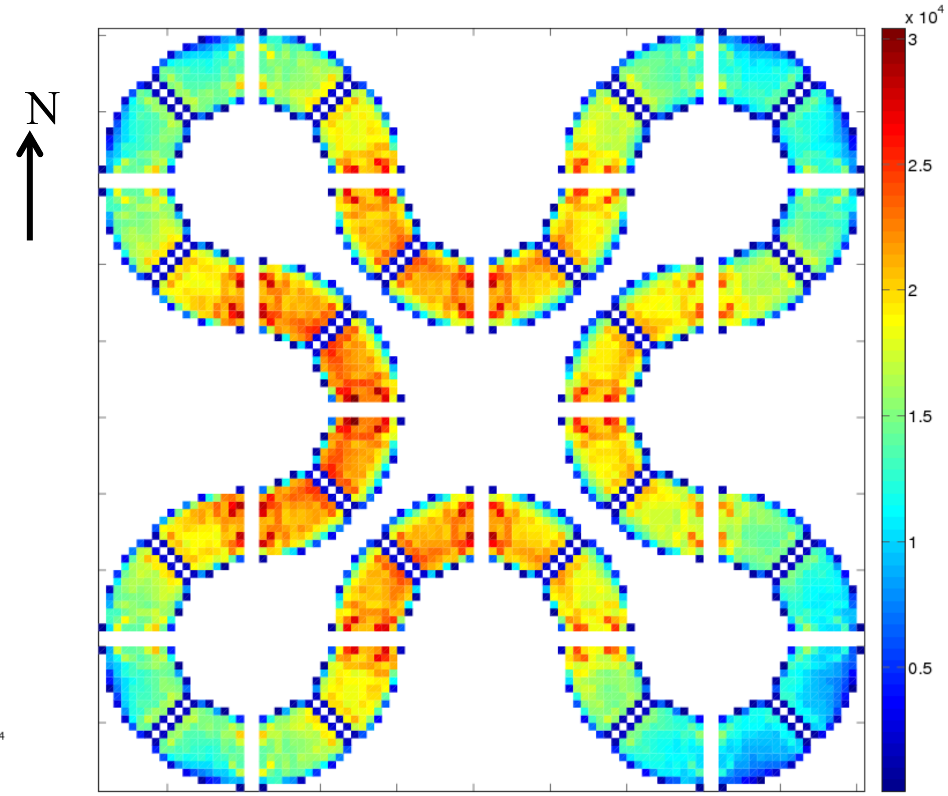

Fundamental mode, 100x100 spatial mesh

ATR - Eigenmodes (100x100 spatial mesh)

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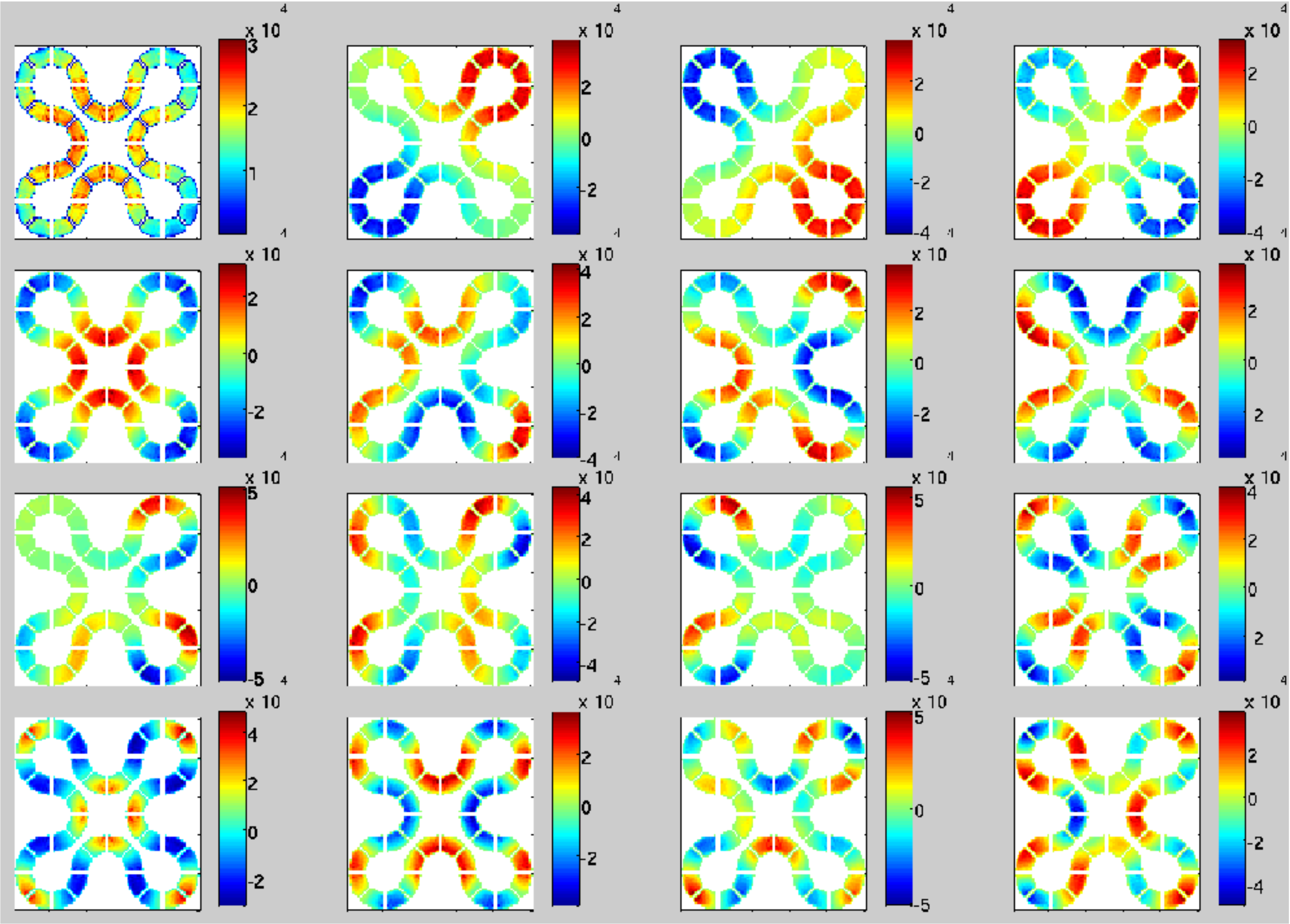
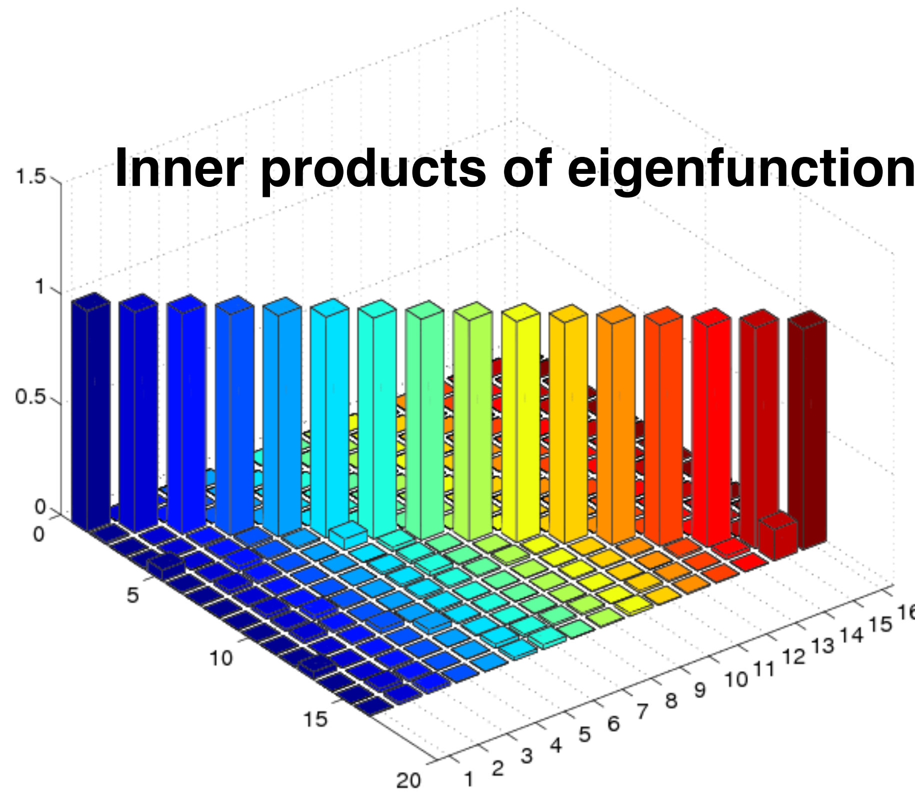


ATR - Fission Matrix Orthogonality

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

100x100x1 spatial mesh, no sparsification
55 cycles, 1 M neutrons/cycle
fission matrix tallies for cycles 4-55

Inner products of eigenfunctions



Conclusions

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- **Fission matrix capability has been added to MCNP (R&D for now)**
- **Tested on variety of real problems (3D, continuous-energy)**
- **Can obtain fundamental & higher eigenmodes**
  - **Empirical evidence for existence of higher modes, real, discrete eigenvalues, very nearly orthogonal eigenmodes** (for reactor-like problems)
  - **Higher eigenmodes are important for BWR void stability, Xenon oscillations, control rod worth, higher-order perturbation theory, inter-cycle correlation effects on predicting statistics, quasi-static transient analysis, accident behavior, etc., etc.**
- **Can provide very effective acceleration of source convergence**
- **Adjoint Fission Matrix can provide source importance, relevant to POI & other calculations**