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Title: Higher-Mode Applications of Fission Matrix Capability for MCNP

Author(s): Carney, Sean E.
Brown, Forrest B.
Kiedrowski, Brian C.
Martin, William R.

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Higher-Mode Applications of Fission Matrix Capability for MCNP

Sean Carney, Forrest Brown,

Brian Kiedrowski, William Martin

Monte Carlo Codes Group, LANL

NERS Dept., University of Michigan

Nuclear Criticality Safety Program

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  - Preliminary theory
  - Past findings

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Carney, Brown, Kiedrowski, Martin, "Fission Matrix Capability for MCNP Monte Carlo", TANS 107, San Diego, 2012

Brown, Carney, Kiedrowski, Martin, "Fission Matrix Capability for MCNP, Part I - Theory", M&C-2013, 2013

Carney, Brown, Kiedrowski, Martin, "Fission Matrix Capability for MCNP, Part II - Applications", M&C-2013, 2013

Motivation

- **Problem: Direct & precise calculation of small changes from fine-tuning design with Monte Carlo is time-consuming:**
  - computationally (precise deltas from stochastic results)
  - man-power (search of design space)
- **Perturbation theory: search design space more efficiently, condense design calculations**
- **2nd order perturbation theory: extend applicability in design space**
  - Forward problems
    - Burnup
    - Control rod movement/interaction
    - BWR/Xenon power oscillations
  - Inverse problems
    - Detector response-guided calculations
  - Requires higher-mode flux information--both forward and adjoint

- **Additionally: further insight into power iteration with higher modes**

Preliminary Theory

Start with the k-eigenvalue form of the transport equation

$$\mathbf{M} \cdot \Psi_n(\vec{r}, E, \hat{\Omega}) = \frac{1}{K_n} \frac{\chi(\vec{r}, E)}{4\pi} S_n(\vec{r})$$

Infinite number of solutions: most recognized & physical is fundamental (*n=0*)

Net loss operator

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

Forward fission source, mode n

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

Theory

- Using,
  - Green's function
  - Integral transport equation
  - Discretization of space into *N* mesh cells

Eigenvalue problem (without approximation):

$$S_{n,I} = \frac{1}{K_n} \sum_{J=1}^{N} F_{I,J} \, S_{n,J}$$

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

Discrete fission source

$$S_{n,I} = \int_{\vec{r} \epsilon V_I} d\vec{r} \, S_n(\vec{r})$$

Fission matrix element

$$F_{I,J} = \int_{\vec{r} \epsilon V_I} d\vec{r} \int_{\vec{r}_0 \epsilon V_J} d\vec{r}_0 \, F(\vec{r}_0 \rightarrow \vec{r}) \frac{S_0(\vec{r}_0)}{S_{0,J}}$$

Energy & angle-integrated Green's function, "fission kernel"

$$F(\vec{r}_0 \rightarrow \vec{r}) = \iiiint dE d\hat{\Omega} dE_0 d\hat{\Omega}_0 \, \nu \Sigma_F(\vec{r}, E) G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega}) \frac{\chi(\vec{r}_0, E_0)}{4\pi}$$

Fission Matrix Error—Mesh Considerations

- **In the equation for F,**
  - $S(r_0)/S_J$ is a local weighting function within region J--unknown if unconverged
  - **As $V_J \rightarrow 0$:**
    - **Discretization errors → 0**
    - **Can accumulate tallies of $F_{I,J}$ even if not converged**
    - **Left eigenvectors correspond to adjoint fission source modes:**

$$S_n^\dagger(\vec{r}) = \int \int dE' d\hat{\Omega}' \frac{\chi(\vec{r}, E')}{4\pi} \Psi_n^\dagger(\vec{r}, E', \hat{\Omega}')$$

- **Higher-order modes require finer mesh for convergence (mode -0 local weighting function deviates from higher modes)**

Past Findings

Fission Matrix Calculations – Recent History

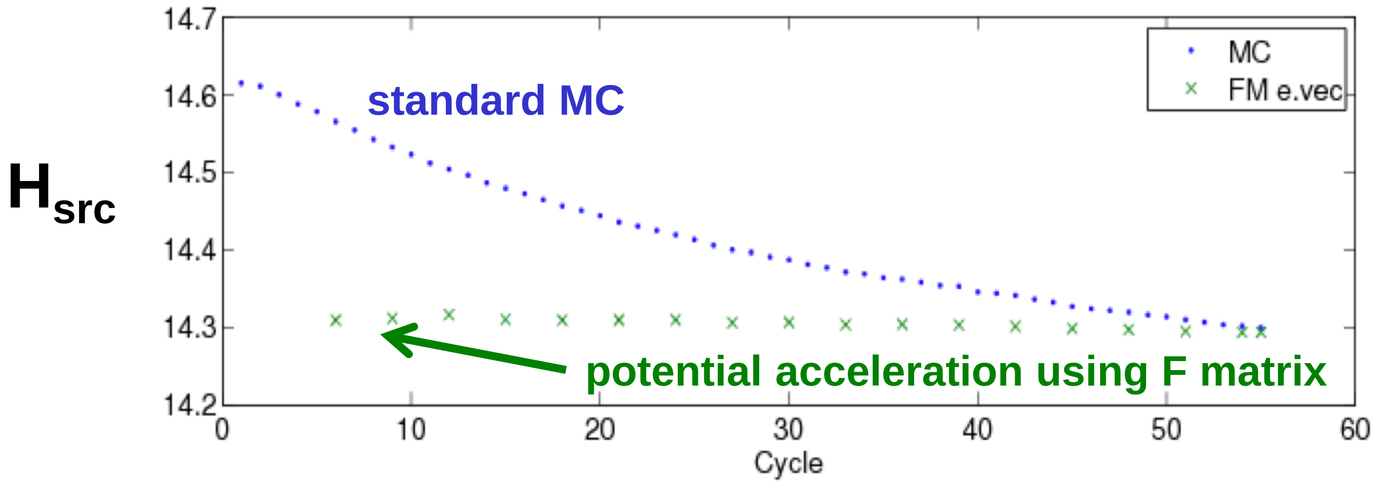
- $F_{I,J}$ **tallies:**
  - Previous F-matrix work: tally during neutron random walks
  - **Present F-matrix work:** **tally only point-to-point, using fission-bank in master proc (~free)**
  - Accumulate tallies over all cycles
    - skip first ~2 to reduce discretization error
- **Sparse storage—coupling between mesh cells is localized**
  - Compressed row storage
  - Very fine mesh—initially allocate some max number of elements
- **Solve eigenvalue problem**
  - Aggregate elements during post-processing
  - Sparse-solvers: Hotelling Deflation (this work), Arnoldi (much faster)

Convergence Acceleration Using Fission Matrix

- **Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles**
- **Duplicate/remove sites in fission bank to match F matrix fund. mode**
- **Impressive convergence improvement**

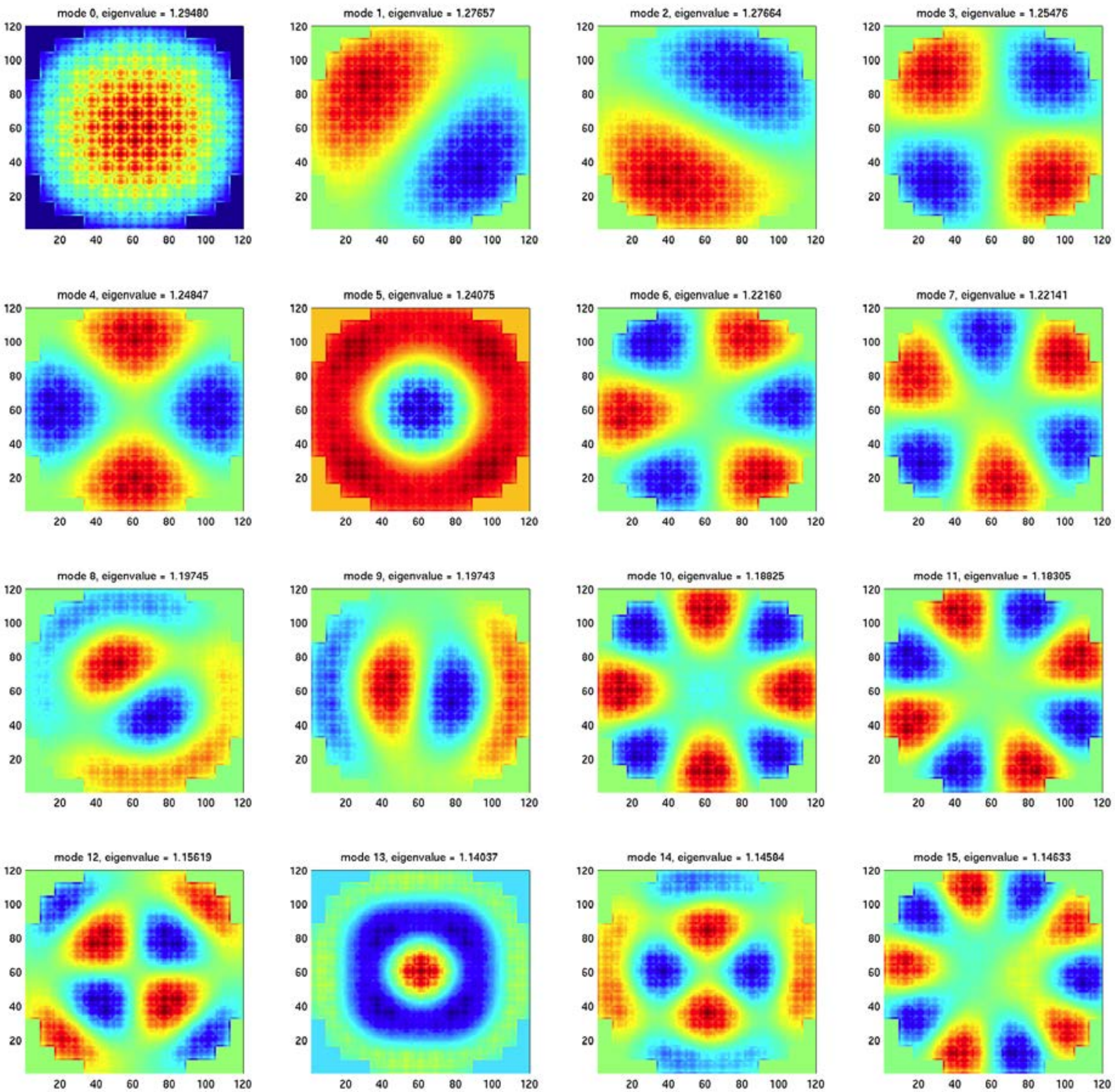
Kord Smith Challenge
(3D Whole-Core)

42x42x20 spatial mesh
1 M neutrons/cycle, Tallied for cycles 4-55



PWR – Eigenmodes for 120x120x1 Spatial Mesh

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



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

Eigenmode Expansion

Expansion of Fission Source Distribution into Eigenmodes

- Source convergence in Monte Carlo criticality calculations involves "powering out" the higher modes excited from the initial distribution

- Using pre-calculated forward/adjoint source modes, and biorthogonality, the cycle-by-cycle contributions of these modes can be estimated

Expansion of cycle-*c* source into $\hat{N}$ modes

$$F^c(\vec{r}) = \sum_{n=0}^{\hat{N}} a_n^c S_n(\vec{r})$$

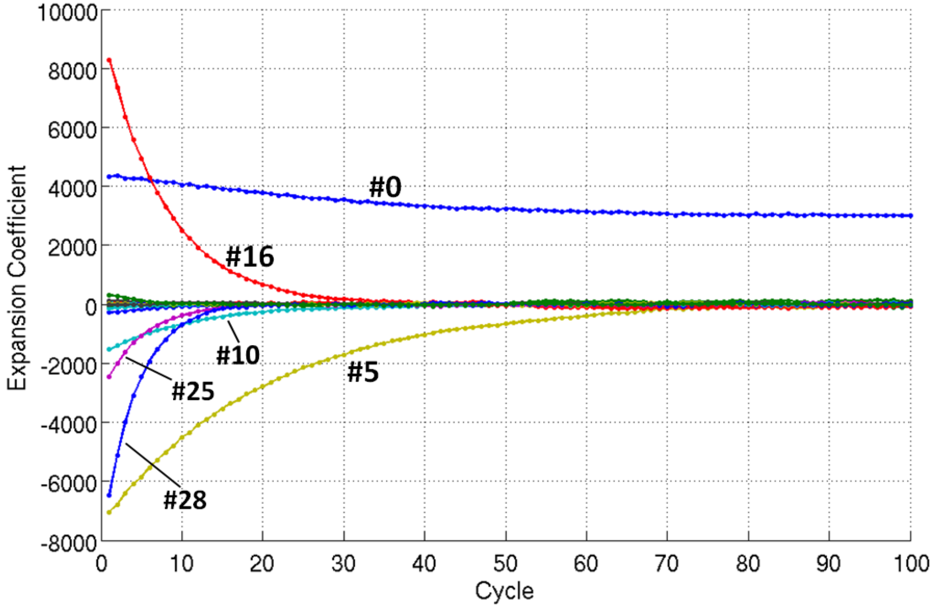
Magnitude of the expansion coefficients (found using inter-cycle fission sites)

$$a_n^c = \frac{\langle F^c(\vec{r}) S_n^\dagger(\vec{r}) \rangle}{\langle S_n(\vec{r}) S_n^\dagger(\vec{r}) \rangle}$$

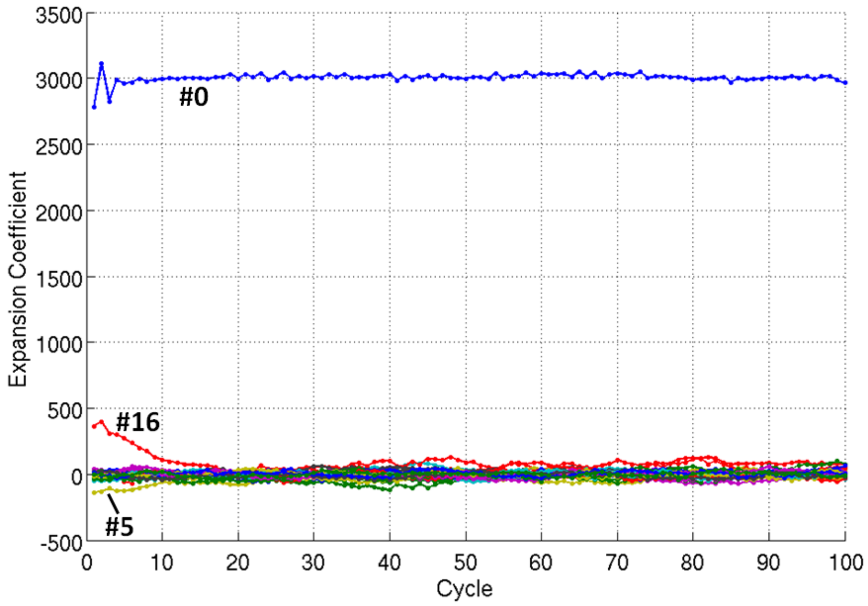
- Three initial guesses ran for 2D PWR problem:
  - center point
  - corner point
  - flat distribution
- Source modes calculated with: 300 cycles, 500k batch size, 50x50x1 mesh

Center-Point & Flat Guesses

Center point guess
100k batch size, 100 cycles

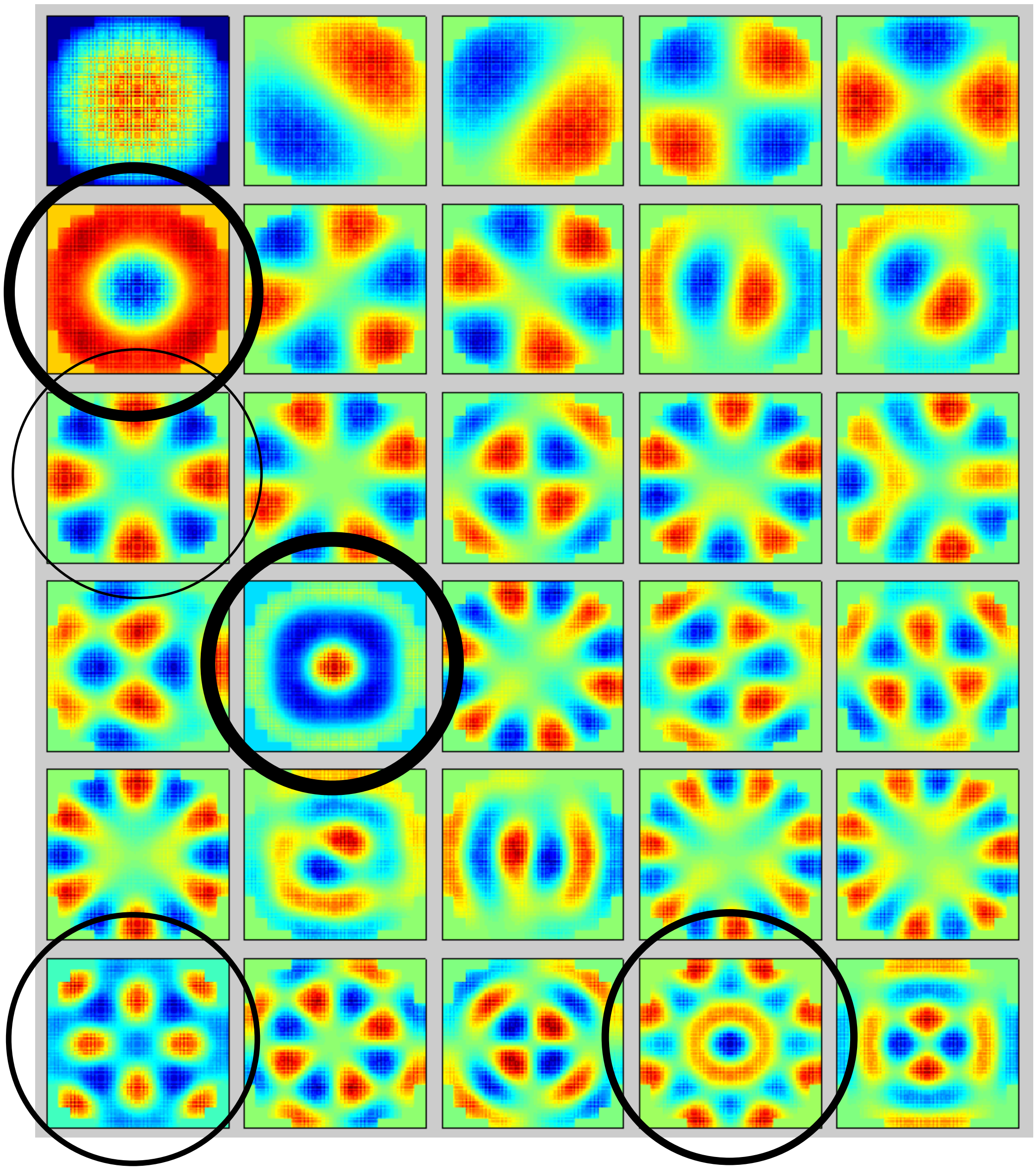


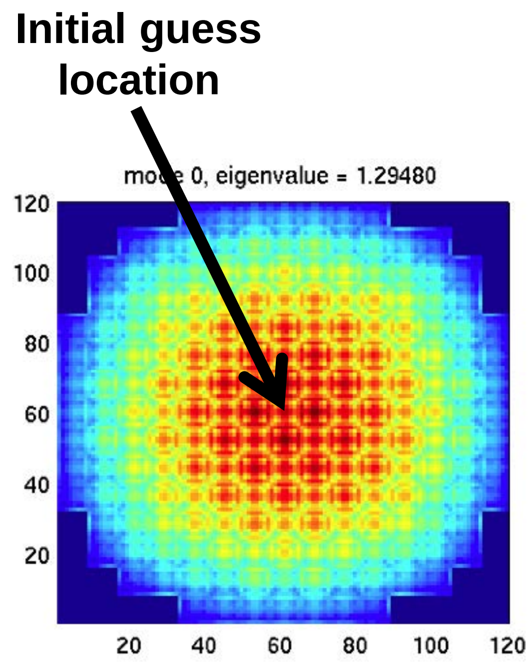
Flat guess
500k batch size, 100 cycles



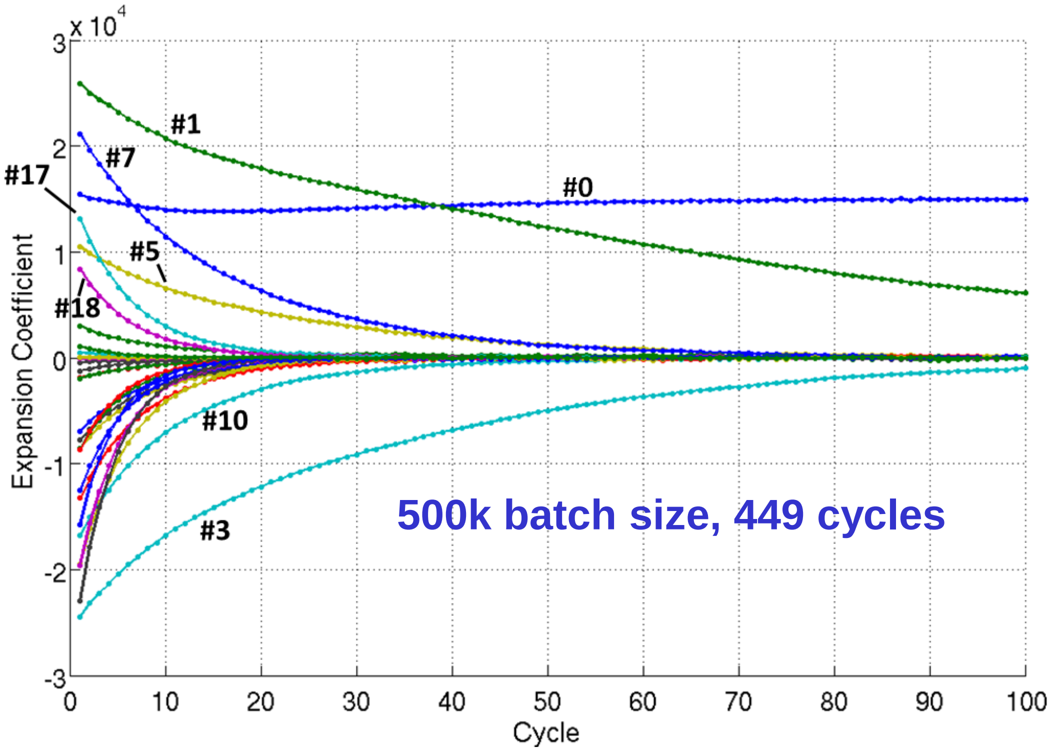
Radially-symmetric modes excited in both cases—more so for center-point

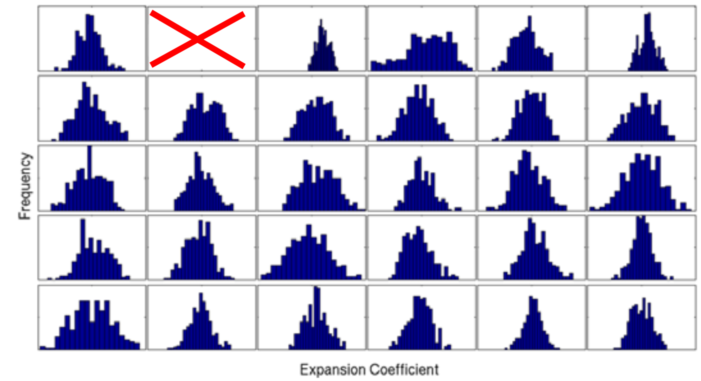
PWR – First 30 Eigenmodes



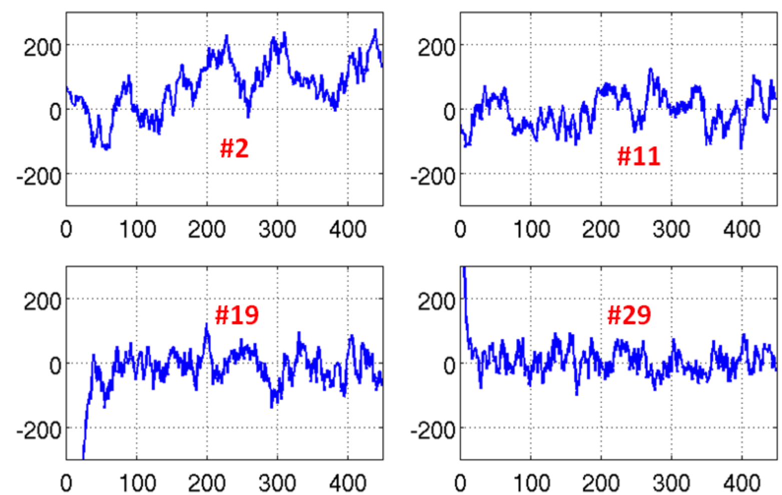


Corner-Point Guess





Converged coefficients are near-normal



Lag-correlation of modes is a function of K_n/K_0

Mode #	Cycle range for fit	Empirical decay rate	K_n/K_0
1	1-150	0.98609	0.98530
3	1-100	0.96945	0.96756
5	1-50	0.95810	0.95619
7	1-50	0.94412	0.94058
8	1-15	0.90134	0.92119
9	1-20	0.89848	0.92118
10	1-45	0.92062	0.91388

Decay rates can be predicted by eigenvalue

PWR – First 30 Eigenmodes

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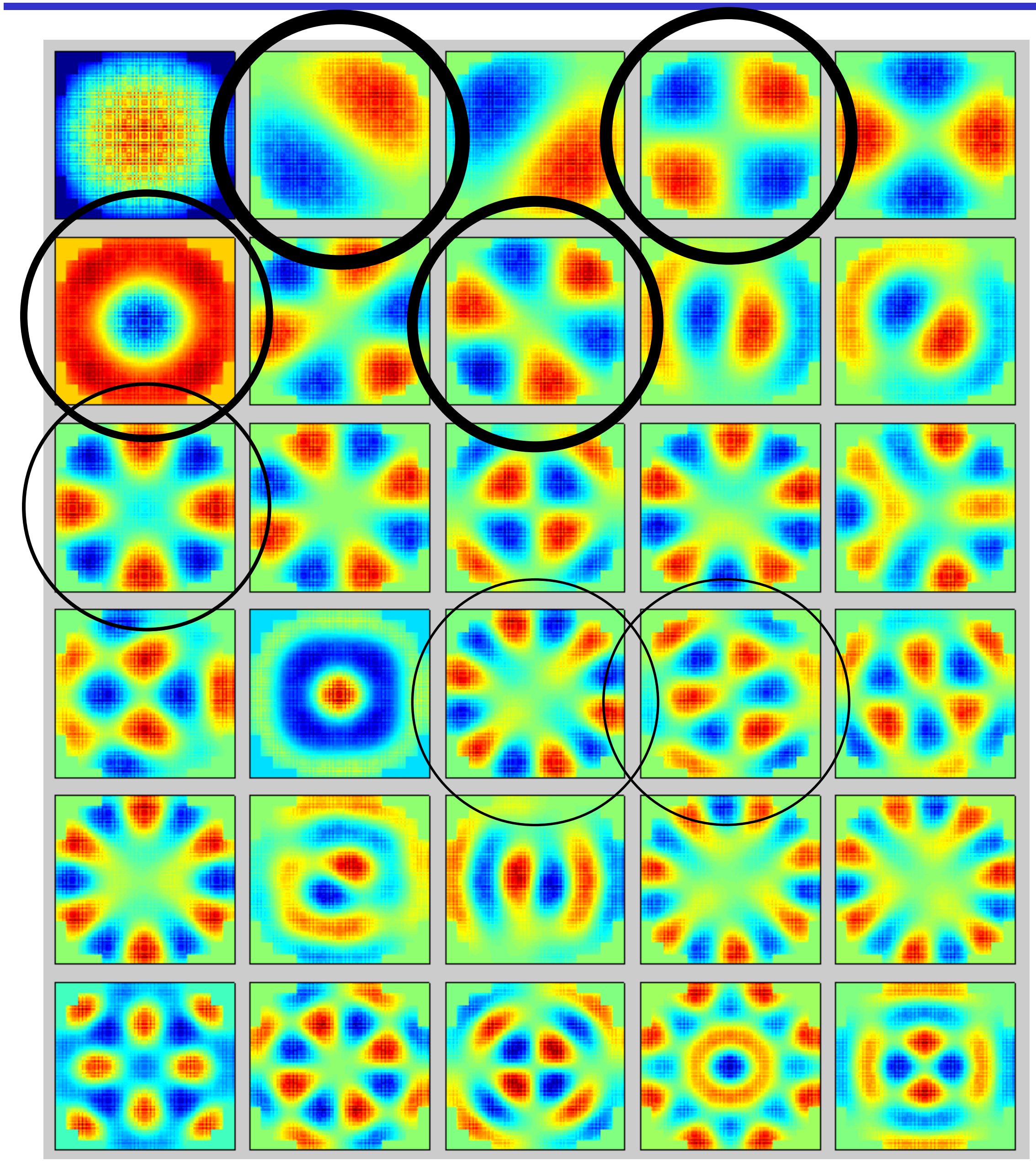
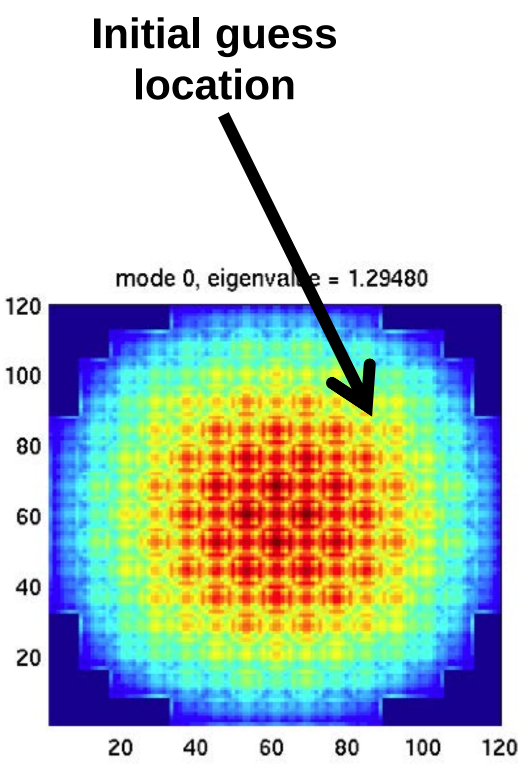




Forward Flux Modes

Calculation of Forward Flux Modes

- **Forward flux modes are calculated by running fixed source calculations on forward fission source modes**

$$\Psi_n(\vec{r}, E, \hat{\Omega}) = \frac{1}{K_n} \mathbf{M}^{-1} \cdot \frac{\chi(\vec{r}, E)}{4\pi} S_n(\vec{r}) \qquad n = 0, 1, \ldots, \hat{N}$$

- **Source is sampled in an analog manner**
  - Alias table used for efficiency
  - Point within mesh cell is resampled until within fissionable material
  - Flag is added for sign of particle weight
  - Fission is treated as absorption (`NONU` card)

- **Track-length flux mesh tally module FMESH used**

- **Possible efficiency gain: Sample source uniformly, keep vector of weights for different mode values**

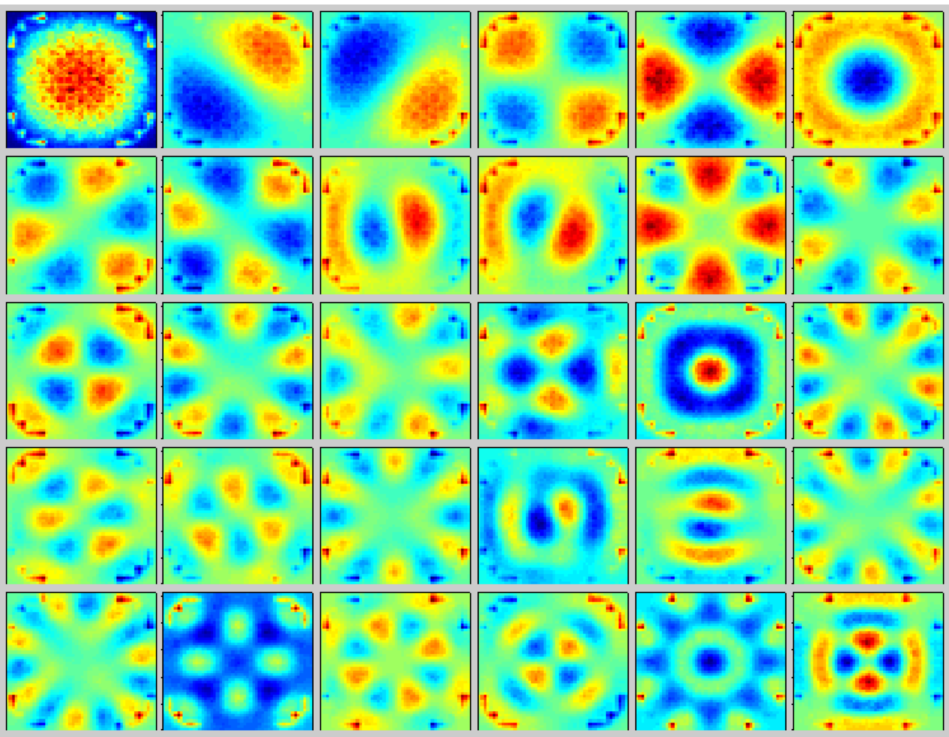
Forward Flux Modes for 2D PWR problem

Source modes acquired with matrix tallied for 500 cycles, 500k batch size

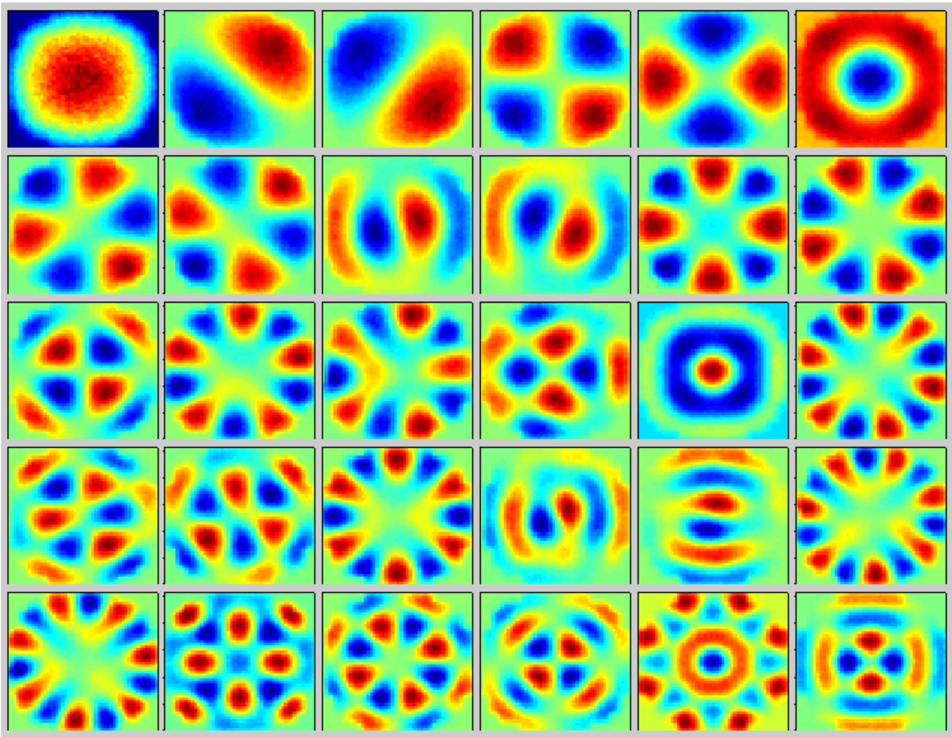
Fixed source calculations performed with 500k histories

50x50x1 mesh

$$\int_{\vec{r}\epsilon V_i} d\vec{r} \int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\hat{\Omega}\, \Psi_n(\vec{r}, E, \hat{\Omega})$$



Thermal flux modes (0 - 0.625 eV)



Above-thermal flux modes (0.625 eV - 20 MeV)

Relative Uncertainty of Forward Flux Modes for 2D PWR problem

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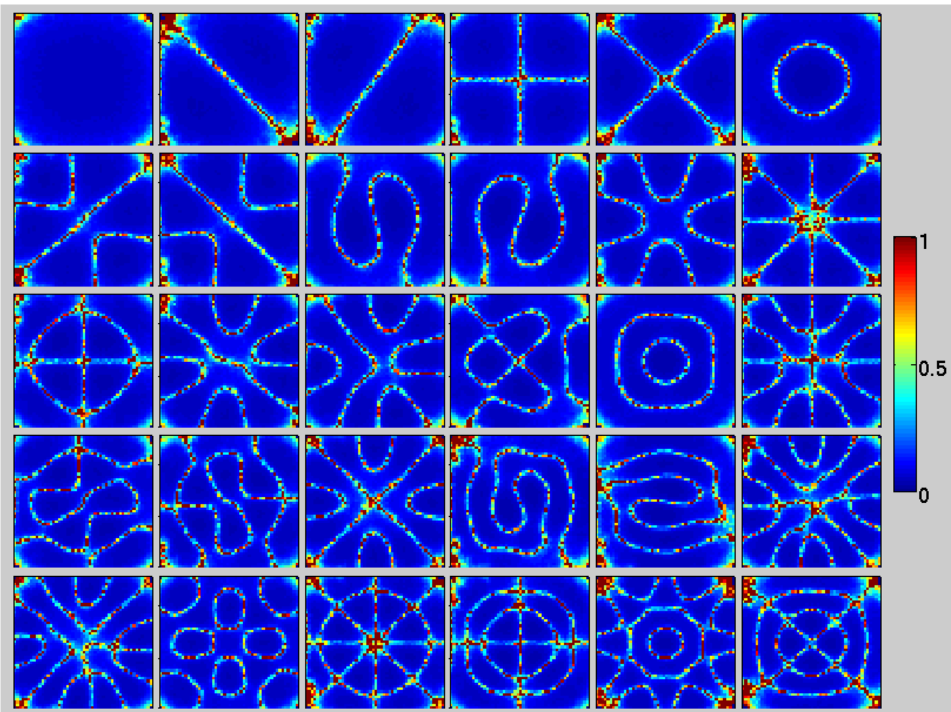
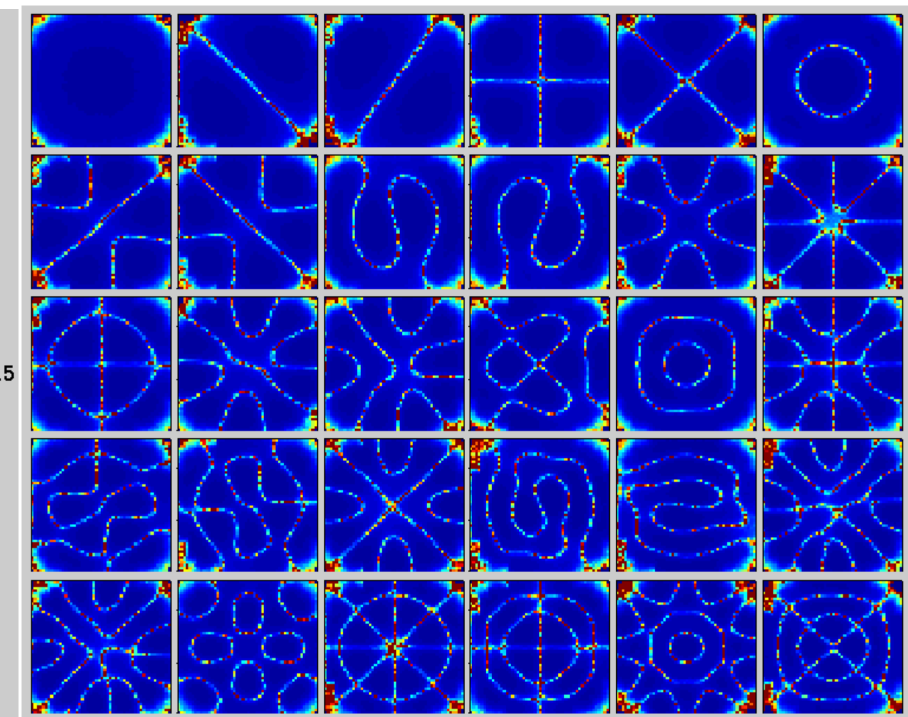
Relative uncertainty of thermal flux modes (0 - 0.625 eV)



Relative uncertainty of above-thermal flux modes (0.625 eV - 20 MeV)



High relative uncertainties are strongly localized to inflection lines

Fission Kernel Deflation

Motivation

- **Desired applications of modal information:**
  - 2nd order perturbation theory (capture effect of flux pert. on eigenvalue)
  - Quasi-static calculations (model BWR instabilities, Xenon oscillations)
- **These methods require weighting with higher-mode adjoint fluxes**
- **Continuous-energy Monte Carlo adjoint transport is intractable**

- **Mode-0 adjoint-weighted tallies are performed in MCNP using iterated fission probability (weigh by size of long-time fission chain):**
  - In original generation, tallies are associated with a progenitor neutron
  - After *L* latent generations, the progeny of progenitors are followed for enough cycles to reach their asymptotic distribution (the fundamental mode)
  - In asymptotic generation, the progeny population is used for weighting of original tallies

$$\Psi^{\dagger}(\vec{r}_0, E_0, \hat{\Omega}_0) \ \alpha \ \langle F(\vec{r}\,' \rightarrow \vec{r})^L \cdot \iint dE' d\hat{\Omega}' G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}\,', E', \hat{\Omega}') \nu \Sigma_F(\vec{r}\,', E') \rangle_{\vec{r}}$$

- **Aside: With higher modes, the number of necessary latent generations can be quantified (as a function of space)**

Higher Mode Adjoint-Weighting

- **Standard matrix deflation eliminates the effect of eigenvectors**

Hotelling deflation (used in calculation of eigenvectors)

$$F_n = F - \sum_{n'=0}^{n-1} K_{n'} \frac{S_{n'} S_{n'}^{\dagger}}{\langle S_{n'}^{\dagger}, S_{n'} \rangle}$$

$$F_n S_{n'<n} = 0, \quad F_n S_n = K_n S_n$$

- **Analogous deflation in continuous phase space:**

$$F_n(\vec{r_0} \to \vec{r}) =$$
$$= \iiiint dE d\hat{\Omega} dE_0 d\hat{\Omega}_0 \nu \Sigma_F(\vec{r}, E) \Big(G(\vec{r}_0, E_0, \hat{\Omega}_0 \to \vec{r}, E, \hat{\Omega}) - \sum_{n'=0}^{n-1} K_{n'} \frac{\Psi_{n'}(\vec{r}, E, \hat{\Omega}) \Psi_{n'}^{\dagger}(\vec{r}_0, E_0, \hat{\Omega}_0)}{\langle S_{n'}^{\dagger}(\vec{r'}) S_{n'}(\vec{r'}) \rangle} \Big) \frac{\chi(\vec{r}_0, E_0)}{4\pi}$$

- **Supposition…**
  - Mode-0 adjoint weighting looks at neutron population after iterative application of the regular kernel
  - Can higher mode adjoint weighting be performed with iterative application of the deflated kernel?

Aside: Relationship Between Green's Function and Flux Modes

K-eigenvalue transport:

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

Expand (approximation):

$$\Psi(\vec{r}, E, \hat{\Omega}) = \sum_{n=0}^{\infty} c_n \Psi_n(\vec{r}, E, \hat{\Omega}) \quad , \quad S(\vec{r}) = \sum_{n=0}^{\infty} s_n S_n(\vec{r})$$

Find coefficients using biorthogonality & transport eq.:

$$s_n = \frac{\langle \Psi_n^{\dagger}(\vec{r}, E, \hat{\Omega}), \frac{\chi(\vec{r},E)}{4\pi} S(\vec{r}) \rangle}{\langle \Psi_n^{\dagger}(\vec{r}, E, \hat{\Omega}), \frac{\chi(\vec{r},E)}{4\pi} S_n(\vec{r}) \rangle} \quad , \quad c_n = \frac{K_n}{K_0} s_n$$

Insert into flux expansion:

$$\Psi(\vec{r}, E, \hat{\Omega}) = \frac{1}{K_0} \sum_{n=0}^{\infty} K_n \frac{\langle \Psi_n^{\dagger}(\vec{r}, E, \hat{\Omega}), \frac{\chi(\vec{r},E)}{4\pi} S(\vec{r}) \rangle}{\langle \Psi_n^{\dagger}(\vec{r}, E, \hat{\Omega}), \frac{\chi(\vec{r},E)}{4\pi} S_n(\vec{r}) \rangle} \Psi_n(\vec{r}, E, \hat{\Omega})$$

Recall the integral transport eq:

$$\Psi(\vec{r}, E, \hat{\Omega}) = \frac{1}{K_0} \iiint d\vec{r}_0 dE_0 d\hat{\Omega} \frac{\chi(\vec{r}_0, E_0)}{4\pi} S(\vec{r}_0) G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega})$$

Indicates Green's function expansion:

$$G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega}) = \sum_{n=0}^{\infty} K_n \frac{\Psi_n(\vec{r}, E, \hat{\Omega}) \Psi_n^{\dagger}(\vec{r}_0, E, \hat{\Omega})}{\langle S_n^{\dagger}(\vec{r}\,'), S_n(\vec{r}\,') \rangle}$$

Kernel Deflation--Implementation

- **Normal deflation alters a matrix--our 'matrix' is the random walk**
- **Approximate deflated kernel by separating its application on a source into,**
  - Normal random walk
  - Matrix multiplication of outer product

$$F_n(\vec{r_0} \rightarrow \vec{r}) \cdot S^c(\vec{r_0}) = F_0(\vec{r_0} \rightarrow \vec{r}) S^c(\vec{r_0}) - \sum_{n'=0}^{n-1} K_{n'} \frac{\langle S^\dagger_{n'}(\vec{r_0}) S^c(\vec{r_0}) \rangle}{\langle S^\dagger_{n'}(\vec{r'}) S_{n'}(\vec{r'}) \rangle} S_{n'}(\vec{r})$$

Deflated fission kernel applied to fission bank

Standard transport

Normalized inner-products of adjoint source modes & fission bank

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Deflated fission kernel applied to fission bank

Standard transport

Normalized inner-products of adjoint source modes & fission bank

- **To apply deflated fission kernel *F_n* to fission bank,**
  - Precompute forward/adjoint fission sources & eigenvalues with fission matrix
  - Start problem again with adjoint weighting on; before each cycle…
    - Bin fission bank into same spatial mesh as eigenvectors
    - Compute *n-1* inner products and save for after next cycle
    - Run cycle--perform normal transport on fission bank
    - Bin new fission bank and subtract scaled forward fission source modes
    - Duplicate/delete sites in fission bank to replicate new vector
  - Aside: A vector of weights could be used to represent all modes desired

Test of Kernel Deflation

Tested kernel deflation with a 3-group (not self-adjoint), 40 cm slab problem

Vacuum boundary conditions

g	Σ_t	Σ_f	Σ_γ	χ	$\Sigma_{s,g'1}$	$\Sigma_{s,g'2}$	$\Sigma_{s,g'3}$	$\bar{\nu}$
1	0.7	0	0.05	1	0.45	0.2	0	0
2	1.2	0	0.05	0	0	0.55	0.6	0
3	1.2	0.05	0.05	0	0	0	1.1	2.17

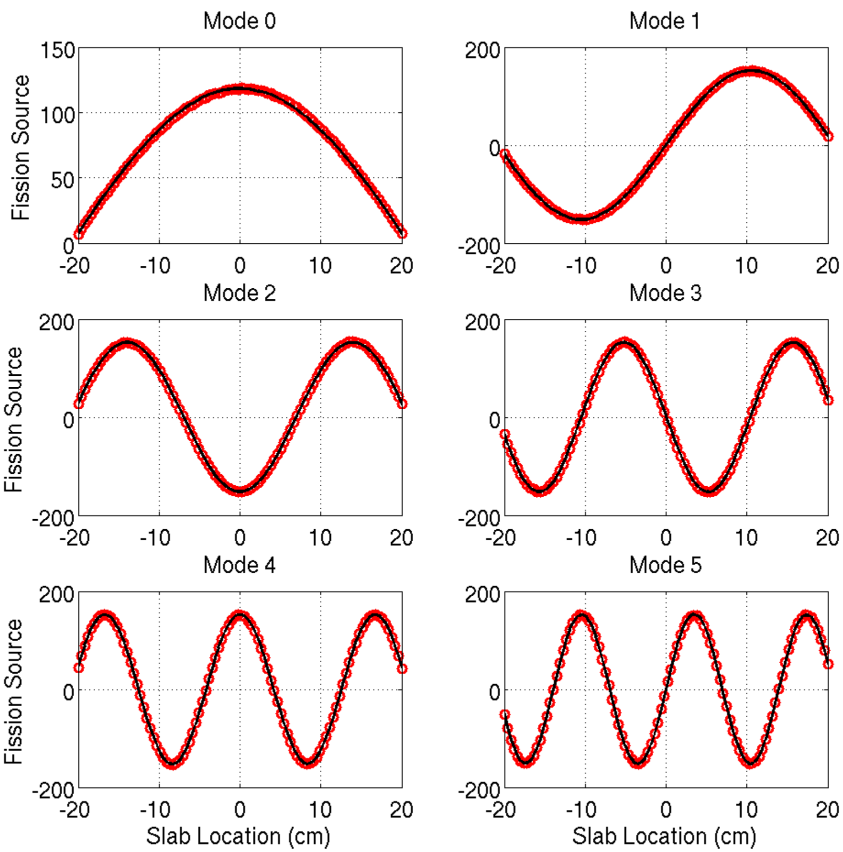
- **1000 cycles ran, 10k batch size**
- **initial guess: flat distribution**

Not shown: Verification with 1-group problem

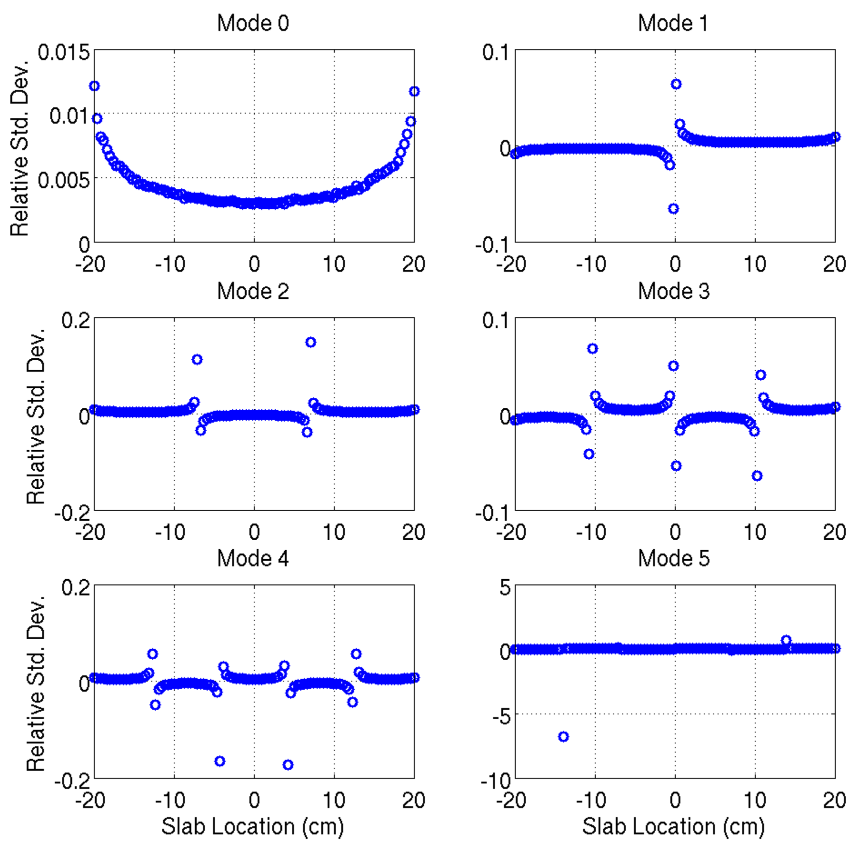
Deflation Results

Ran 1000 cycles, 10k batch size, flat distribution as initial guess
Statistics found from cycles 100-1000, wherein modes 0-5 were converged

Mean fission bank distribution
& fission matrix right-eigenvectors



Relative Standard Deviation
of Mean Fission Bank Distribution



Deflated fission banks stably oscillate about the true fission source mode

Adjoint Flux Weighting

Adjoint Flux Weighting

- **Higher-mode adjoint weighting uses iterated fission probability, but with repeated application of deflated fission kernel**
  - 0^{th} mode—weigh tallies by fission rates of progeny in asymptotic generation
  - Higher modes—weigh by total population of progeny in asymptotic generation

- **Verification--tally adjoint-weighted flux (compare with Matlab S_N code):**

$$\int_{\vec{r}\epsilon V_i} d\vec{r} \int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\hat{\Omega}\; \Psi_n^\dagger(\vec{r}, E, \hat{\Omega}) \Psi_n(\vec{r}, E, \hat{\Omega})$$

- **Positive/negative tally considerations:**
  - Weighting factors in asymptotic generation are always positive
  - Flux tallies in original generation vary with sign
  - Absolute value of adjoint-weighted flux tallies at end-of-run are taken—assumes adjoint and forward flux are of same sign for given location in space

- **Note: for perturbation & quasi-static calculations, want to compute:**

$$\int_{\vec{r}} d\vec{r} \int_0^\infty dE \int_{4\pi} d\hat{\Omega}\; \Psi_n^\dagger(\vec{r}, E, \hat{\Omega}) \mathbf{A} \Psi_m(\vec{r}, E, \hat{\Omega})$$

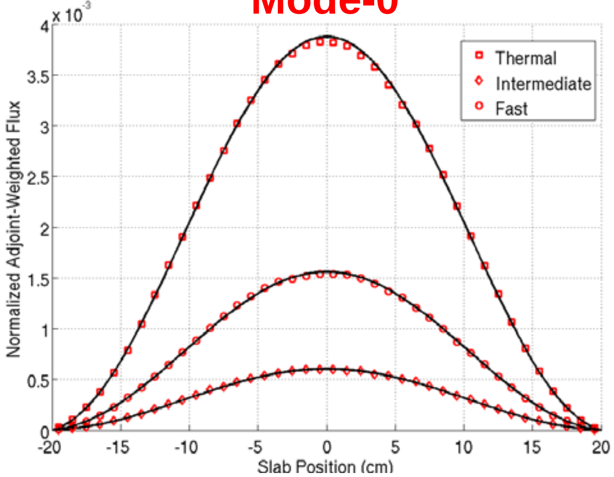
***A* is any operator**

Adjoint Flux Weighting Results

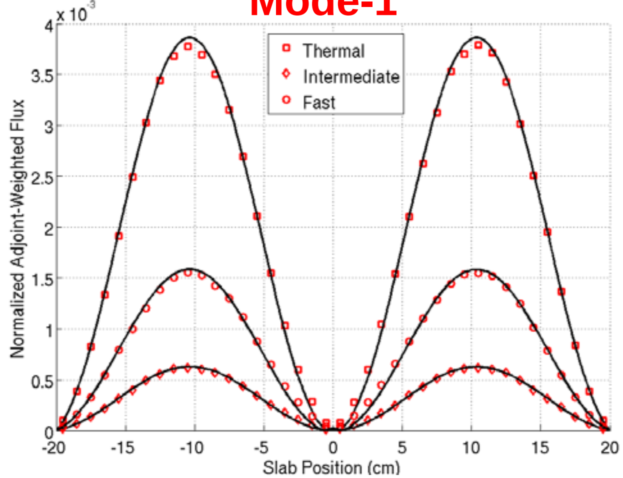
Ran 3015 cycles, 50k batch size, 20 latent generations
Use relevant fission matrix source mode as initial guess
Plot Monte Carlo & S_{16} adjoint-weighted flux

$$\int_{\vec{r}\epsilon V_i} d\vec{r} \int_{E_g}^{E_{g-1}} dE \int_{4\pi} d\hat{\Omega}\; \Psi_n^\dagger(\vec{r},E,\hat{\Omega})\Psi_n(\vec{r},E,\hat{\Omega})$$

Mode-0

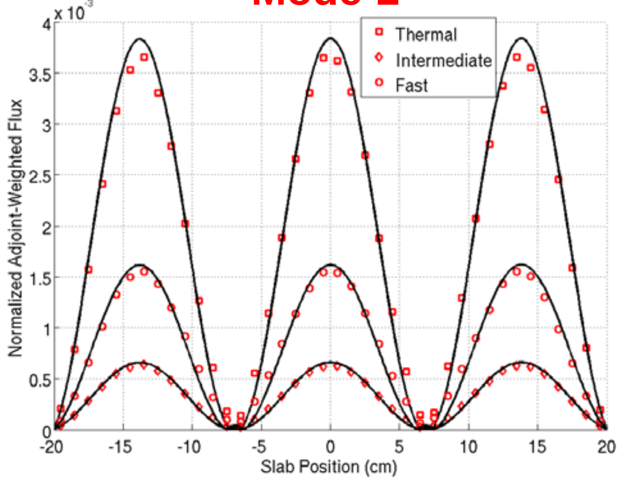


Mode-1

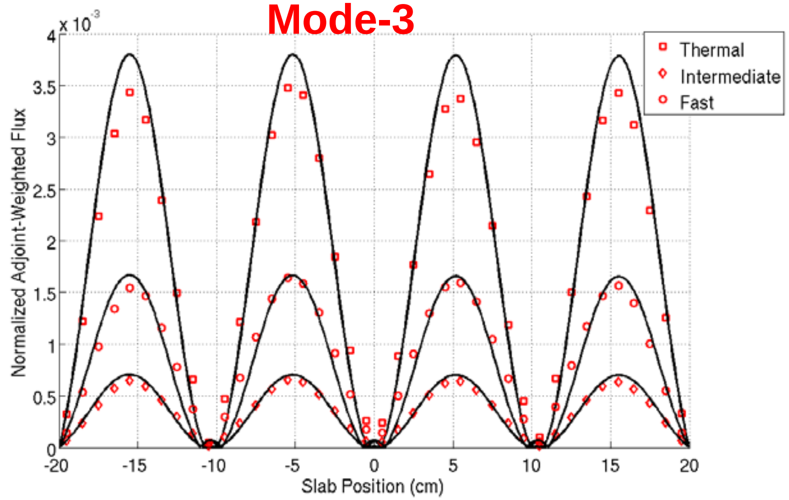


- **Increasing bias for higher mode number (std. dev. is minor)**
- **Overestimation near inflection points**
- **Less analog treatment may be needed**

Mode-2



Mode-3



Conclusions & Future Work

- **Conclusions**
  - Fission matrix source modes can give insight into power iteration
  - Running fixed source calculations on source modes give statistically-tractable tallies of forward flux modes
  - Fission kernel deflation on a 3-group slab problem is stable, and gives correct estimates of forward source modes
  - Higher-mode adjoint-weighting gives reasonable estimates for the 3-group slab problem
- **Future Work**
  - Investigate bias seen in higher-mode adjoint-weighting, improve method
  - Do higher-mode adjoint weighting on harder problems (asymmetric, multi-D, continuous energy)
  - 2^{nd} order perturbation theory & quasi-static methods
  - Investigate sensitivity of higher source modes to meshing and statistics

Questions?