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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Los Alamos National Laboratory

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

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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

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

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Fission Matrices Transition Coefficients

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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:

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

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

$$\mathcal{C}_{ij} = \mathbf{s}_{i, \mathsf{original}} \cdot \mathbf{s}_{j, \mathsf{modified}}^{\dagger}$$

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

Fission Matrices Transitions

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

$$\mathbf{s}_{\mathsf{n}} pprox \sum_{j=1}^{m} C_{1,j} \left(rac{k_j}{k_1}
ight)^n \mathbf{s}_{j,\mathsf{modified}}$$

Assumes:

All modes have the same mean neutron generation time

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There are no delayed neutrons

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

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

| Storage type | Storage | |
|--------------|-------------|--|
| Full matrix | 8 TB | |
| Sparse | pprox 10 GB | |

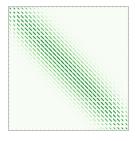


Figure: An Example Fission Matrix Sparsity Plot

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Fission Matrices Calculating Eigenpairs

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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 |
|-------------|---------------|-----------------|
| 3600×3600 | 3.09 s | 4878 s |
| 900×900 | 0.234 s | 353 s |
| 225×225 | 0.0337 s | 30.6 s |

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

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- Studied transitions
- Studied statistics

Methods Core Models - PWR

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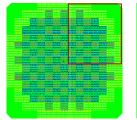
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Inserted SS304 control rods in 1/4 of the core



(a) PWR Full Core

(b) PWR Original

(c) PWR Modified

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Note the barely visible orange pins.

Methods Core Models - ATR

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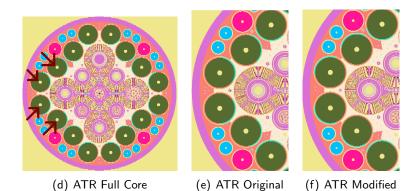
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Rotated 4 control drums out 50°



Rotated hafnium out, beryllium in.

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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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Results Eigenmodes - PWR

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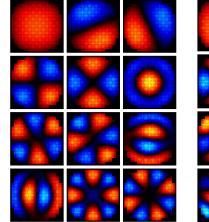
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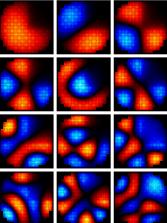
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Eigenmodes of PWR



(g) PWR Modes Initial



(h) PWR Modes Final

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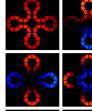
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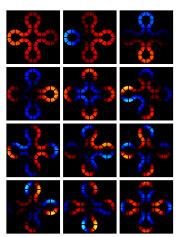








(i) ATR Modes Initial



(j) ATR Modes Final

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Results Verification of Eigenmodes

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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 = Aν_C - λ_Cν_C
 - Norm (*I*₂) consistently below *N**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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Results Transition Coefficients

Transition Coefficients



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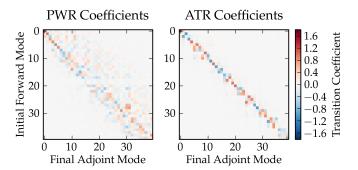
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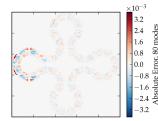
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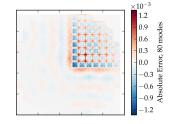
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Fundamental mode reconstruction error with 80 eigenmodes



(k) ATR $(I_2 = 0.0243)$



(I) PWR ($l_2 = 0.0423$)

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Results Reconstruction Error, Quantitative

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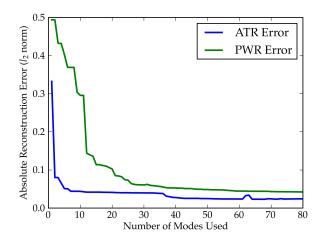
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Fundamental mode reconstruction error as a function of eigenmode count



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Results Optimality of Approximation

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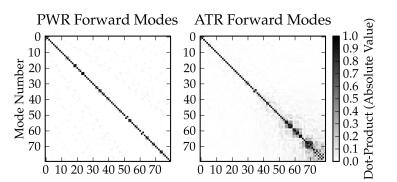
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Optimality of the series truncation closely related to orthogonality of eigenmodes



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Results Statistics, Fundamental and Secondary Modes

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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	imes 50	imes 50 | 0.995017 | 0.000021 | 0.900928 | 0.000033 |
| 25	imes25	imes25 | 0.995011 | 0.000021 | 0.898198 | 0.000033 |
| 10 	imes 10 	imes 10 | 0.994977 | 0.000021 | 0.879747 | 0.000036 |
| 5 	imes 5 	imes 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

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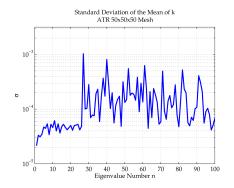
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Statistics for first 100 eigenvalues were calculated for 50 \times 50 \times 50 case.



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Why the spike at 27?

Results 3D Mode Plots

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We plotted the modes to see what went wrong.







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(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

Results 3D Mode Plots

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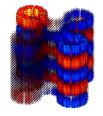
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Turns out, run 20 had very large abnormalities. Removing the aberrant values:



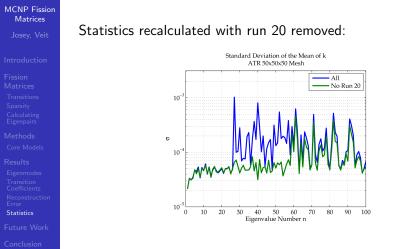
(s) Run 20 - Mode 27

(t) Average - Mode 27

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The modes are now nearly identical.

Results Statistics, By Eigenvalue Number



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

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Results Complex Eigenvalues

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

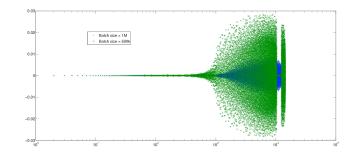


Figure: From F.B. Brown, S.E. Carney, B.C. Kiedrowski, W.R. Martin, LA-UR-13-20429.

Future Work

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

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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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