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# Fission Matrix Capability for MCNP

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- Introduction
- Theoretical Basis of the Fission Matrix
- Examples – Higher Eigenmodes
- Conclusions & Future work

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

# Introduction – Who Cares?

- **Knowledge of fundamental & all higher modes**
  - "Crown Jewels" of analysis – explains everything
- **Reactor theory & mathematical foundations**
  - Existence of higher modes
  - Eigenvalue spectrum – discrete ? real ?
  - Forward & adjoint modes, orthogonality
- **Fundamental reactor physics & crit-safety analysis**
  - **Higher-mode eigenvalues & eigenfunctions**
  - Stability analysis of Xenon & void oscillations
  - High-order perturbation theory
  - **Startup, probability of initiation**
  - **Subcritical multiplication problems**
- **Source convergence testing & acceleration**
  - **May provide robust, reliable, automated convergence test**
  - **Acceleration of source convergence**

# Forward & Adjoint Fission Matrix Equations

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- **Obtain integral equations for fission source from k-effective form of exact continuous-energy transport equation, forward & adjoint**
- **Segment the physical problem into N disjoint spatial regions**
- **Integrate the forward & adjoint integral fission source equations over $r_0$ & r**

**Initial: $r_0 \in V_J$, Final: $r \in V_I$ H = Green's function**

**Forward**

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

$$S_J = \int_{\vec{r}'\in V_J} S(\vec{r}')d\vec{r}'$$

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

**Adjoint**

$$F^{\dagger}_{I,J} = \int_{\vec{r}\in V_I} d\vec{r} \int_{\vec{r}_0\in V_J} d\vec{r}_0 \frac{S^{\dagger}(\vec{r}_0)}{S^{\dagger}_J} \cdot H(\vec{r} \to \vec{r}_0)$$

$$S^{\dagger}_J = \int_{\vec{r}'\in V_J} S^{\dagger}(\vec{r}')d\vec{r}'$$

$$S^{\dagger}_I = \frac{1}{K} \cdot \sum_{J=1}^{N} F^{\dagger}_{I,J} \cdot S^{\dagger}_J$$

**<u>Exact</u> equations for integral source $S_I$ & $S^{\dagger}_I$**

**N = # spatial regions, F = N x N matrix, <u>nonsymmetric</u>**

# Forward & Adjoint Fission Matrix - Comments

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

- Compare $F_{I,J}$ & $F^{\dagger}_{J,I}$, interchange integration order for $F^{\dagger}_{J,I}$

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

$$F^{\dagger}_{J,I} = \int_{\vec{r}_0 \in V_J} d\vec{r}_0 \int_{\vec{r} \in V_I} d\vec{r} \cdot \frac{S^{\dagger}(\vec{r})}{S^{\dagger}_I} \cdot H(\vec{r}_0 \to \vec{r})$$

Same form, but different spatial weighting functions

- If the spatial discretization is fine enough that

$$\frac{S(\vec{r}_0)}{S_J / V_J} \approx 1 \quad \text{for } \vec{r}_0 \in V_J \qquad \text{and} \qquad \frac{S^{\dagger}(\vec{r})}{S^{\dagger}_I / V_I} \approx 1 \quad \text{for } \vec{r} \in V_I$$

then

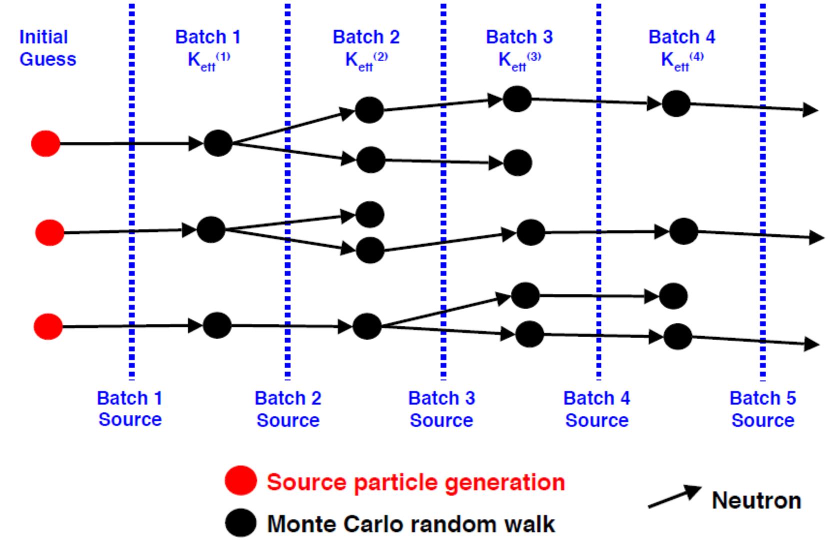
- Can neglect spatial weights, discretization errors ~ 0
- Can accumulate tallies of $F_{I,J}$ even if not converged
- For fine spatial mesh, $F^{\dagger}$ = transpose of F

$$\bar{\bar{F}}^{\dagger} = \bar{\bar{F}}^{T}$$

# Monte Carlo Estimation of Fission Matrix

## Monte Carlo K-effective Calculation

1. Start with fission source & k-eff guess
2. Repeat until converged:
   - Simulate neutrons in cycle
   - Save fission sites for next cycle
   - Calculate k-eff, renormalize source
3. Continue iterating & tally results




## For Fission Matrix calculation

During standard k-eff calculation, at the end of each cycle:

- Estimate $F_{I,J}$ tallies from start & end points in fission bank ( ~ free )
- Accumulate $F_{I,J}$ tallies, over all cycles (even inactive cycles)

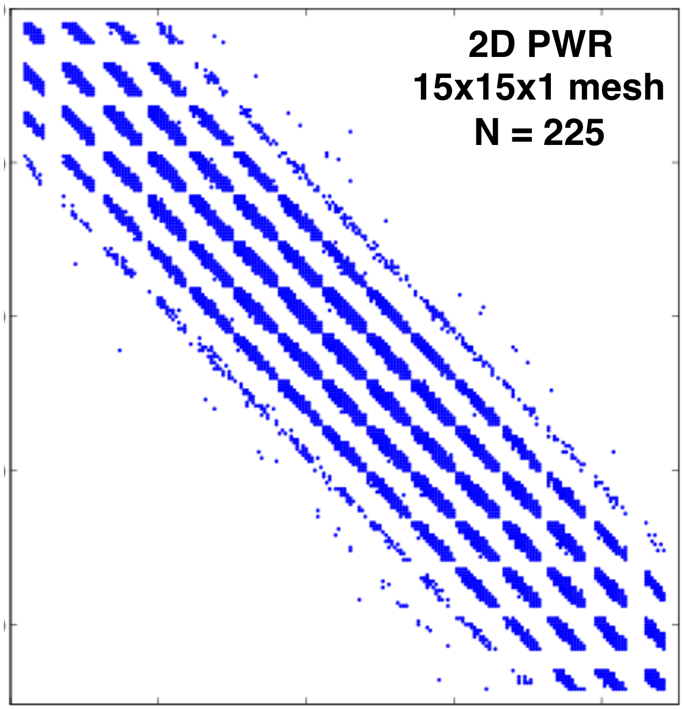
After Monte Carlo completed:

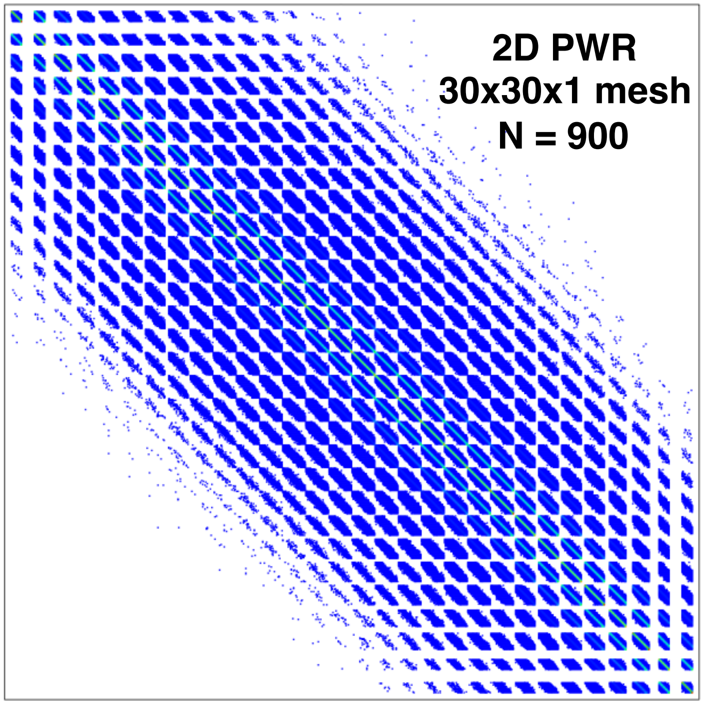
- Normalize $F_{I,J}$ accumulators, divide by total sources in J regions
- Find eigenvalues/vectors of F matrix (power iteration, with deflation)

# 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

- **Compressed row storage scheme**
  - Don't store near-zero elements, general sparsity
  - Reduced F matrix storage, no approximation
  - Can easily do 100x100x100 mesh on 8 GB Mac

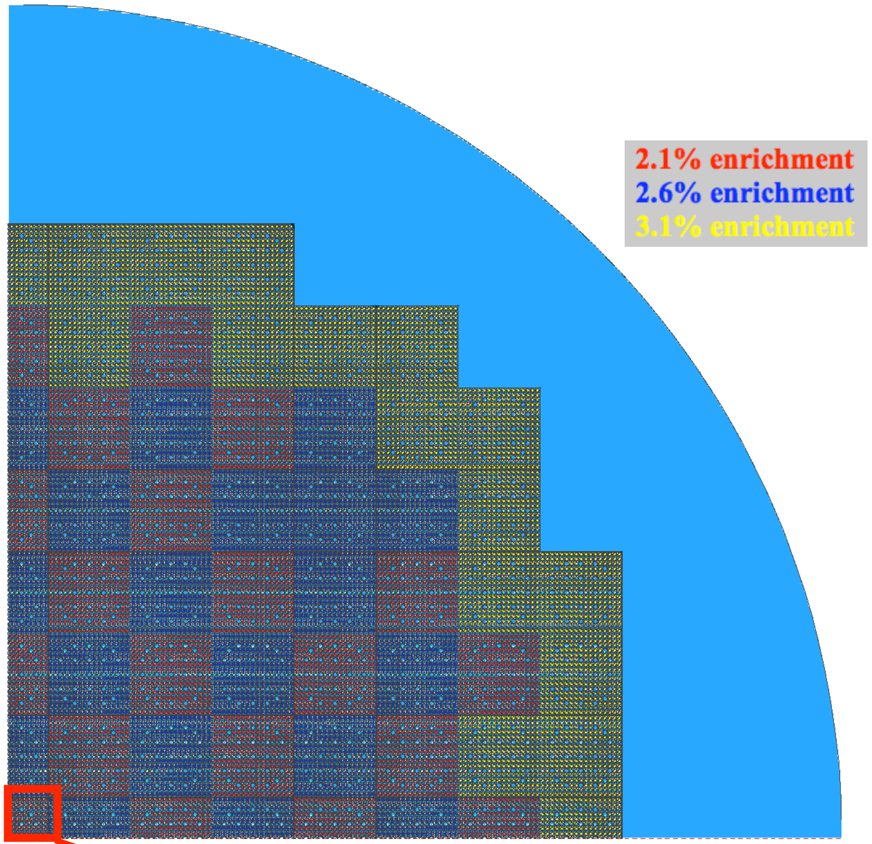


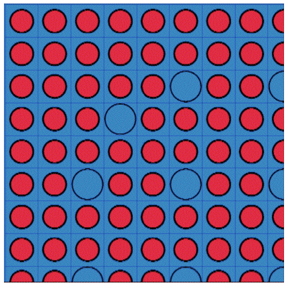



# Whole-core 2D PWR Model

## 2D PWR (Nakagawa & Mori model)

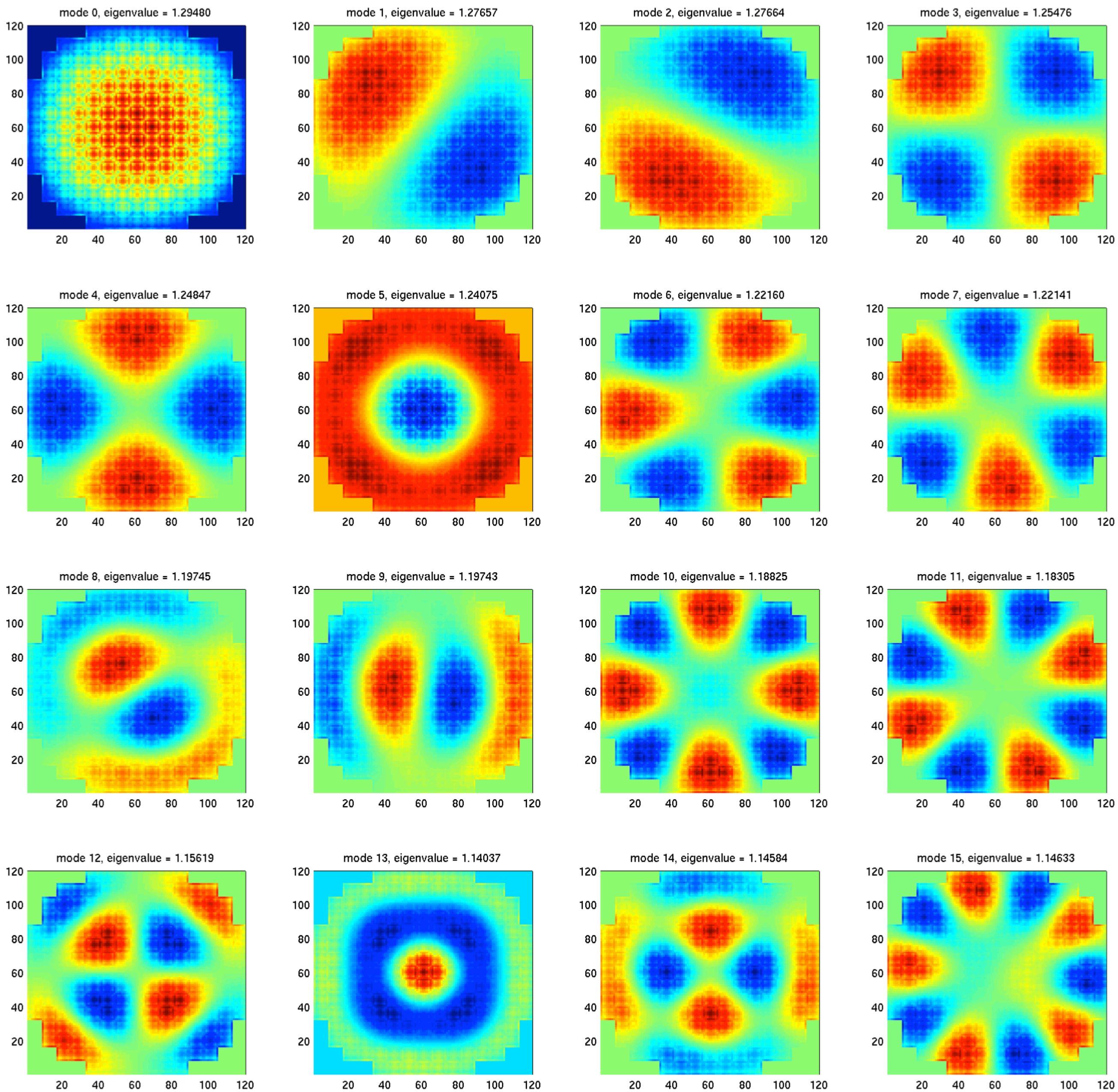
- 48 1/4 fuel assemblies:
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes for control rods or detectors
- Each assembly:
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- Dominance ratio ~ .98
- Calculations used whole-core model, symmetric quarter-core shown at right
- ENDF/B-VII data, continuous-energy
- Tally fission rates in each quarter-assembly



# PWR – Eigenmodes for 120x120x1 Spatial Mesh

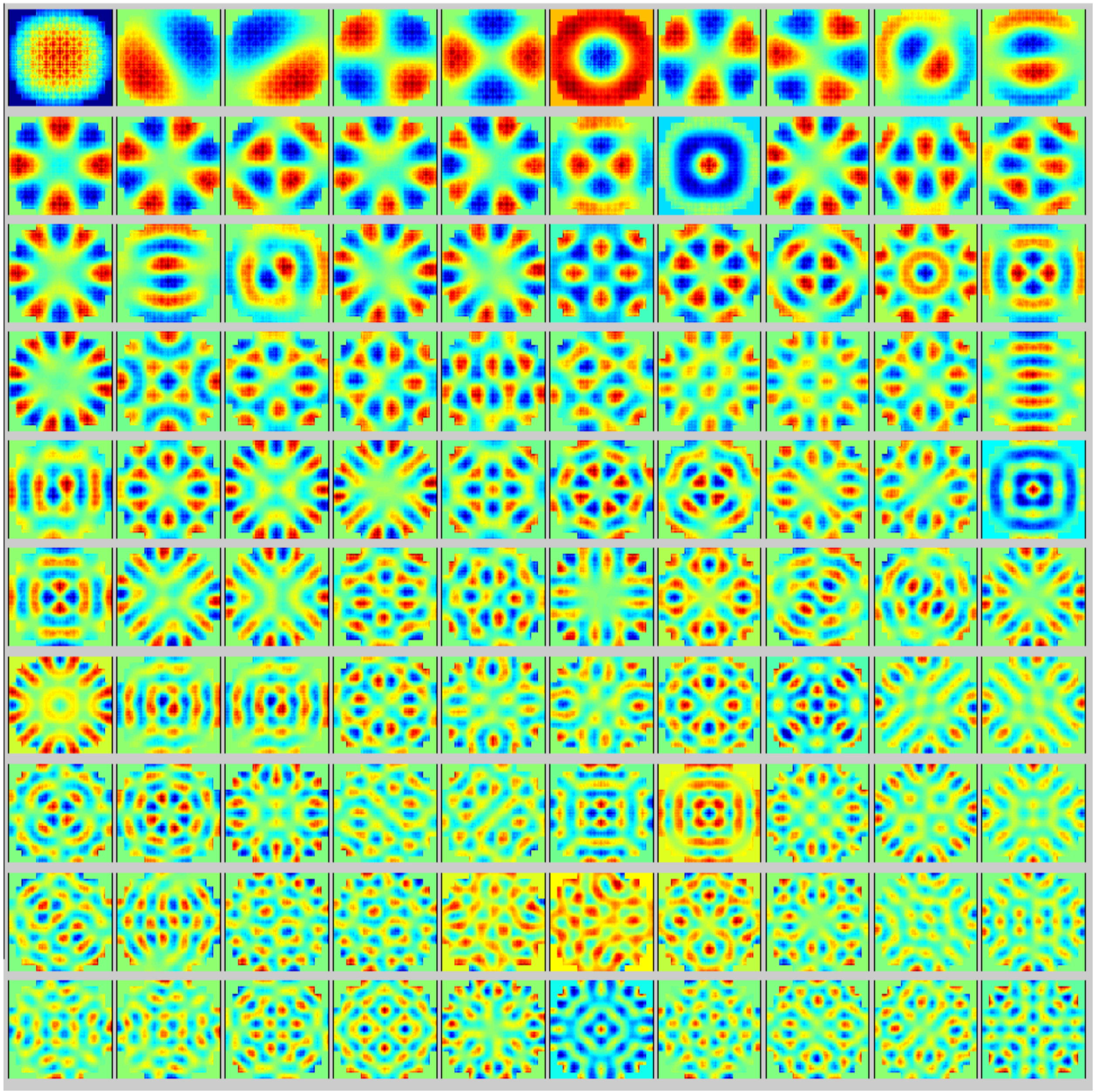





| n | $K_n$ |
|---|---|
| 0 | 1.29480 |
| 1 | 1.27664 |
| 2 | 1.27657 |
| 3 | 1.25476 |
| 4 | 1.24847 |
| 5 | 1.24075 |
| 6 | 1.22160 |
| 7 | 1.22141 |
| 8 | 1.19745 |
| 9 | 1.19743 |
| 10 | 1.18825 |
| 11 | 1.18305 |
| 12 | 1.15619 |
| 13 | 1.14633 |
| 14 | 1.14617 |
| 15 | 1.14584 |

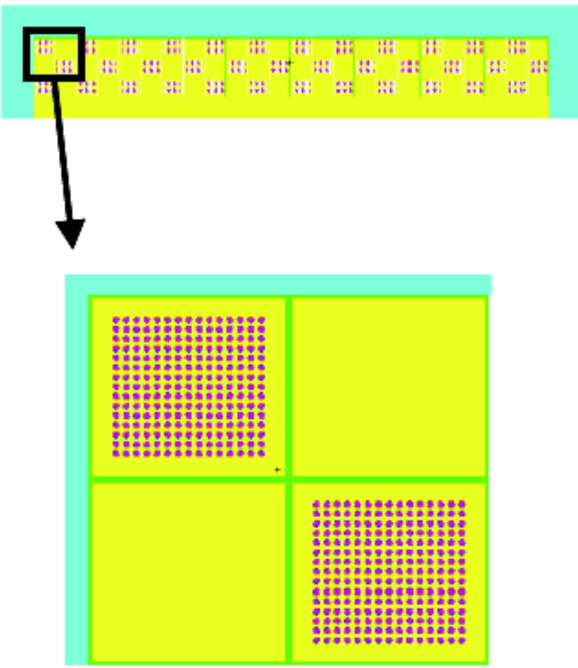
# PWR – First 100 Eigenmodes



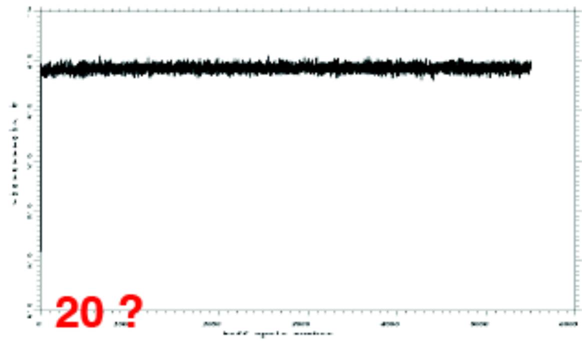


# Fuel Vault Problem

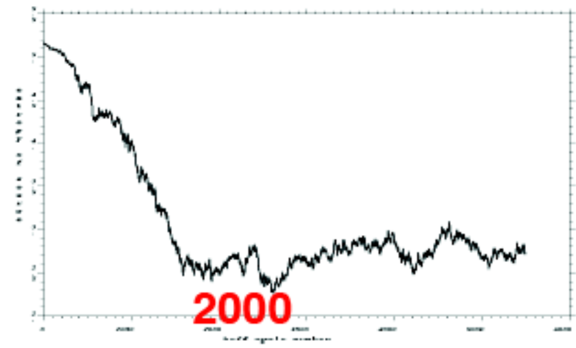
## Fuel Storage Vault



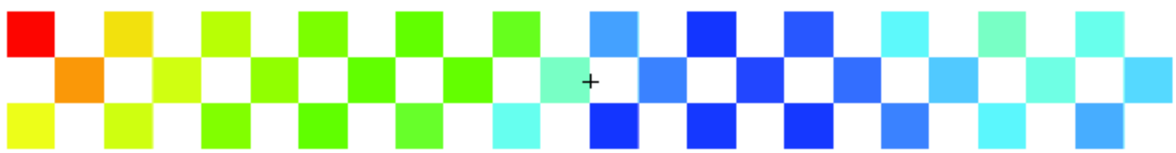
## K vs cycle




## $H_{src}$ vs cycle




## Assembly Heating Distribution



**For this calculation,**

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

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

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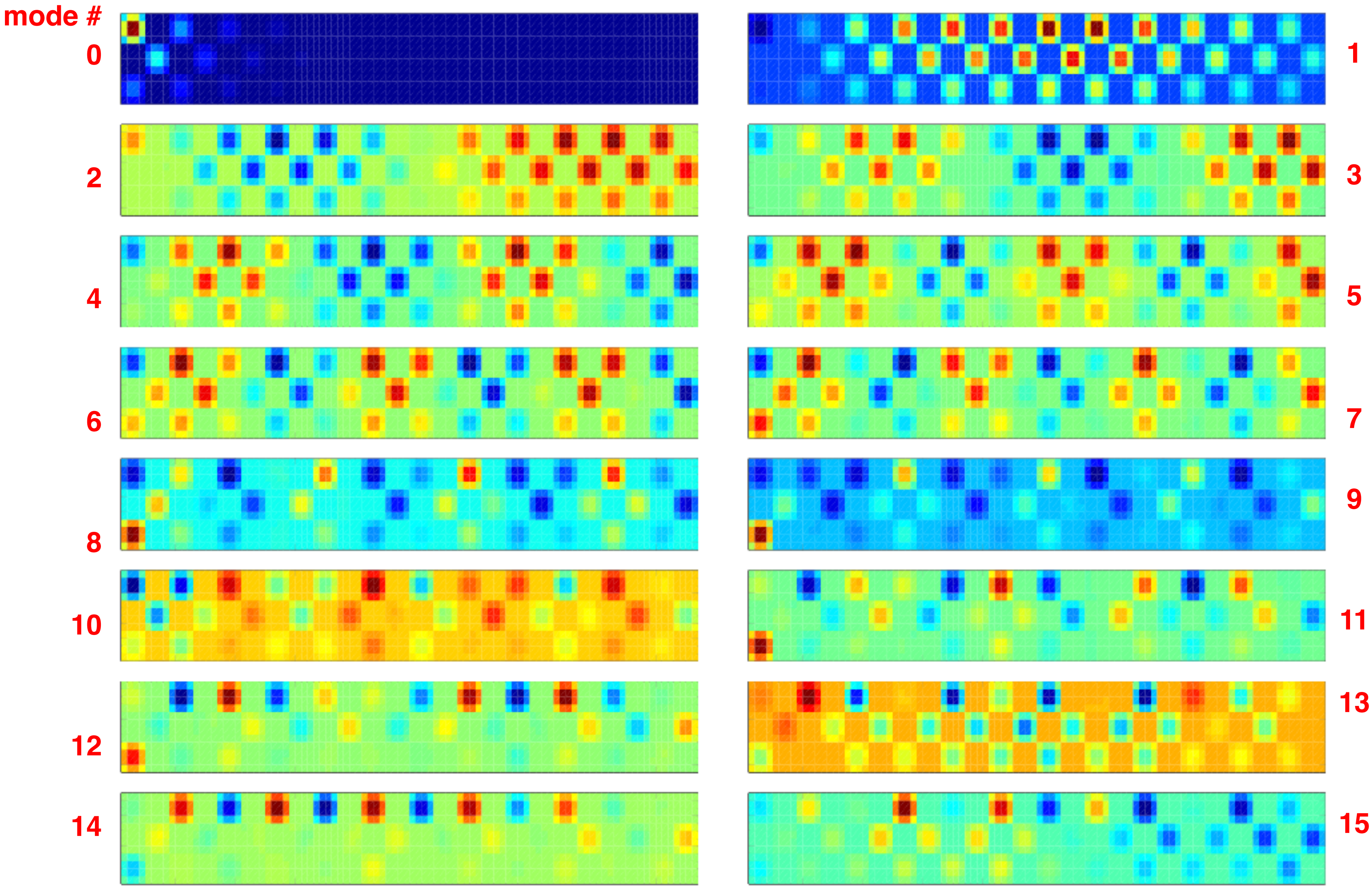
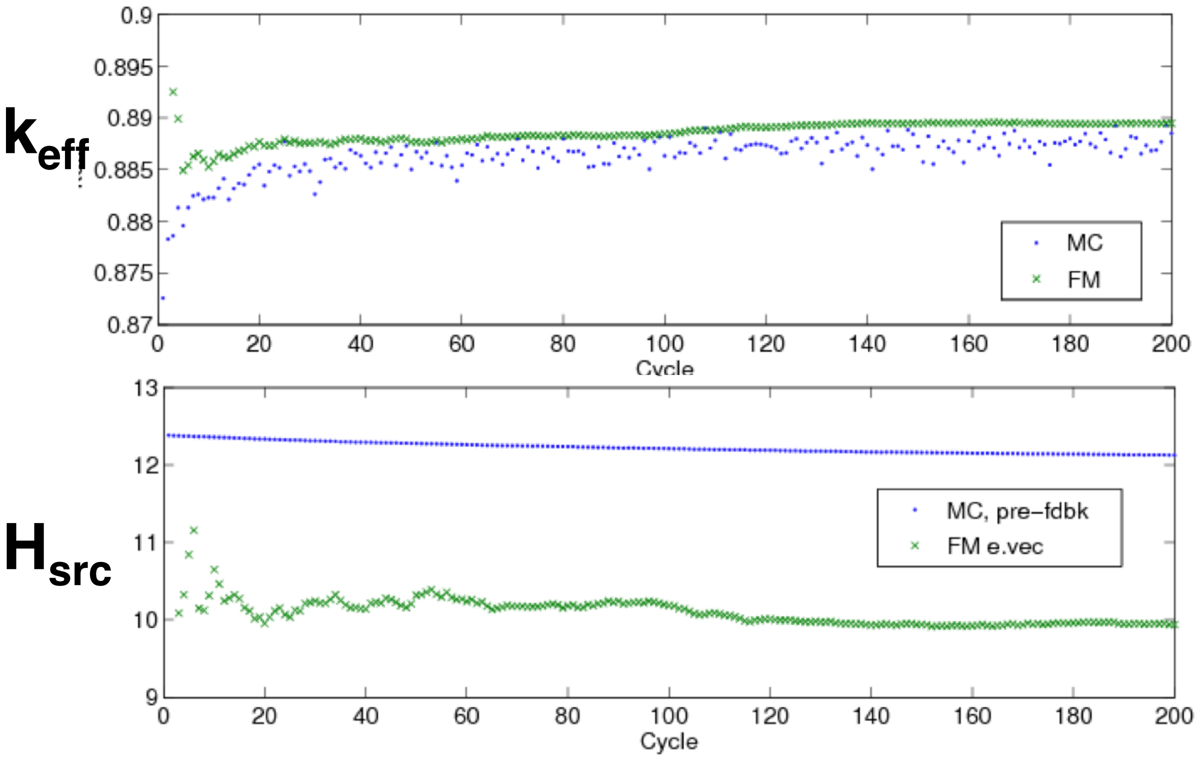



XY planes mid-height. Axial shape is cosine, #10,13,15 have change in sign in z

# Fuel Vault Problem - Convergence Acceleration

**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**

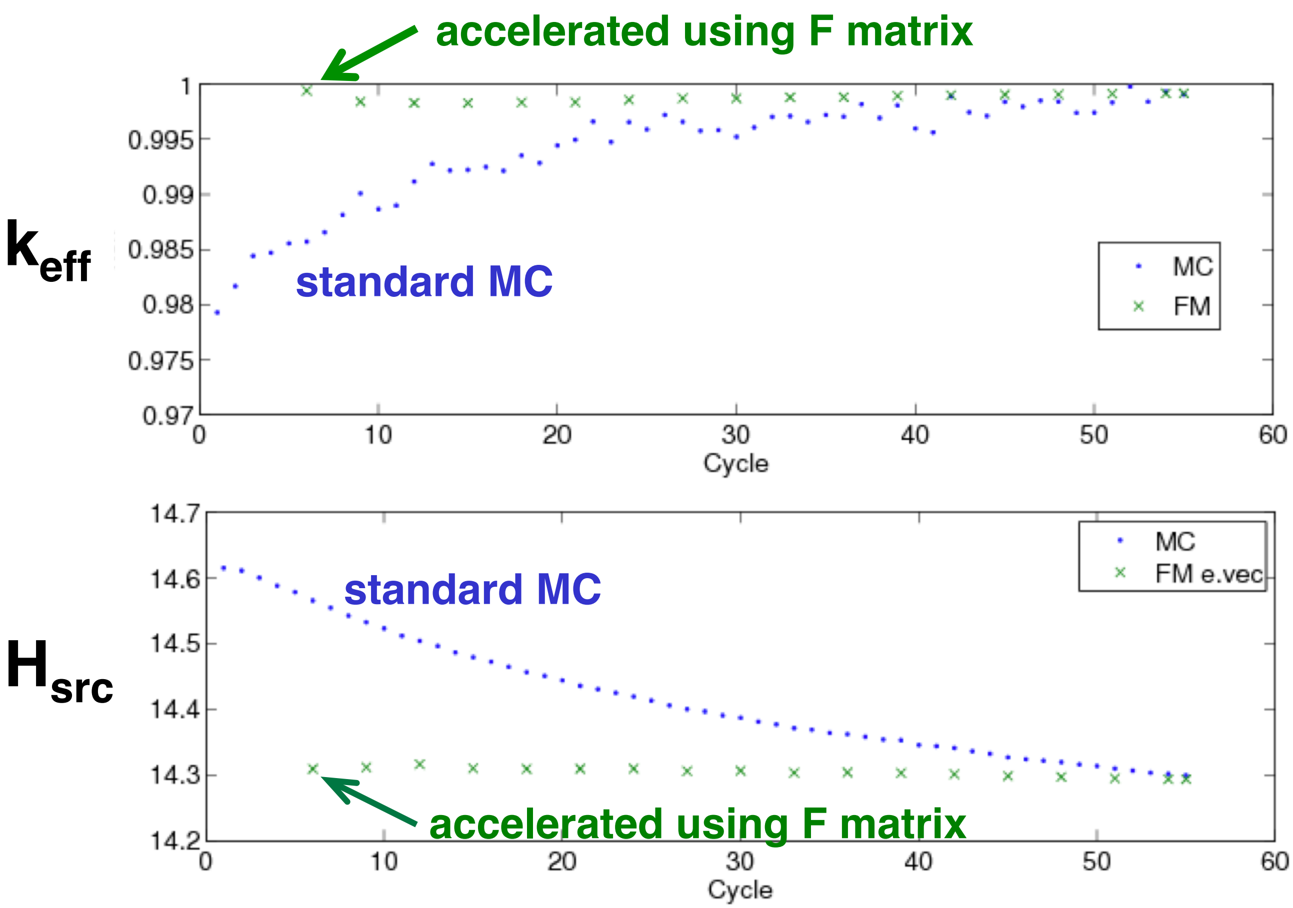
**accelerated using F matrix**

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

# Convergence Acceleration Using Fission Matrix



- Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles
- Requires only fundamental forward mode
- Very impressive convergence improvement




**3D reactor**

**Kord Smith Challenge Problem**

# Conclusions

- **Derived theory underlying fission matrix method**
  - Rigorous Green's function approach, no approximations
  - Specific conditions on spatial resolution required for fission matrix accuracy
  - If spatial resolution fine enough, adjoint fission matrix identical to transpose of forward fission matrix

- **Fission matrix capability has been added to MCNP6 (R&D for now)**

- **Applied to realistic continuous-energy MC analysis of typical reactor models. Can obtain fundamental & higher eigenmodes**

- **Higher eigenmodes are important for**

| | |
|---|---|
| **BWR void stability,** | **higher-order perturbation theory,** |
| **Xenon oscillations,** | **quasi-static transient analysis,** |
| **control rod worth,** | **correlation effects on statistics,** |
| **accident behavior,** | **etc., etc., etc.** |

- **Can provide very effective acceleration of source convergence**

# Future Work

- **Use fission matrix to accelerate source convergence**
  - Already demonstrated; very effective; **needs work to automate**
- **Use fission matrix for automatic, on-the-fly determination of source convergence**
  - **Automate the determination of "inactive cycles"**
- **Use fission matrix to assess problem coverage**
  - Need more neutrons/cycle to get adequate tallies?
- **Higher modes can be used to reduce/eliminate cycle-to-cycle correlation bias in statistics**
  - Replicas & ensemble statistics may be better, for exascale computers
- **Apply higher-mode analysis to reactor physics problems**
  - Higher-order perturbation theory, Xenon & void stability, slow transients, etc.

# Questions ?

**See Sun Valley M&C-2013 papers & talks for more examples, applications, ideas.**

**[on mcnp.lanl.gov website]**