LA-UR-13-26464
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Title: Eigenfunction Decomposition of Reactor Perturbations & Transitions Using MCNP Monte Carlo

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Intended for: MCNP documentation
Web

Issued: 2013-08-15

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Eigenfunction Decomposition of Reactor Perturbations & Transitions Using MCNP Monte Carlo

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8 August 2012

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- MCNP6 has new fission matrix capabilities
- These capabilities can accelerate the convergence of k eigenvalue calculations
- They can also be used to solve for non-fundamental modes
- Has applications in stability analysis and accident modeling

Fission Matrices
Basic Theory

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Using only a spatial discretization, the neutron transport equation

$$M\Psi(\mathbf{r}, E, \hat{\Omega}) = \frac{1}{k}\frac{\chi(E)}{4\pi}S(\mathbf{r})$$

can be reduced to

$$\mathbf{s} = \frac{1}{k}\bar{F}\mathbf{s},$$

Fission Matrices

Transition Coefficients

Given two sets of eigenvectors, $\mathbf{s}_{i,\text{original}}$ and $\mathbf{s}_{j,\text{modified}}$, we can reconstruct any of the original eigenvectors using the new ones with the following equation:

$$\mathbf{s}_{i,\text{original}} = \sum_{j=1}^{N} C_{ij} \mathbf{s}_{j,\text{modified}}$$

If we also have $\mathbf{s}^{\dagger}$, the adjoint source, found by calculating the eigenvectors of $\bar{F}^{T}$, we can solve for C_{ij}:

$$C_{ij} = \mathbf{s}_{i,\text{original}} \cdot \mathbf{s}^{\dagger}_{j,\text{modified}}$$

Setting $i = 1$, the fundamental eigenmode can be reconstructed in the new eigenspace.

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Basic quasistatic time-dependent transitions can be calculated. Source after n generations:

$$\mathbf{s}_{\mathrm{n}} \approx \sum_{j=1}^{m} C_{1,j} \left(\frac{k_j}{k_1} \right)^n \mathbf{s}_{j,\mathrm{modified}}$$

Assumes:

- All modes have the same mean neutron generation time
- There are no delayed neutrons

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Fission Matrices
Sparsity

- 1000×1000 mesh $\rightarrow$ $1M \times 1M$ fission matrix
- Matrix usually sparse, nonsymmetric

For a $1M \times 1M$ matrix:

Storage type	Storage
Full matrix	8 TB
Sparse	$\approx$ 10 GB

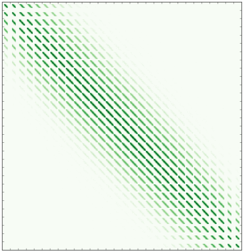

Figure: An Example Fission Matrix Sparsity Plot

Fission Matrices
Calculating Eigenpairs

Sparse nonsymmetric matrices:

- Few algorithms to calculate eigenpairs
- Choice of power iteration, implicitly restarted Arnoldi method (IRAM)
- Power iteration - linear convergence
- IRAM - superlinear convergence (preferred)

On one CPU core for 16 eigenvalues:

Matrix Size	IRAM (ARPACK)	Power Iteration
3600x3600	3.09 s	4878 s
900x900	0.234 s	353 s
225x225	0.0337 s	30.6 s

Methods

- Took MCNP models, perturbed them
- Wrote tools to solve eigenpairs
- Used tools on both problems to check if both were doing it right
- Studied transitions
- Studied statistics

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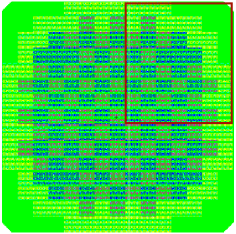
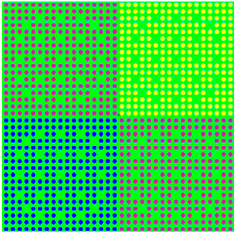
Methods

Core Models - PWR

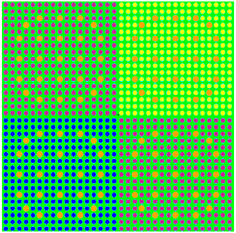
Inserted SS304 control rods in 1/4 of the core



(a) PWR Full Core



(b) PWR Original



(c) PWR Modified

Note the barely visible orange pins.

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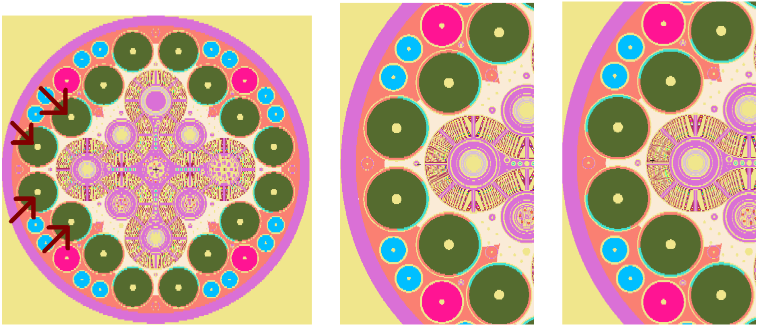
Rotated 4 control drums out 50°



(d) ATR Full Core (e) ATR Original (f) ATR Modified

Rotated hafnium out, beryllium in.

Results

We:

- Calculated eigenmodes
- Verified eigenmodes
- Generated transition coefficient arrays
- Reconstructed primary eigenmode in new eigenspace
- Generated transition animation
- Measured statistical variation compared to `KCODE`

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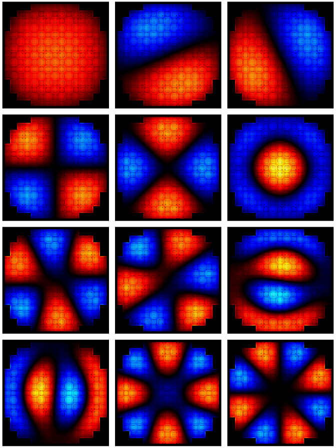
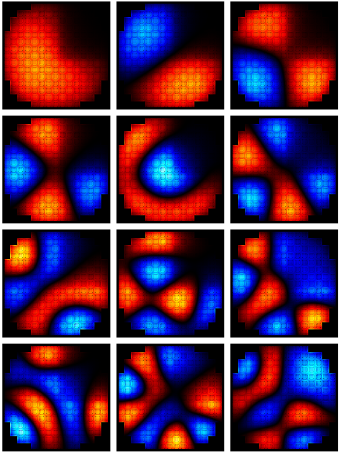
Eigenmodes of PWR



(g) PWR Modes Initial



(h) PWR Modes Final

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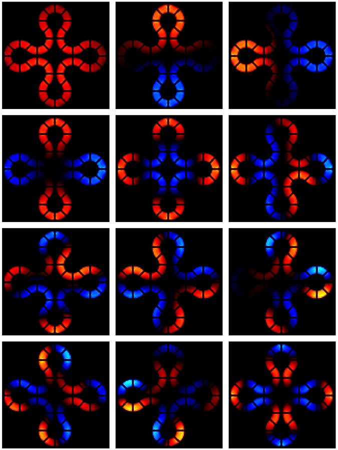
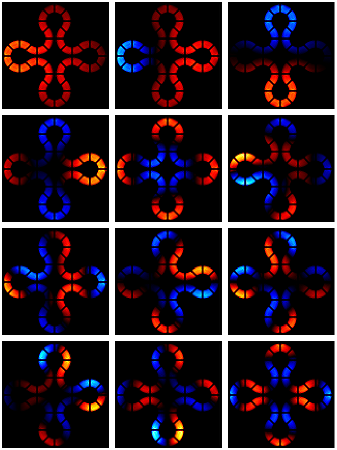
Eigenmodes of ATR



(i) ATR Modes Initial



(j) ATR Modes Final

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We don't know how ARPACK internally verifies its results.

Two independent checks used:

- Are the results eigenmodes?
  - Substitute computed solution into eigenvalue equation, compute residual $r = A\mathbf{v}_C - \lambda_C \mathbf{v}_C$
  - Norm (l_2) consistently below $N{*}\text{eps}$
- Are they linearly independent?
  - Compute SVD, make sure all values nonzero
  - Check passed for 80 modes of both PWR and ATR

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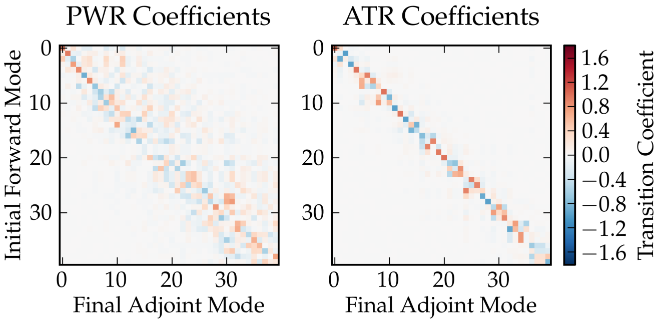
Transition Coefficients



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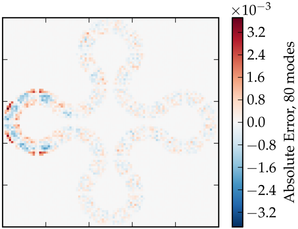
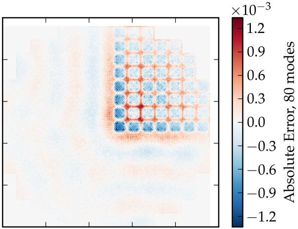
Fundamental mode reconstruction error with 80 eigenmodes



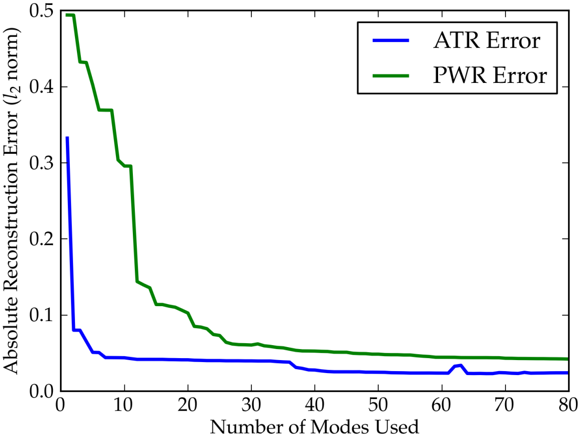
(k) ATR ($l_2 = 0.0243$)



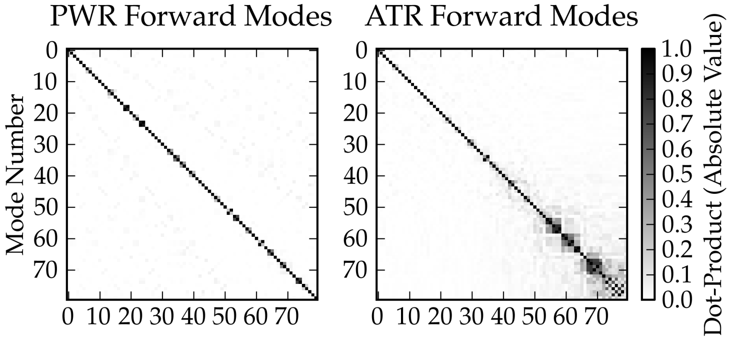
(l) PWR ($l_2 = 0.0423$)

Results
Reconstruction Error, Quantitative

Fundamental mode reconstruction error as a function of eigenmode count



Optimality of the series truncation closely related to orthogonality of eigenmodes



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25 ATR runs were done with different random number seeds. These are the results:

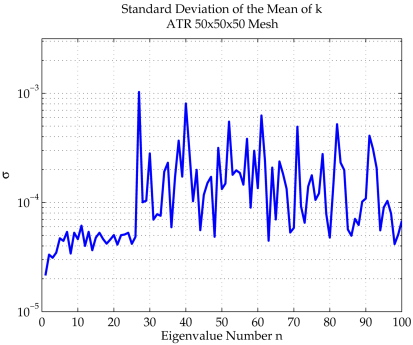
Mesh size	$\bar{k}_1$	$\sigma_{\bar{k}_1}$	$\bar{k}_2$	$\sigma_{\bar{k}_2}$
KCODE	0.995077	0.000023	N/A	N/A
$50 \times 50 \times 50$	0.995017	0.000021	0.900928	0.000033
$25 \times 25 \times 25$	0.995011	0.000021	0.898198	0.000033
$10 \times 10 \times 10$	0.994977	0.000021	0.879747	0.000036
$5 \times 5 \times 5$	0.994924	0.000021	0.831998	0.000042

As shown, fission matrices have comparable standard deviation to KCODE, but small matrices have difficulty beyond the fundamental mode.

Results

Statistics, By Eigenvalue Number

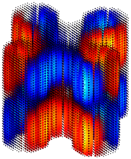
Statistics for first 100 eigenvalues were calculated for $50 \times 50 \times 50$ case.



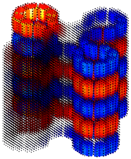
Why the spike at 27?

Results
3D Mode Plots

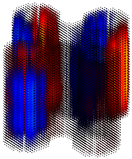
We plotted the modes to see what went wrong.



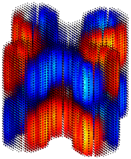
(m) Average - Mode 26



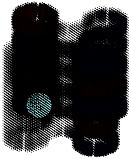
(n) Average - Mode 27



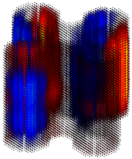
(o) Average - Mode 28



(p) Run 20 - Mode 26



(q) Run 20 - Mode 27



(r) Run 20 - Mode 28

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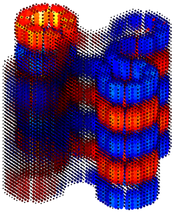
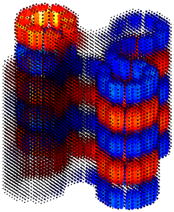
Turns out, run 20 had very large abnormalities. Removing the aberrant values:



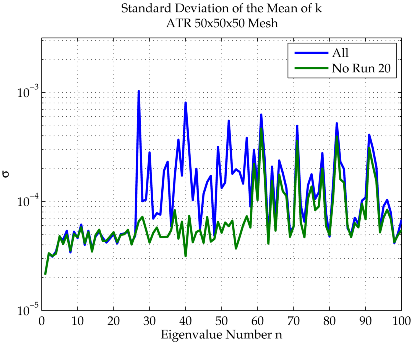
(s) Run 20 - Mode 27



(t) Average - Mode 27

The modes are now nearly identical.

Statistics recalculated with run 20 removed:



Spikes between 27 and 57 disappear, but those beyond persist.

Imaginary coefficients often appear in higher eigenvalues, but we suspect they are just a product of statistical variation.

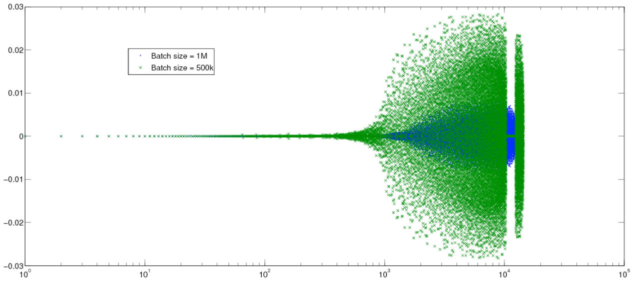


Figure: From F.B. Brown, S.E. Carney, B.C. Kiedrowski, W.R. Martin, LA-UR-13-20429.

Future Work

- Study the statistics of higher eigenpairs
- Study why complex eigenvalues sometimes show up
- Study other perturbations

Summary

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- New algorithms allow fission matrices to be solved quickly and with reasonable memory usage.
- It is easy to solve for small number of eigenmodes and generate transition coefficients.
- Quasistatic transition animations can be computed.
- Small, symmetric perturbations require fewer eigenmodes to reconstruct.
- Fission matrices have good statistical properties for the fundamental mode, but large matrices are needed beyond.

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Questions?