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Title:	Monte Carlo - Advances and Challenges
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Monte Carlo - Advances and Challenges

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Abstract

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Monte Carlo - Advances and Challenges

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With ever-faster computers and mature Monte Carlo production codes, there has been tremendous growth in the application of Monte Carlo methods to the analysis of reactor physics and reactor systems. In the past, Monte Carlo methods were used primarily for calculating k_{eff} of a critical system. More recently, Monte Carlo methods have been increasingly used for determining reactor power distributions and many design parameters, such as β_{eff}, l_{eff}, τ, reactivity coefficients, Doppler defect, dominance ratio, etc. These advanced applications of Monte Carlo methods are now becoming common, not just feasible, but bring new challenges to both developers and users: Convergence of 3D power distributions must be assured; confidence interval bias must be eliminated; iterated fission probabilities are required, rather than single-generation probabilities; temperature effects including Doppler and feedback must be represented; isotopic depletion and fission product buildup must be modeled.

This workshop focuses on recent advances in Monte Carlo methods and their application to reactor physics problems, and on the resulting challenges faced by code developers and users. The workshop is partly tutorial, partly a review of the current state-of-the-art, and partly a discussion of future work that is needed. It should benefit both novice and expert Monte Carlo developers and users. In each of the topic areas, we provide an overview of needs, perspective on past and current methods, a review of recent work, and discussion of further research and capabilities that are required. Electronic copies of all workshop presentations and material will be available. The workshop is structured as several morning and afternoon segments:

- *Morning:*
  - *Introduction*
  - *Criticality Calculations* – k_{eff} bias, convergence diagnostics, acceleration methods, dominance ratio, confidence interval bias, and the iterated fission probability,
  - *Temperature Dependence* – cross-sections, pseudo-materials, feedback, coupling to other codes
- *Afternoon:*
  - *Fission Energy Deposition* – fission energy release & deposition, assumptions, & calculations
  - *Depletion Calculations* – a tutorial on time-step algorithms, fission products, error propagation, etc.
  - *Impact of ENDF/B-VII data*
  - *The "Kord Smith Challenge"*

Agenda

Morning

- **Criticality Calculations** (Brown)
  - Bias, convergence, dominance ratio, confidence intervals, acceleration, iterated fission probability
- **Temperature dependence** (Martin)
  - Cross-sections, pseudo-materials, feedback, & coupling to other codes

Afternoon

- **Fission energy deposition** (Martin)
  - Fission energy release & deposition, assumptions, & calculations
- **Depletion Calculations** (Brown, Mosteller)
  - Tutorial on timesteps, fission products, error propagation, etc.
- **Impact of ENDF/B-VII data** (Mosteller)
- **The "Kord Smith Challenge"** (Martin)

Introduction

Perspective

- As computing power has increased, the use of Monte Carlo methods for reactor analysis has grown
- Also, since more histories give better localized statistics, the principal uses of Monte Carlo have evolved:

1960s:	K-effective
1970s:	K-effective, detailed assembly power
1980s:	K-effective, detailed 2D whole-core
1990s:	K-effective, detailed 3D whole-core
2000s:	K-effective, detailed 3D whole-core, depletion, reactor design parameters

➜ **Recent Monte Carlo R&D is focussed on advanced methods for modeling, depletion, & design parameters**

Monte Carlo for Reactor Applications

- **Monte Carlo strengths**
  - Very general & accurate geometry modeling
  - Direct use of best cross-section data (ENDF/B, JEF, JENDL, …)
  - Continuous-energy neutron transport & physics
  - Readily adapted to parallel computers

  - Examples on next few slides …..

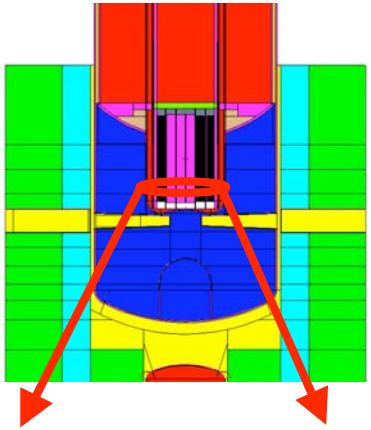
- **This workshop:**

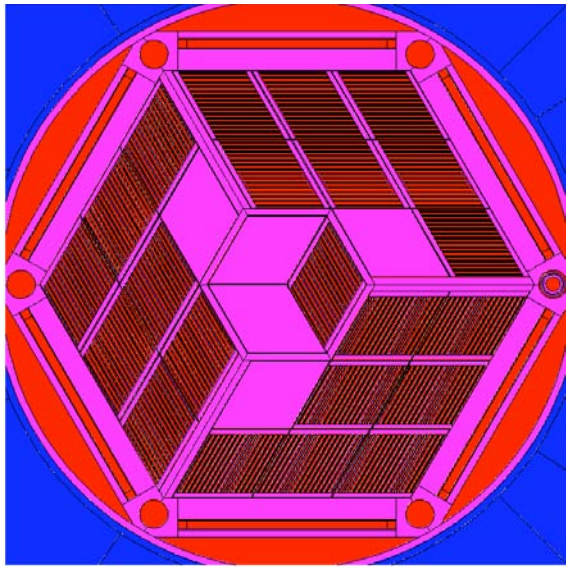
  - **Review the current challenges & advances**

  - **Consider both theory & computations**

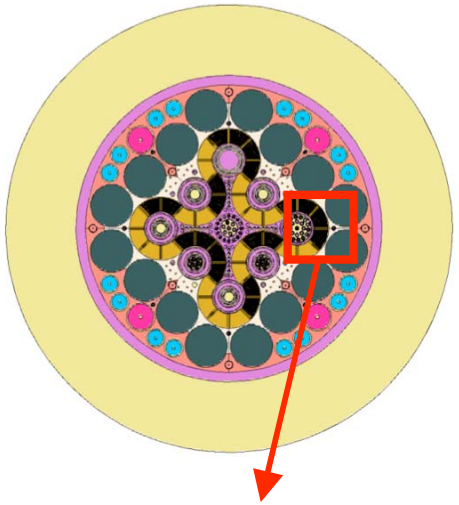
Research Reactors

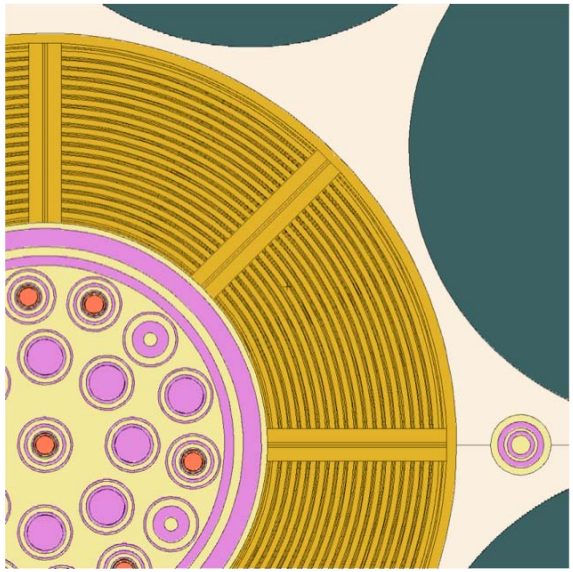
MIT research reactor, with beam ports





Advanced Test Reactor (ATR)

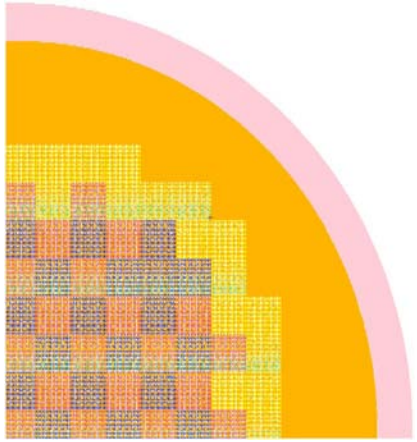




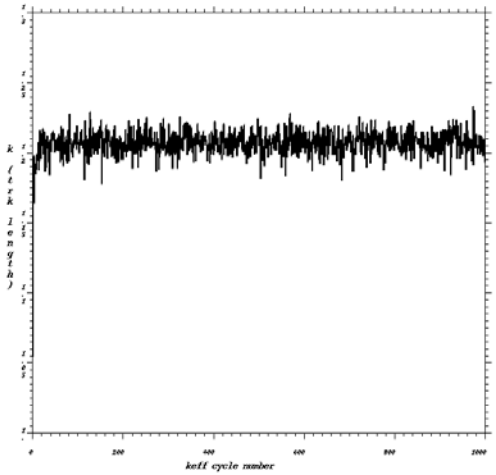
Pictures from mcnp plotter

Commercial Reactors - PWR, BWR

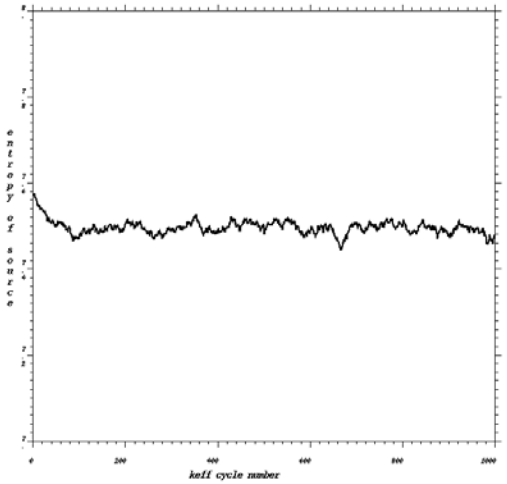
Geometry Model (1/4)



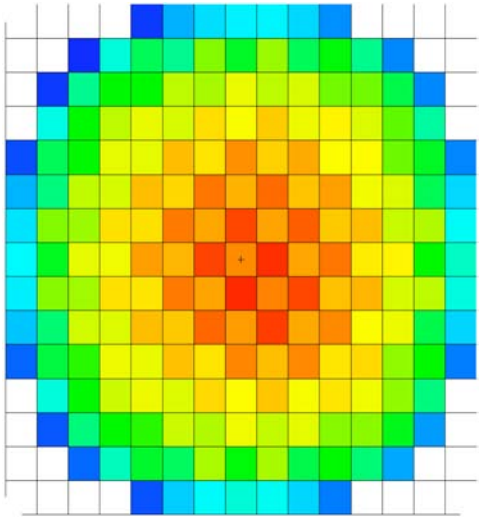
K vs cycle



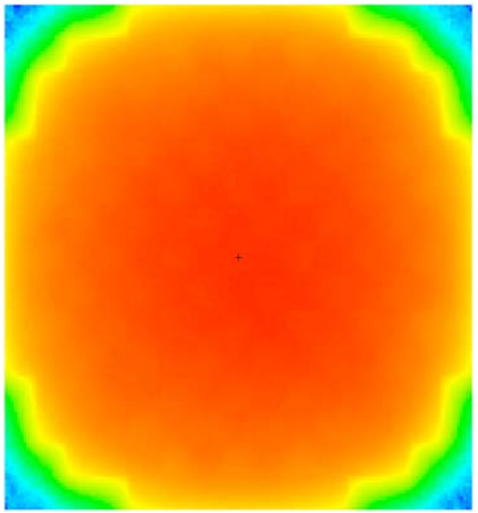
H_{src} vs cycle



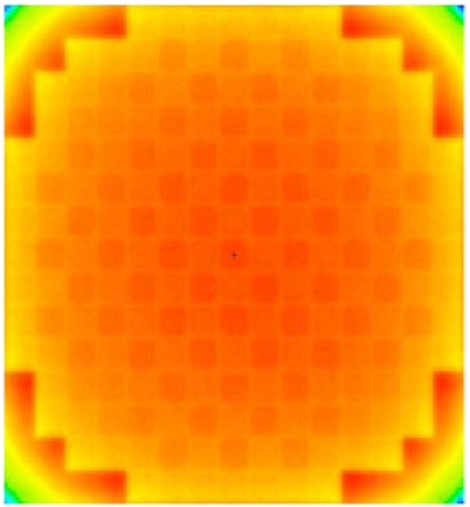
Assembly Powers



Fast Flux

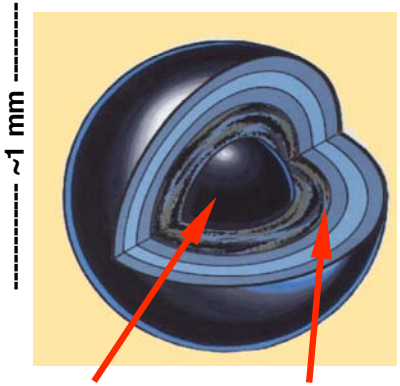


Thermal Flux



Pictures from mcnp plotter

Advanced Reactors - VHTR, HTGR, ...

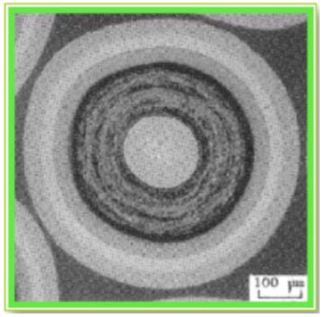


TRISO Fuel Particles:

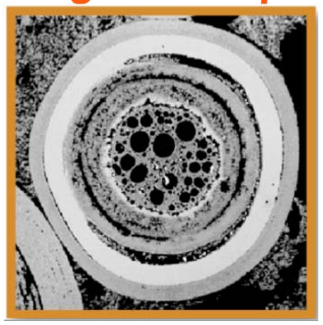
- Fission product gases trapped within coatings
- Coatings remain intact, even with high T & burnup

Fuel concept is same for block or pebble bed

Fresh Fuel



High Burnup

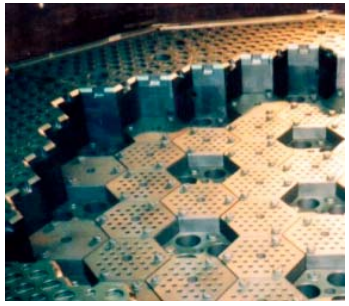


(From General Atomics)

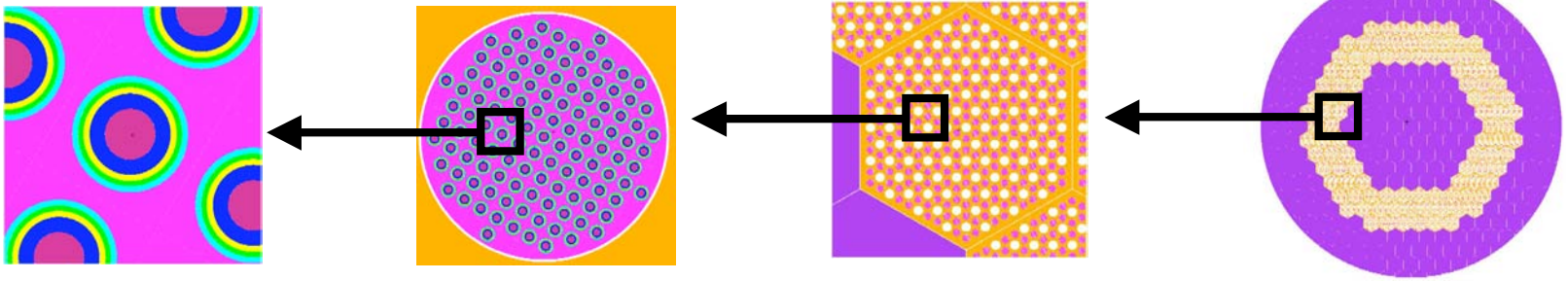
PARTICLES

COMPACTS

FUEL BLOCK



CORE



Accurate & explicit modeling at multiple levels

Challenges in Monte Carlo Criticality Calculations

Longstanding problems with the fundamental theory:

1. Bias in Keff
2. Convergence of source distribution
3. Underprediction bias in confidence intervals
4. Lack of adjoint weighting for tallies
5. Determining adequate population size
6. Propagation of error (xsecs, depletion, etc.)
7. Existence & completeness of higher modes (Keff calculations)
8. …..

Current computational difficulties:

1. Fission products for depletion calculations
2. Scaling of codes to extreme problem sizes
3. Multiphysics - coupling to T/H, heat transfer, & structural codes
4. Multicore threading vs GPGPU vectors
5. Particle parallelism vs domain decomposition
6. Uncertainties in nuclear data
7. Validation of codes & nuclear data
8. Run-time needed for pin powers & depletion
9. …..

Criticality Calculations

- Bias in Keff
- Convergence of source distribution
- Dominance ratio
- Underprediction bias in confidence intervals
- Acceleration
- Iterated Fission Probability

Bias in Keff

Bias in Keff

- **Power iteration is used for Monte Carlo Keff calculations**
  - For one cycle (iteration):
    - $\mathbf{M_0}$ neutrons from source distribution
    - $\mathbf{M_1}$ neutrons produced during random walks
    - E[$\mathbf{M_1}$] = Keff · $\mathbf{M_0}$ (mcnp uses weight, rather than number of neutrons)
  - At end of each cycle, must **renormalize**
    - By factor $\mathbf{M_0 / M_1}$
    - Adjust number of neutrons, or adjust total weight
    - Effectively, dividing by stochastic quantity ($\mathbf{M_1}$) $\Rightarrow$ introduces bias
- **Bias in Keff, due to renormalization**

$$\text{bias in } K_{eff} = -\frac{\sigma_k^2}{K_{eff}} \cdot \begin{pmatrix} \text{sum of lag-i correlation} \\ \text{coeff's between batch K's} \end{pmatrix} \propto \frac{1}{M_0}$$

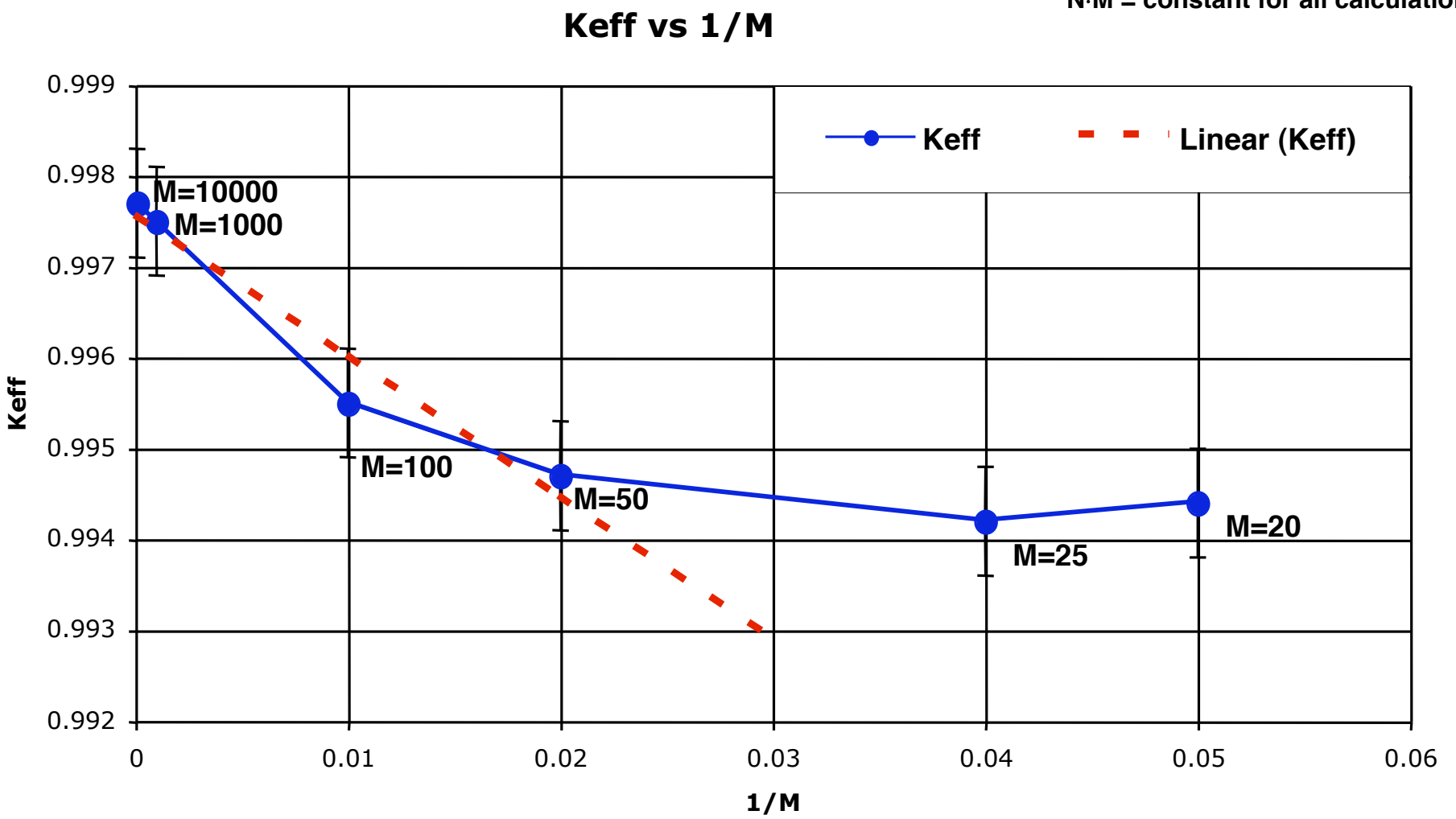
Note: σ_k^2 = population variance; $\sigma_{keff}^2 = \sigma_k^2 / N$

References: Gelbard & Prael, Brissenden & Garlick, Ueki

Bias in Keff

- **For a simple Godiva reactor calculation:**

N = # cycles
M = neutrons/cycle
N·M = constant for all calculations



Bias in Keff

- **Past work - eliminating bias**
  - **MacMillan** (see appendix in Gast & Candelore)
    - Weight the tallies for each cycle **n** by

$$W_n = \frac{\prod_{J=1}^{n-1} k_J}{K^{n-1}}, \qquad \text{where} \quad K = \left(\prod_{J=1}^{N} k_J \right)^{1/N}, \qquad N = \text{number of active cycles}$$

    - Difficulty: Must save all tallies for all cycles, combine at end of problem
  - **Gast & Candelore**
    - Increase M (neutrons/cycle) each cycle by 10 neutrons
    - Difficulty: For finite number of cycles, bias still exists
- **Practical solution - use large M (neutrons/cycle)**
  - **Years ago**
    - Slow computers, M ~ 500 $\Rightarrow$ bias could be a problem
  - **Today**
    - Fast computers, typically M ~ 10K or 100K $\Rightarrow$ bias negligible
    - Large M gives more efficient parallel calculations

References

E.M. Gelbard and R.E. Prael, "Monte carlo Work at Argonne National Laboratory", in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).

R. C. Gast and N. R. Candelore, "Monte Carlo Eigenfunction Strategies and Uncertainties," in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).

R. J. Brissenden & A. R. Garlick, “Biases in the Estimation of Keff and Its Error by Monte Carlo Methods,” Ann. Nucl. Energy, 13, 2, 63-83 (1986)

T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations", Nucl. Sci. Eng. 141, 101-110 (2002)

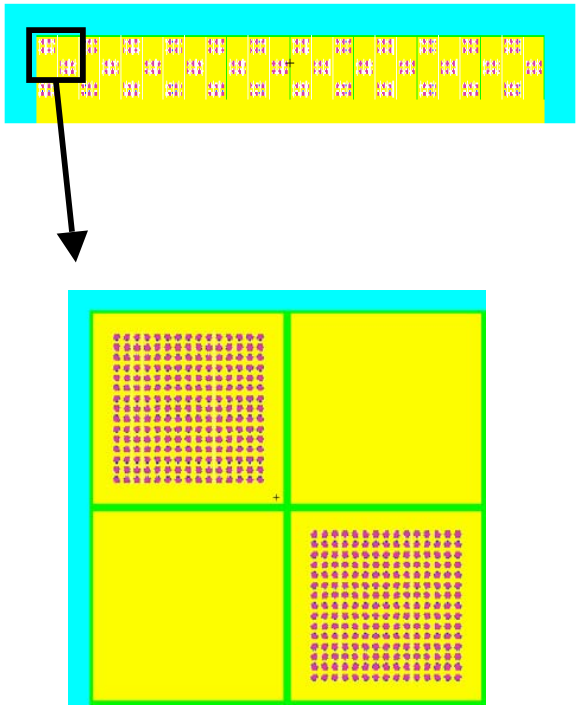
J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," *Nukleonik* 11,213 (1968).

L.V. Maiorov, "Estimates of the Bias in the Results of Monte Carlo Calculations of Reactors and Storage Sites for Nuclear Fuel", *Atomic Energy*, Vol 99, No 4, 681-693 (2005).

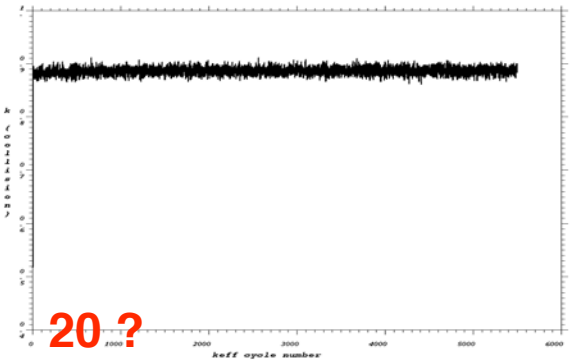
Convergence of Source Distribution

Keff vs Source Convergence

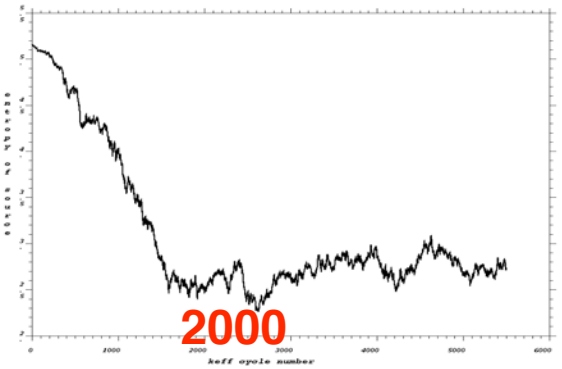
Fuel Storage Vault



K vs cycle



H_{src} vs cycle



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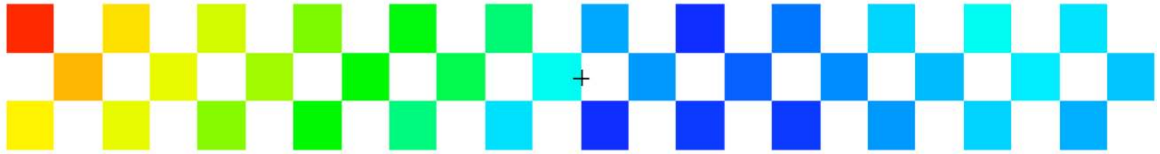
Assembly Heating Distribution



For this calculation,

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

Introduction

- **Monte Carlo codes use power iteration to solve for K_{eff} & Ψ for eigenvalue problems**

$$(L + T - S)\Psi^{(n)} = \frac{1}{K^{(n-1)}} M\Psi^{(n-1)}$$

L = loss to leakage **S = gain from scatter-in** **n = cycle no.**
T = loss to collisions **M = gain from fission multiplication**

- **Power iteration convergence is well-understood**

$$\Psi^{(n)}(\vec{r}) = \vec{u}_0(\vec{r}) + a_1 \cdot \rho^n \cdot \vec{u}_1(\vec{r}) + \ldots$$

$$k_{eff}^{(n)} = k_0 \cdot \left[1 - \rho^{n-1}(1-\rho) \cdot g_1 + \ldots\right]$$

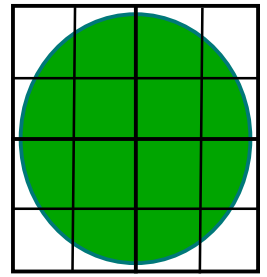
  - **First-harmonic source errors die out as ρ^n, $\rho = k_1 / k_0 < 1$**
  - **First-harmonic K_{eff} errors die out as $\rho^{n-1}(1-\rho)$**
  - **Source converges slower than K_{eff}**

- **Most codes only provide tools for assessing K_{eff} convergence.**

⇒ **MCNP5 also looks at Shannon entropy of the source distribution, H_{src}.**

K_{eff} Calculations - Convergence Diagnostics

- Divide the fissionable regions of the problem into **N_S spatial bins**
  - Typical choices: -- 1 bin for each assembly
    -- regular grid superimposed on core



- **Shannon entropy of the source distribution**

$$H(S) = -\sum_{J=1}^{N_S} p_J \cdot \ln_2(p_J), \quad \text{where} \quad p_J = \frac{\text{(\# source particles in bin J)}}{\text{(total \# source particles in all bins)}}$$

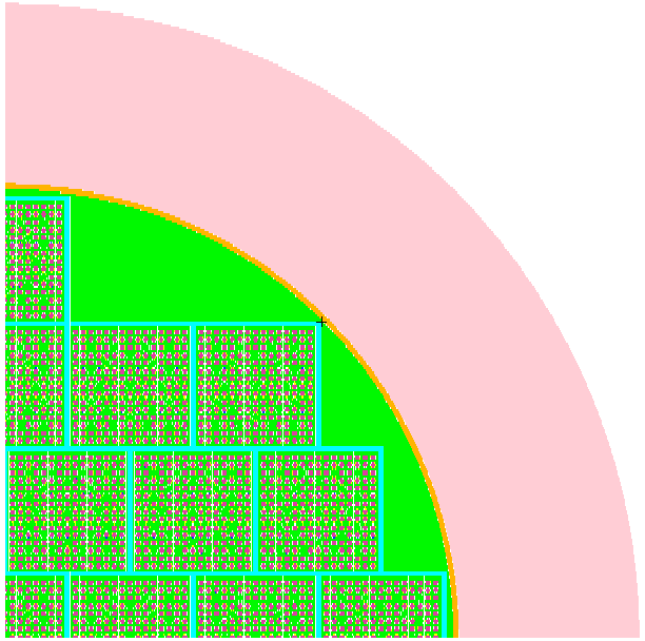
  - **For a <u>uniform</u> source distribution,** **$H(S) = \ln_2(N_S)$**
  - **For a <u>point</u> source (in a single bin),** **$H(S) = 0$**
  - **For any <u>general</u> source,** **$0 \le H(S) \le \ln_2(N_S)$**

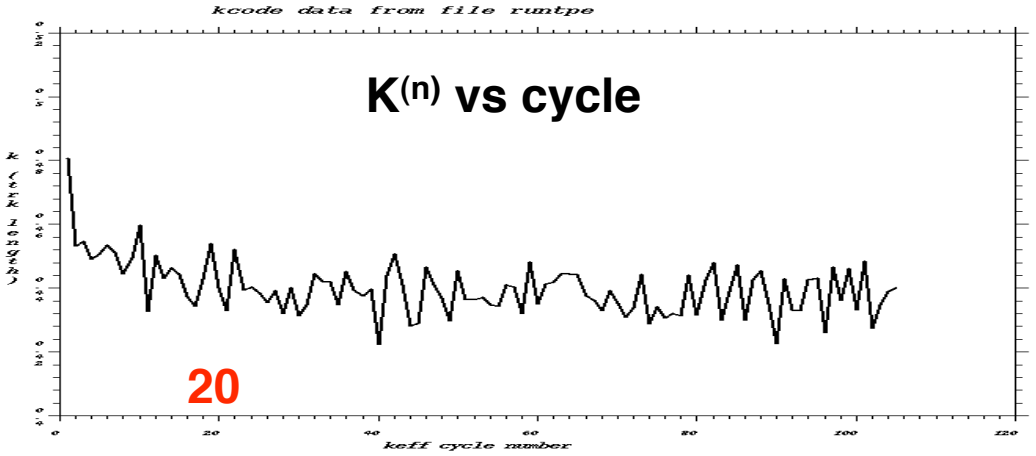
- **$H(S^{(n)})$ provides a single number to characterize the source distribution for iteration n (no physics!)**

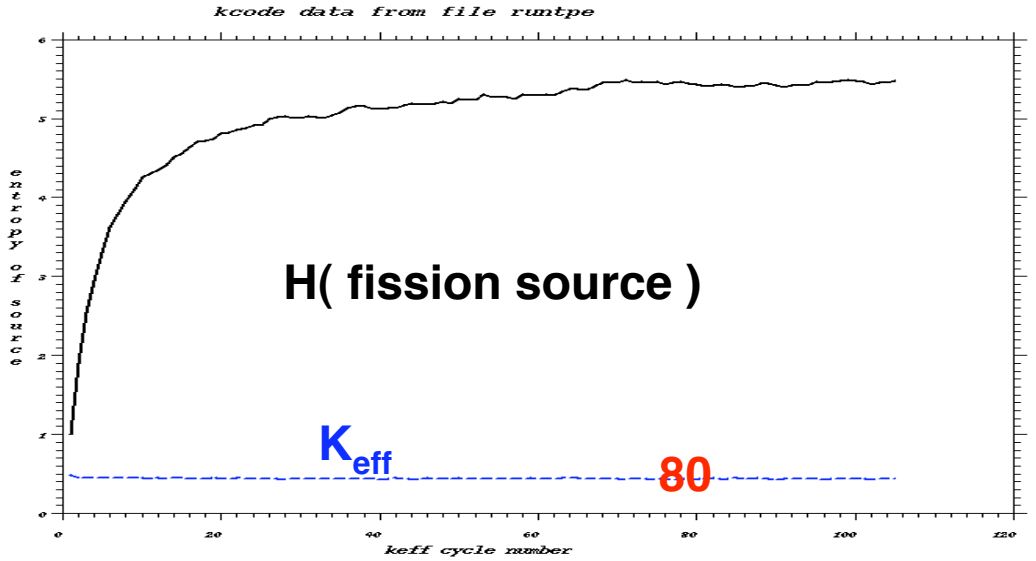
$\Rightarrow$ As the source distribution converges in 3D space, a line plot of $H(S^{(n)})$ vs. n (the iteration number) converge

Criticality Calculations - Convergence

- **Reactor core (Problem inp24)**







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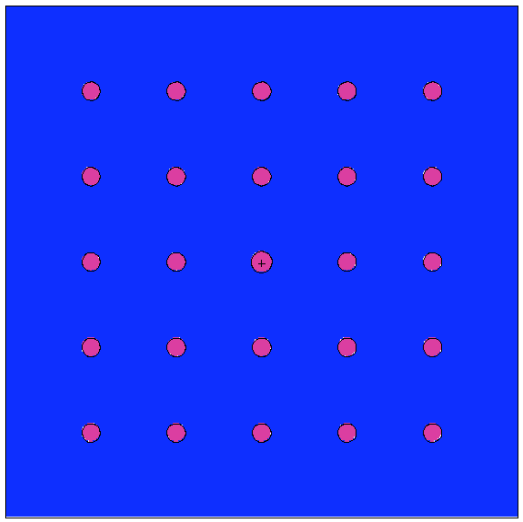
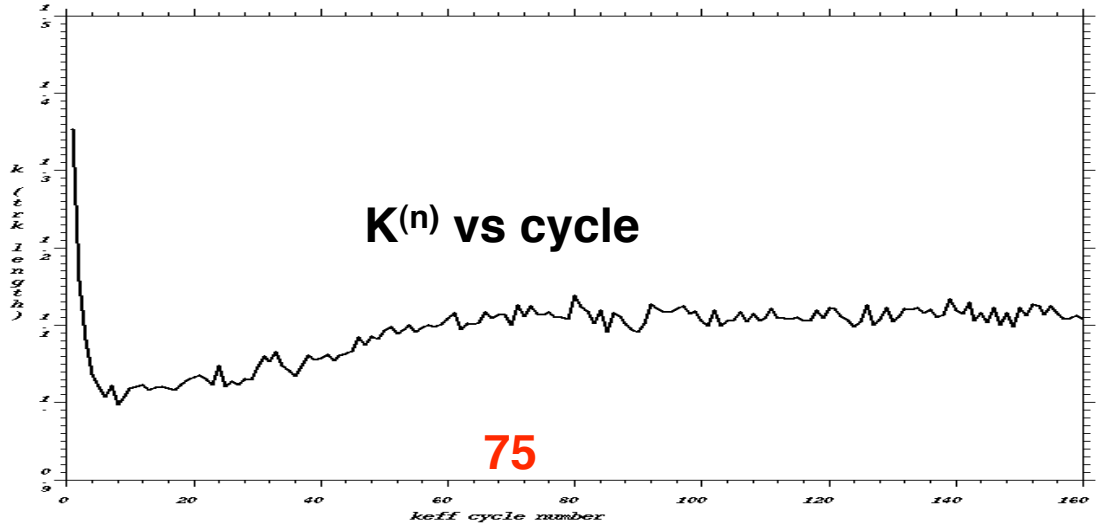
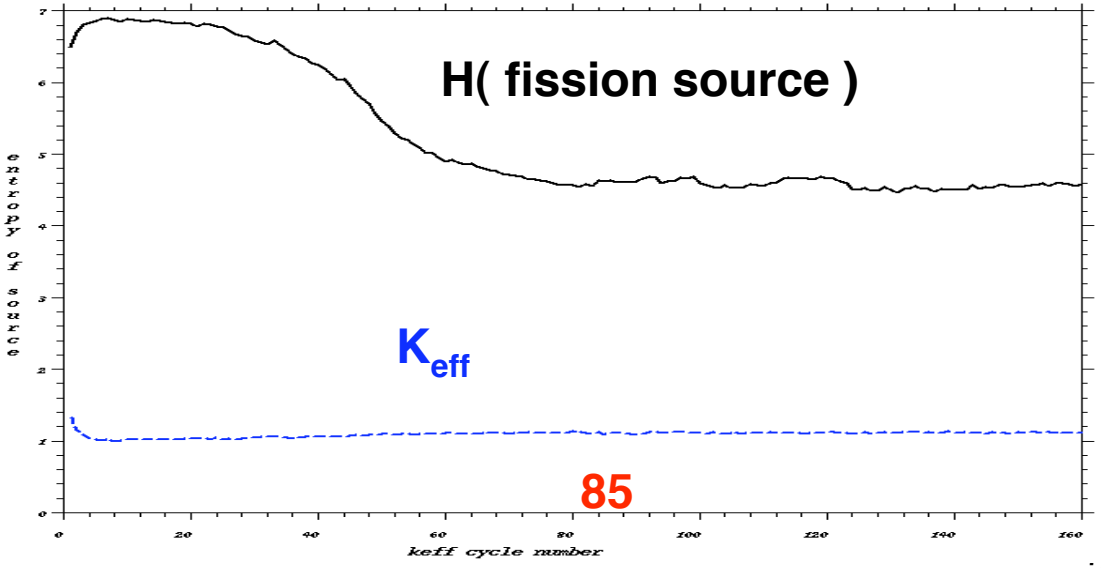
Criticality Calculations - Convergence

- Loosely-coupled array of spheres (Problem test4s)







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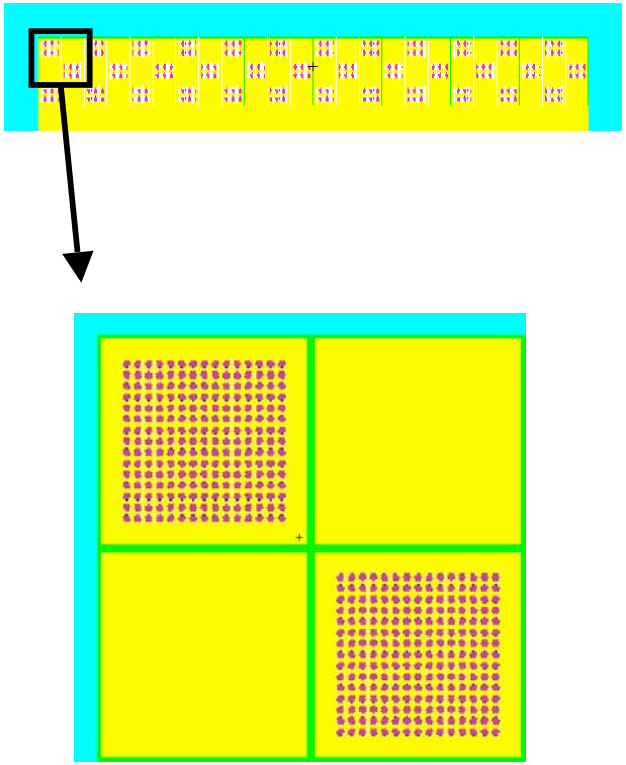
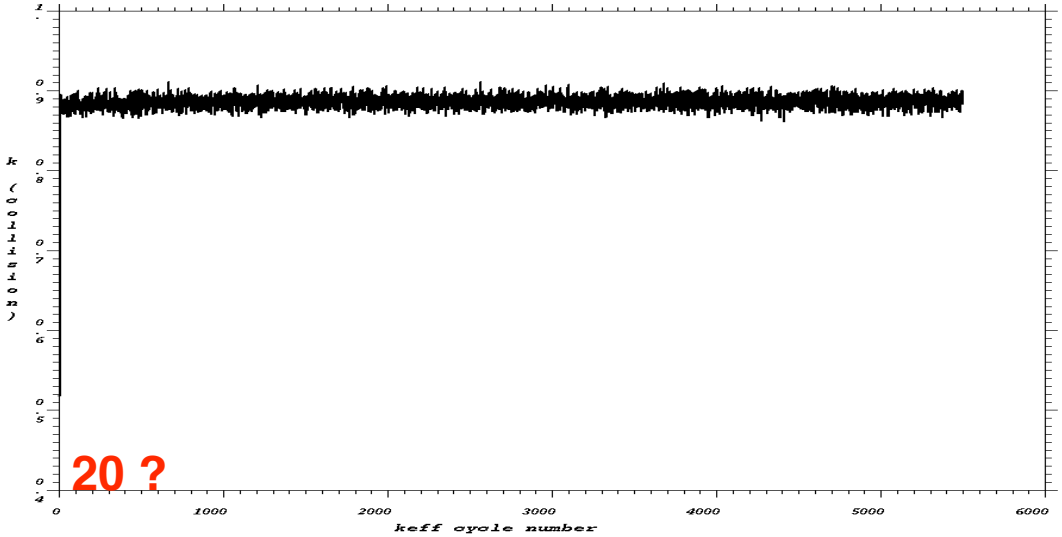
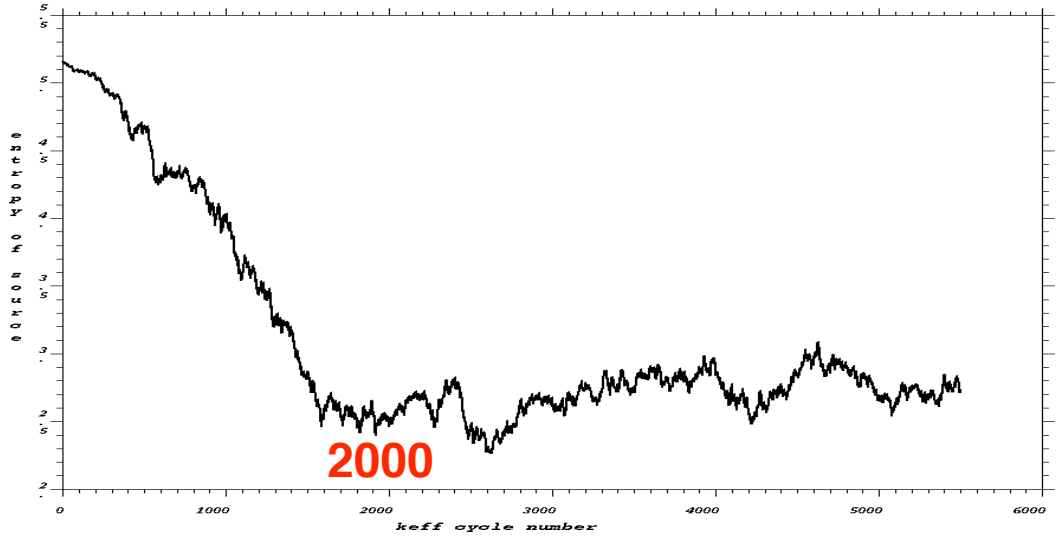
Criticality Calculations - Convergence

- **Fuel Storage Vault (Problem OECD_bench1)**







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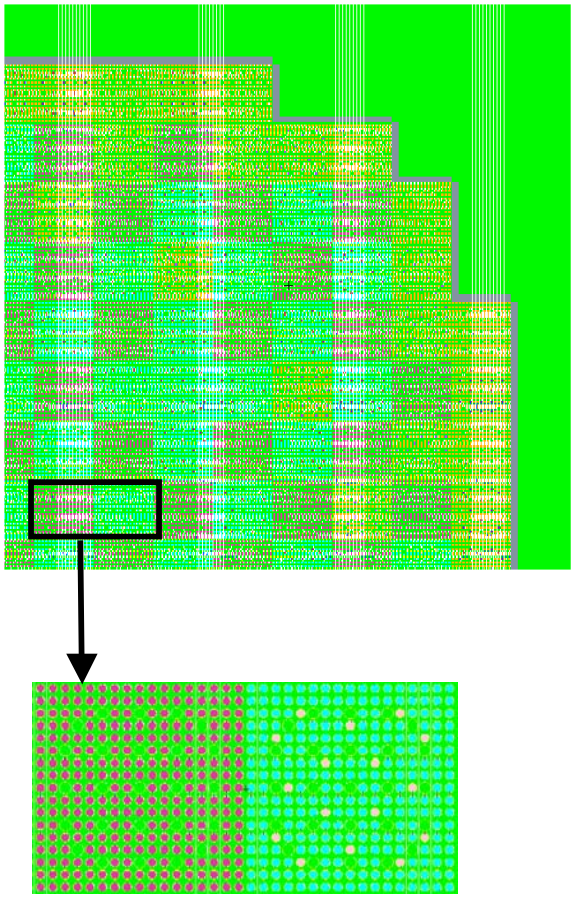
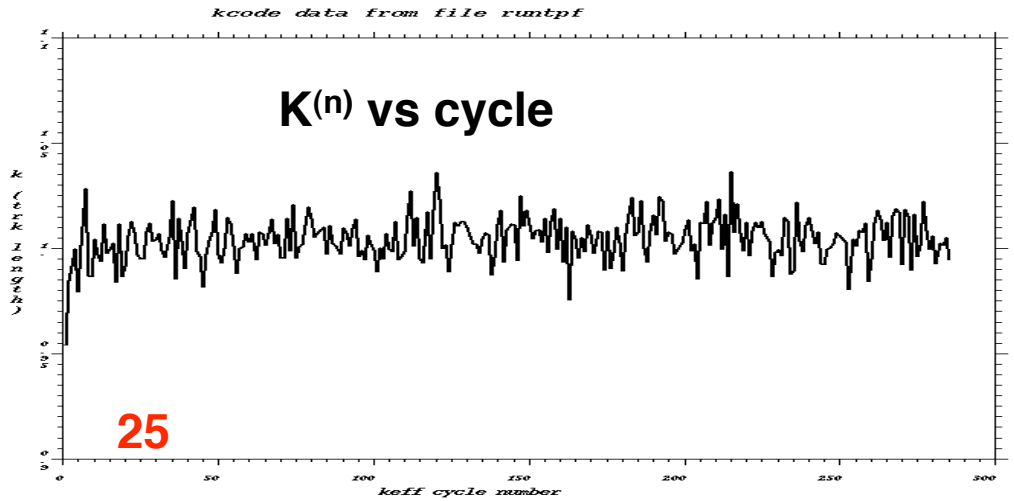
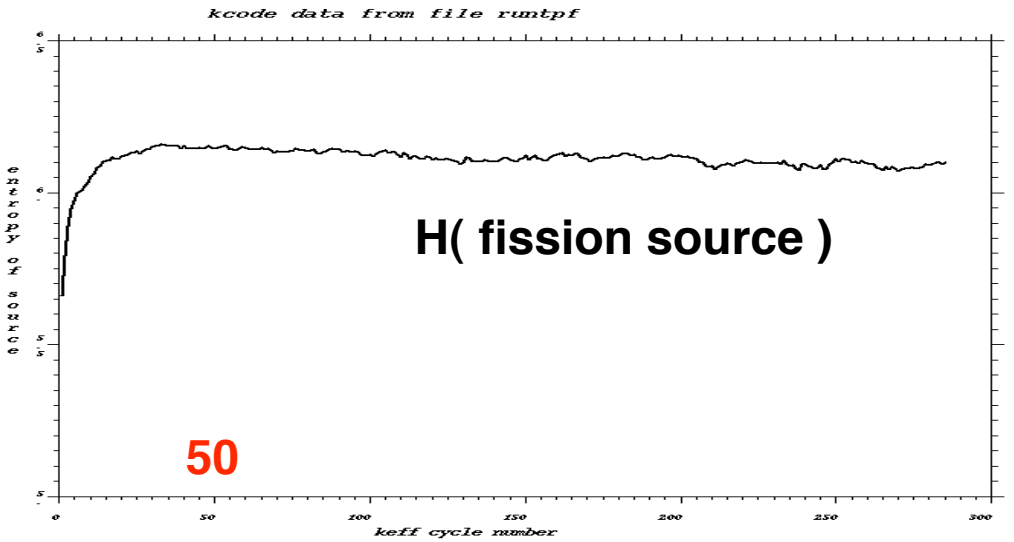
Criticality Calculations - Convergence

- **PWR 1/4-Core (Napolitano)**







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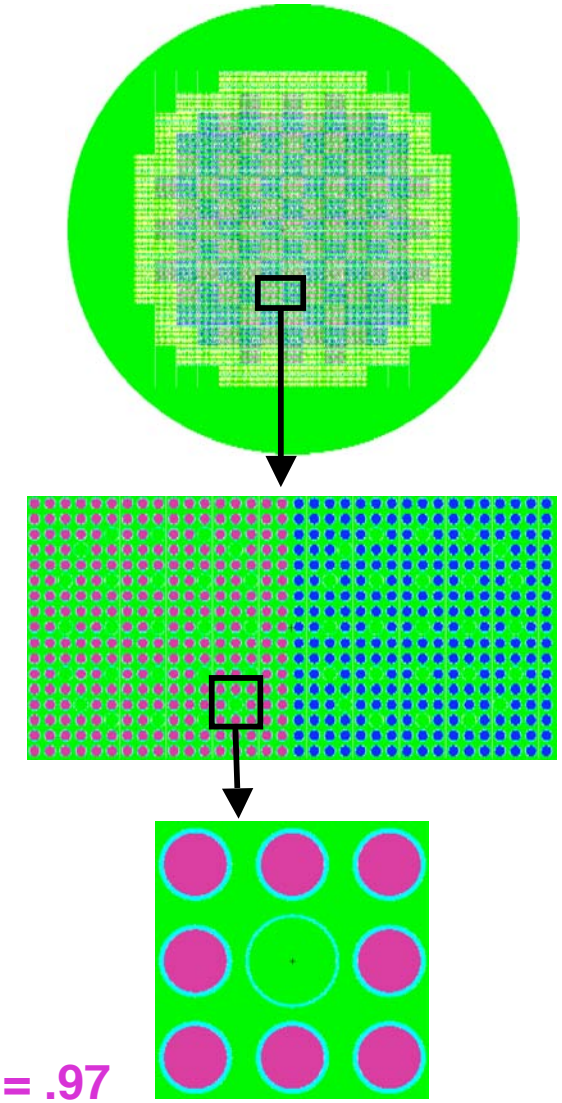
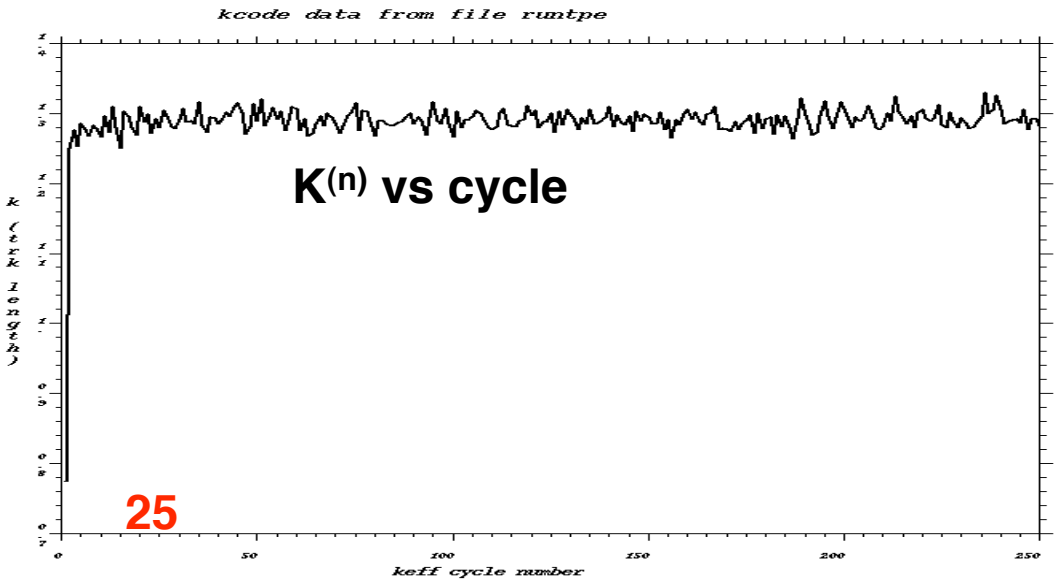
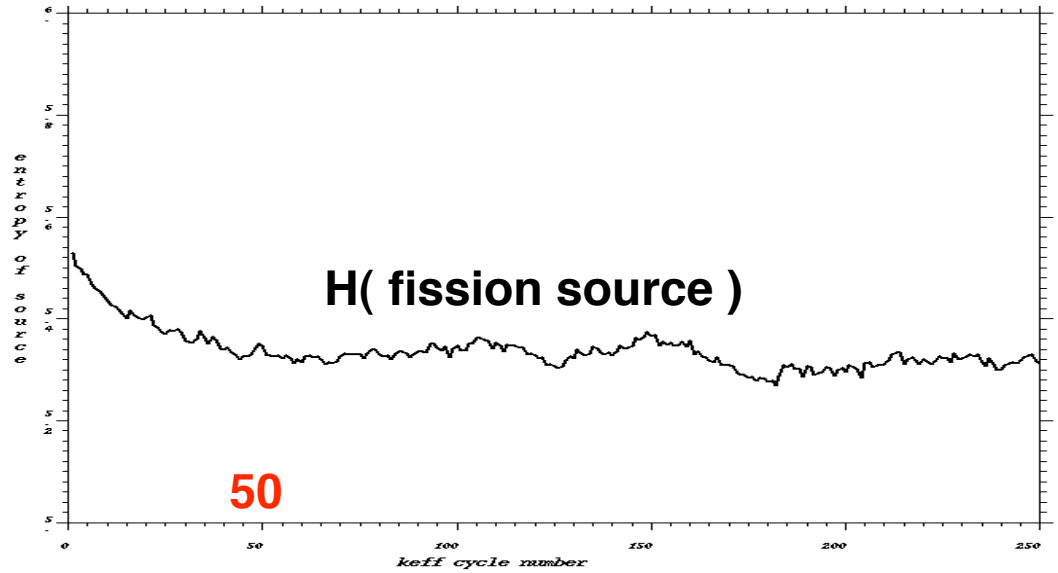
Criticality Calculations - Convergence

- 2D PWR (Ueki)



DR = .97





Conclusions - H_{src}

- Shannon entropy is a highly effective means of characterizing convergence of the fission distribution

- If you are computing more than just K_{eff} (eg, local reaction rates, dose fields, fission distributions, heating distributions, etc.):

  Should check both k_{eff} and H_{src} for convergence

- MCNP5 (1.40) computes & plots H_{src} as an important new tool for assessing problem convergence.

References - Shannon Entropy & Convergence

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Dominance Ratio Calculations

(For future versions of MCNP5)

DR - Overview

- **Time-series methods for computing DR**
  - Ueki - developed a method [NSE 145, 279-290, 2003]
  - Nease & Ueki - a practical method, CMPM [NSE 157, 51-64, 2007]
  - Nease, Brown, & Ueki - test in MCNP5 **[PHYSOR-08, 2008]**

  ⇒ **Accurate, regardless of mesh used for collecting statistics**

  ⇒ **Can be used only after source has converged**

- **Fission Matrix method**

  $$\vec{S} = \frac{1}{k}\overline{F} \cdot \vec{S}$$

  F_{ij}=prob fission in cell j, given fission in cell i

  - Tally F_{ij}, then find eigenvalues & eigenvectors of F
  - Very old - used by dozens of researchers (Morrison, Mendelson, …)

  ⇒ **Approximate, results are very sensitive to mesh**

  ⇒ **Can be used before source has converged**

Coarse Mesh Projection Method (Nease & Ueki)

- **Tally the source distribution for cycle m on a coarse mesh**
  - Typically, use the same mesh as for determining Shannon entropy
  - Tally the source only after convergence, for **N** active cycles
  - Collapse the source tallies to 1, 2, or 3 intervals in each of x,y,z
- **Using the source vectors $S^{(m)}$, determine the noise propagation matrix A_0 & determine the eigenvectors, d_i**

$$\mathbf{L}_0' = \mathbf{E}\left[\hat{\mathbf{S}}^{(m)}(\hat{\mathbf{S}}^{(m)})^{\mathbf{T}}\right] \qquad \mathbf{A}_0 = \mathbf{L}_1'\mathbf{L}_0'^{-1} - \mathbf{I}$$

$$\mathbf{L}_1' = \mathbf{E}\left[\hat{\mathbf{S}}^{(m+1)}(\hat{\mathbf{S}}^{(m)})^{\mathbf{T}}\right] \qquad \mathbf{A}_0^{\mathbf{T}}\vec{\mathbf{d}}_i = \lambda_i\vec{\mathbf{d}}_i$$

- **Use the eigenvectors d_i as projection vectors & compute the dominance ratio**

$$\mathbf{DR} = \frac{\sum_{m=2}^{M}\left(\vec{\mathbf{d}}_1^{\mathbf{T}}\cdot\hat{\mathbf{S}}^{(m-1)}\right)\left(\vec{\mathbf{d}}_1^{\mathbf{T}}\cdot\hat{\mathbf{S}}^{(m)}\right)\Big/(\mathbf{N}-1)}{\sum_{m=1}^{M}\left(\vec{\mathbf{d}}_1^{\mathbf{T}}\cdot\hat{\mathbf{S}}^{(m)}\right)\left(\vec{\mathbf{d}}_1^{\mathbf{T}}\cdot\hat{\mathbf{S}}^{(m)}\right)\Big/\mathbf{N}}$$

$$var(\mathbf{DR}) \approx \frac{1}{\mathbf{N}}(1-\mathbf{DR}^2)$$

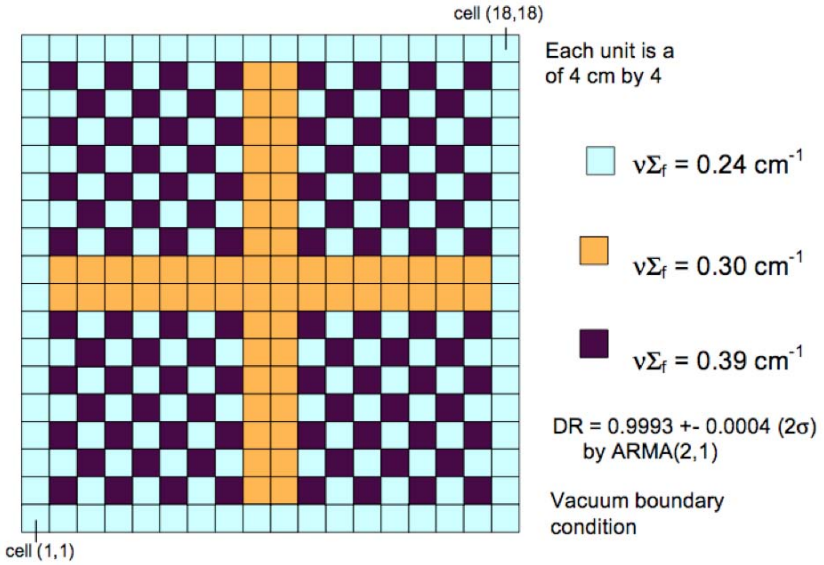
Example - Godiva Problem

- **Bare sphere of HEU**

	mesh size	matrix size	DR
F-matrix	2 x 2 x 2	8 x 8	.56
	4 x 4 x 4	64 x 64	.60
	8 x 8 x 8	512 x 512	.65
CMPM	2 x 2 x 2	8 x 8	.68 ± .03
ARMA(2,1) analysis			.63 ± .04

Example - 1-Group 2D Test Problem

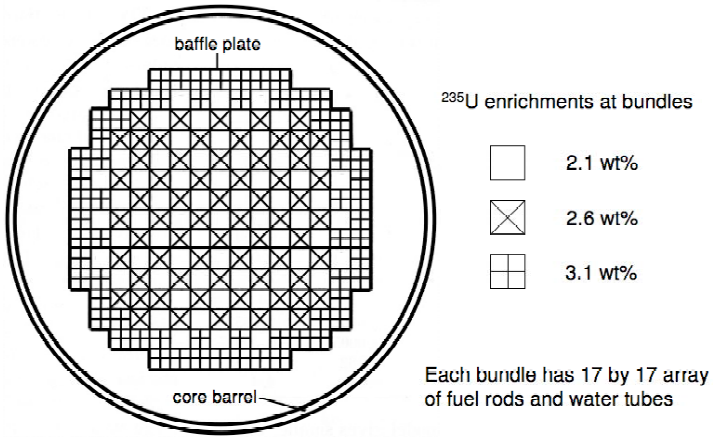
- **From Nease & Ueki**
  (NSE, Sept 2007)

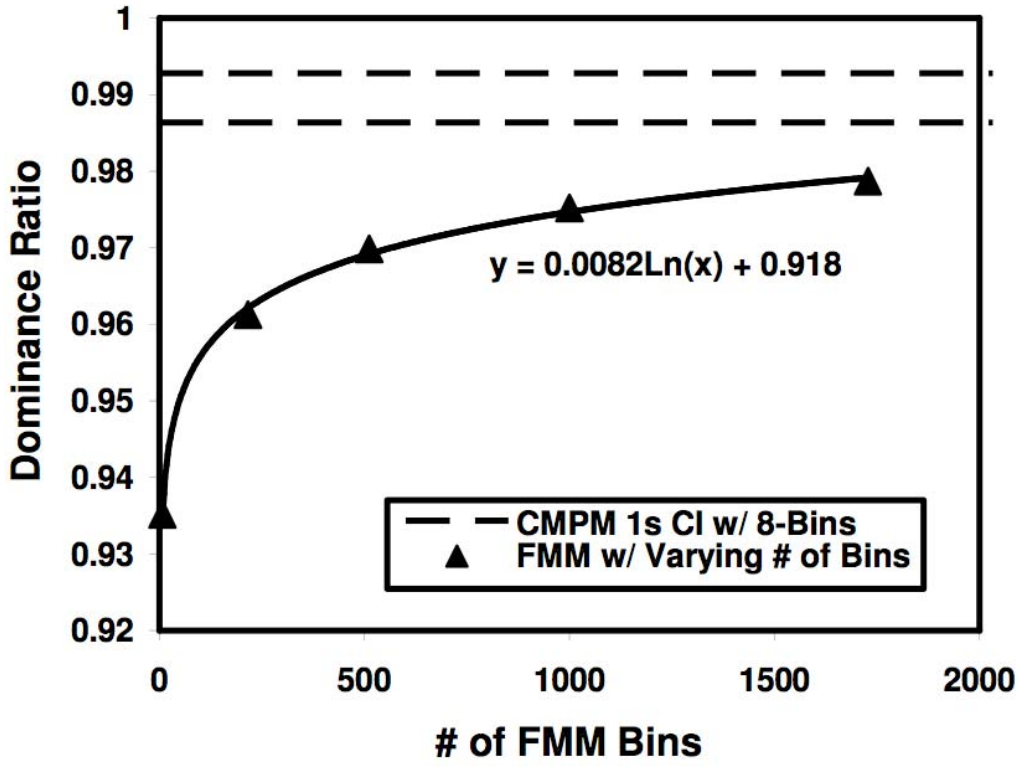


	mesh size	matrix size	DR
F-matrix	4 x 4 x 1	16 x 16	.988
	9 x 9 x 1	81 x 81	.993
	18 x 18 x 1	324 x 324	.997
CMPM	2 x 2 x 1	4 x 4	.998 ± .002
ARMA(2,1) (Ueki & Nease 2006)			.9993 ± .0004

Example - 3D PWR Problem

- **3D PWR as specified by Nakagawa & Mori, 1993**
  - Explicit fuel rods, water tubes, etc.
  - Includes plenum, top & bottom end plugs, top & bottom supports, etc.
  - Continuous-energy xsecs





Matrix size = (# bins)^2

Even with a 12 x 12 x 12 mesh,
& F-matrix 1728 x 1728,
DR from F-matrix gives large error

F-matrix method not practical for large 3D reactor problems

MCNP5 Implementation

- **Both methods for DR computation were added to test version of MCNP5**
- **Negligible extra CPU time for either method**
- **Fission matrix DR**
  - Can be determined early, **before convergence**
  - Sensitive to mesh size
  - Provides **approximate DR**
  - Useful for characterizing problem convergence
  - May be useful for automated convergence tests
- **Coarse Mesh Projection Method with time series analysis for DR**
  - Can only be used **after convergence**
  - Independent of mesh size
  - Provides **accurate DR**

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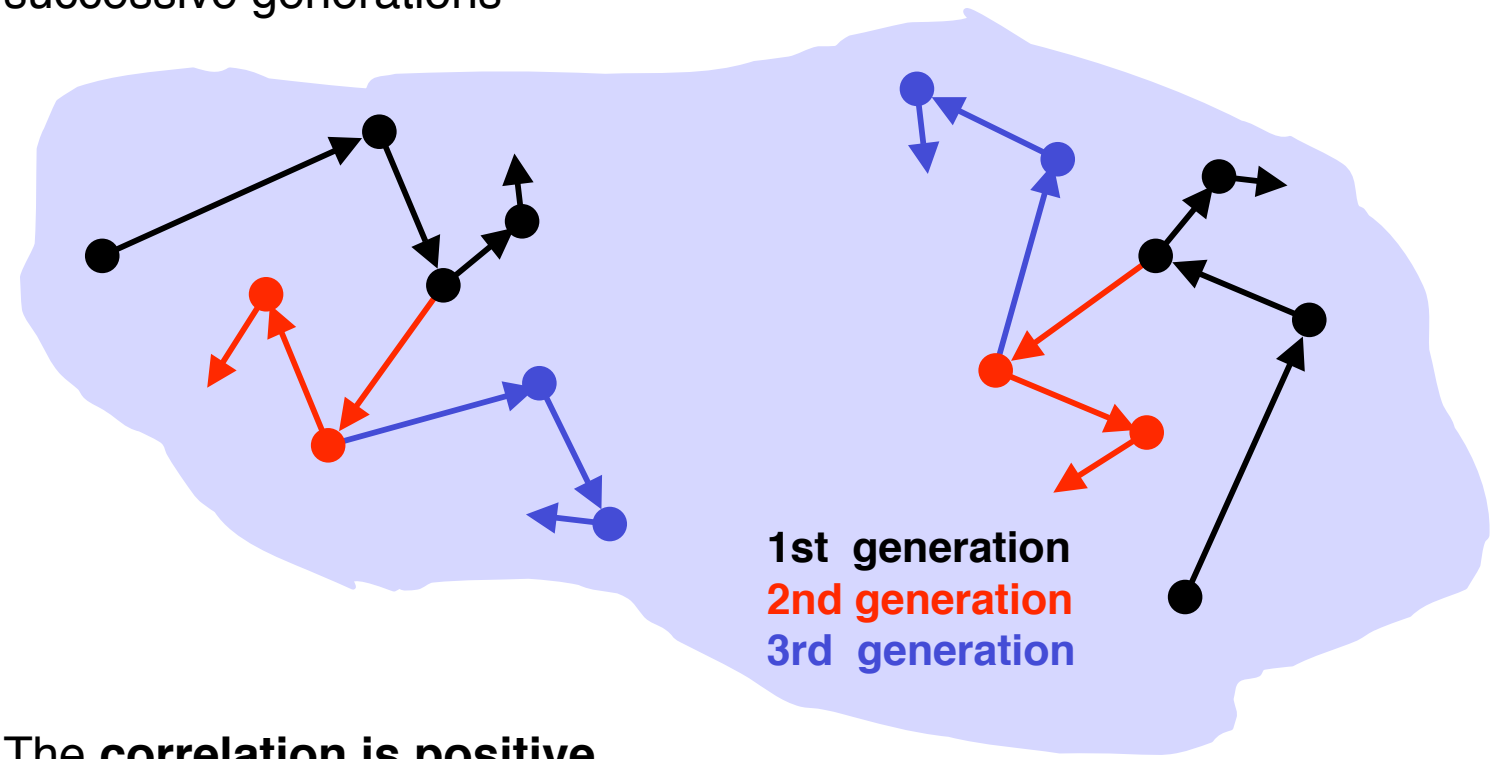
Underprediction Bias in Confidence Intervals

in Monte Carlo Keff Calculations

Tallies & Correlation

- **MC eigenvalue calculations are solved by power iteration**
  - A **generation model** is used in following neutron histories
  - Tallies from one generation (including K) are **correlated** with tallies in successive generations



  - The **correlation is positive**
  - Spatial locations of fission sites in one generation tend to be (somewhat) near the fission sites from the previous generation

Bias in σ^2

- **For tally X, made N times** **(for large N)**

$$\bar{X} = \frac{\sum_{n=1}^{N} X_n}{N} \quad = \quad \text{mean value of X}$$

$$\tilde{\sigma}^2_{\bar{X}} = \frac{1}{N} \cdot \left(\frac{\sum_{n=1}^{N} X_n^2}{N-1} - \bar{X}^2 \right) \quad = \quad \text{variance computed by codes, assuming independence of } X_n\text{'s}$$

$$\sigma^2_{\bar{X}} \approx \tilde{\sigma}^2_{\bar{X}} + \tilde{\sigma}^2_{\bar{X}} \cdot 2 \cdot \sum_{i=1}^{\infty} r_i \quad = \quad \text{True variance, including correlations; } r_i = \text{ lag-i correlation coef. between } X_n\text{'s}$$

- **(True σ^2) > (computed σ^2), since correlations are positive**

$$\frac{\text{True } \sigma^2_{\bar{X}}}{\text{Computed } \sigma^2_{\bar{X}}} = \frac{\sigma^2_{\bar{X}}}{\tilde{\sigma}^2_{\bar{X}}} \approx 1 + 2 \cdot \left(\begin{array}{c} \text{sum of lag-i correlation} \\ \text{coeff's between tallies} \end{array} \right)$$

Variance underprediction bias is **independent of N and M**

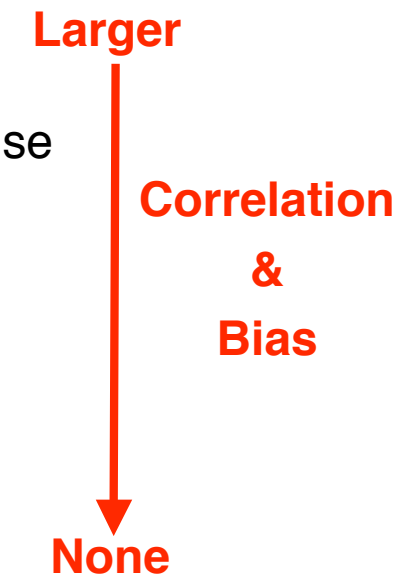
Correlation vs Tallies

- **MC codes ignore correlation in tallies when computing σ^2's**
- **σ^2's computed by MC codes are always too small**

$$\frac{\text{True } \sigma^2_{\bar{x}}}{\text{Computed } \sigma^2_{\bar{x}}} = 1 + 2 \cdot \left(\begin{array}{l} \text{sum of lag-i correlation} \\ \text{coeff's between tallies} \end{array} \right)$$

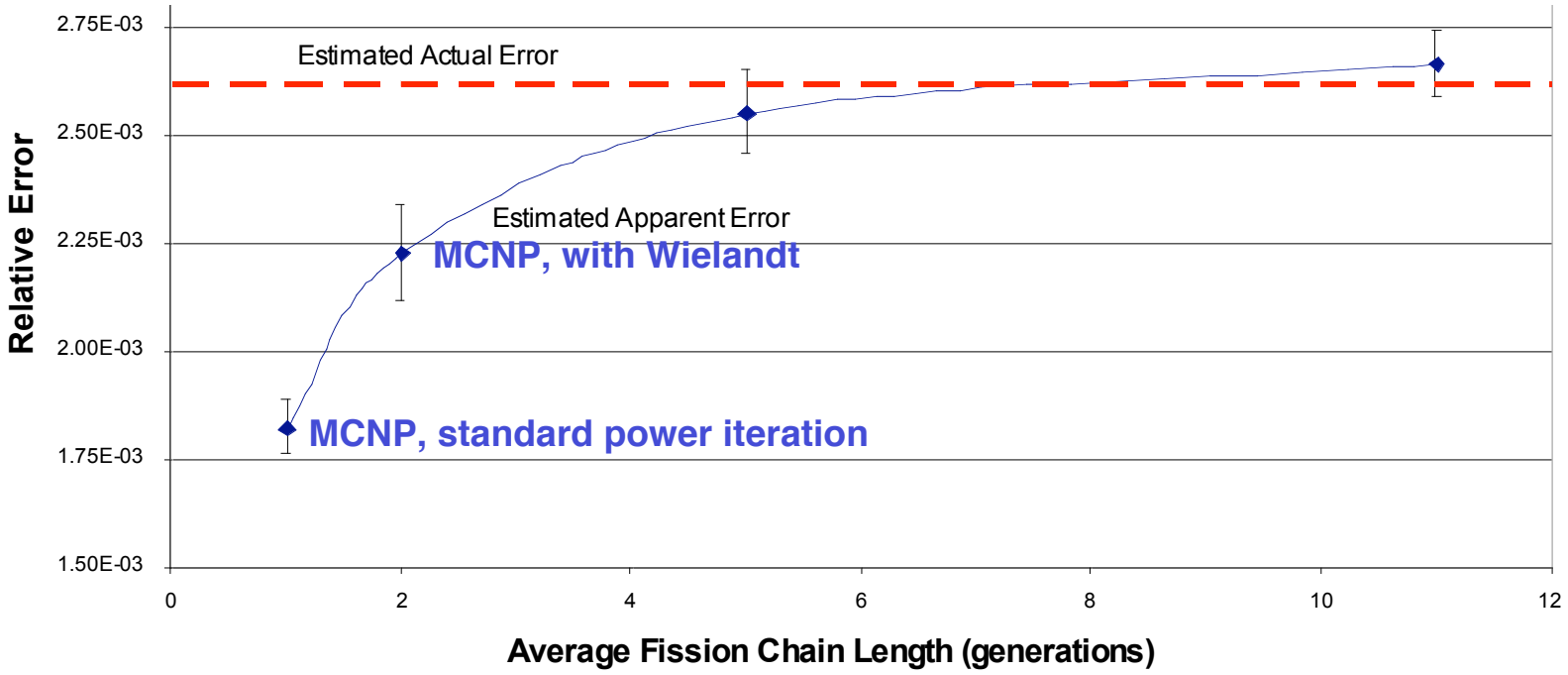
- **The size of underprediction bias in σ^2's depends on how tallies are performed:**

MCNP:	generation tallies for Keff, **history** tallies for everything else
VIM, RACER, RCP, …:	**generation** tallies
MCNP+Wielandt, MONK:	**several generations**
Repeated MC runs, averaged:	**all generations** from each run



Example - Godiva with Region tallies

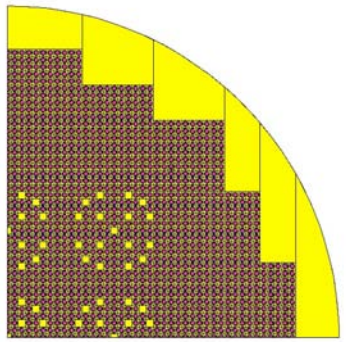
- **Bare HEU sphere, with 3x3x3 mesh tallies of flux**
  - Examine center element flux tally
  - Calculate true relative error (RE) from independent jobs
  - Compare with MCNP computed RE

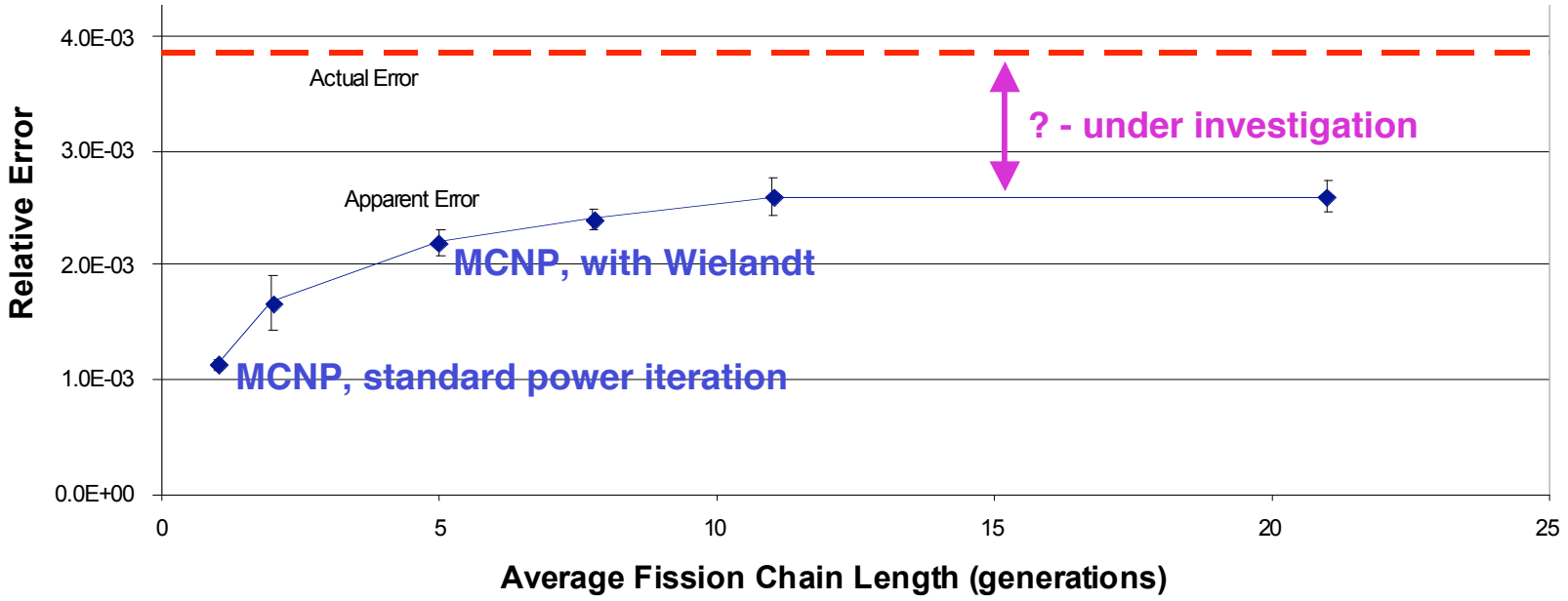


  - Standard MCNP calculation underestimates RE by ~ 30% for this very simple problem with DR ~ .63

Example - B&W XI-2 Critical

- **B&W benchmark, with 3x3 mesh tally in inner core**
  - Examine center element flux tally
  - Calculate true relative error (RE) from independent jobs
  - Compare with MCNP computed RE





  - Standard MCNP calculation underestimates RE by factor of ~ 4x for this problem with DR ~ .91

Approximate Correction for Bias in σ^2

$$\frac{\text{True } \sigma^2_{\bar{x}}}{\text{Computed } \sigma^2_{\bar{x}}} = 1 + 2 \cdot \left(\begin{array}{c} \text{sum of lag-i correlation} \\ \text{coeff's between tallies} \end{array} \right)$$

- **MacMillan assumed**
  - Easy to compute $\mathbf{r_1}$ during MC, lag-1 correlation coefficient for a tally
  - Not practical to compute lag-i correlations for all $i > 1$
  - Assume:

$$\mathbf{r_i} \approx \mathbf{r_1} \cdot \rho_1^{\,i}, \qquad \text{where} \quad \rho_1 = \text{dominance ratio, } k_1 / k_0$$

This is a **conservative** assumption, ie, (true r_i) < (assumed r_i)

Then

$$\frac{\text{True } \sigma^2_{\bar{x}}}{\text{Computed } \sigma^2_{\bar{x}}} = 1 + \frac{2 \cdot r_1}{1 - \rho_1}$$

  - Difficulties: Usually don't know the dominance ratio.
    Computed r_1's may be unreliable due to MC noise.
    Conservative, no way to estimate by how much.

Some Recent Work

Kiedrowski & Brown

Variance bias is caused by correlation

- **The mutual information between 2 source distributions separated by J cycles is**

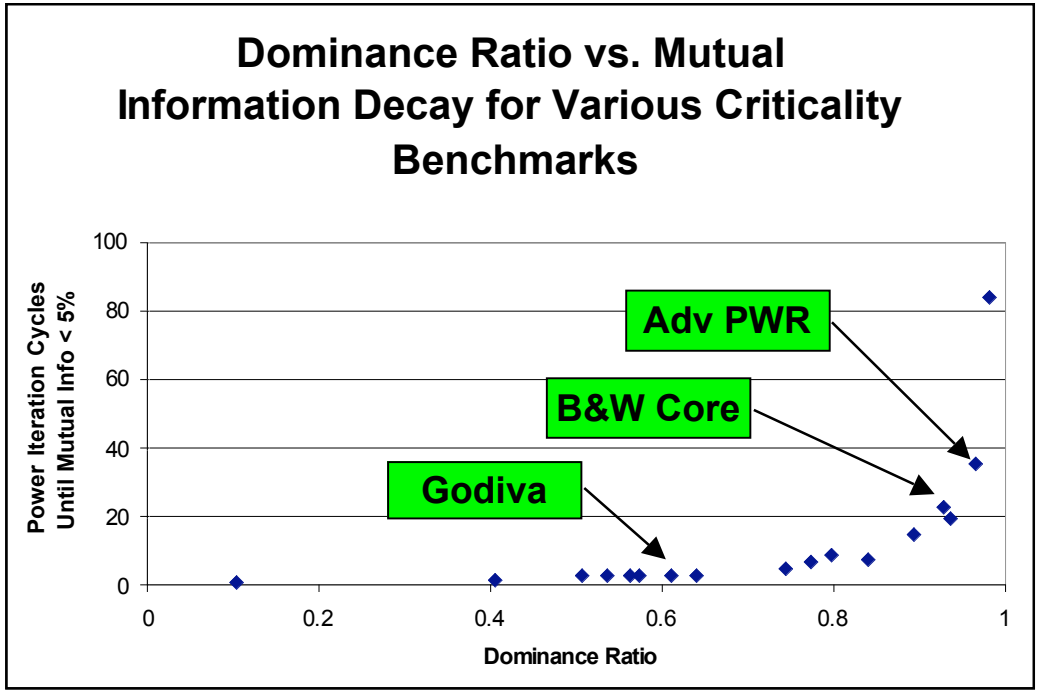
  $$MI = E_I\{ H(S_{I+J}) - H(S_{I+J} \mid S_I) \}$$

- **For a number of problems, determine the number of cycles J for the relative mutual information to fall below 5% (ie, so that correlation effects are small)**

- **Plot J vs the Dominance Ratio**

- **Strongly suggests that problems with high DR show more correlation, hence larger bias in confidence intervals**

- **More to come …..**



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Wielandt Acceleration

(For <u>future</u> versions of MCNP5)

Inspired by: T. Yamamoto & Y. Miyoshi, J. Nucl. Sci. Technol. 41, No 2, 99-107 (2004)

Wielandt Method

- **Basic transport equation for static eigenvalue problems**

$$(L + T - S)\Psi = \frac{1}{K_{eff}} M\Psi$$

L = loss to leakage
T = loss to collisions
S = gain from scatter-in
M = gain from fission multiplication

- **Define a fixed parameter k_e such that $k_e > k_0$ (k_0 = exact eigenvalue)**

$$k_e = k_0 + \Delta, \qquad \Delta > 0$$

- **Subtract $\frac{1}{k_e} M\Psi$ from each side of the transport equation**

- **Solve the modified transport equation by power iteration**

$$(L + T - S - \frac{1}{k_e} M)\Psi^{(n)} = (\frac{1}{K_{eff}^{(n-1)}} - \frac{1}{k_e})M\Psi^{(n-1)}$$

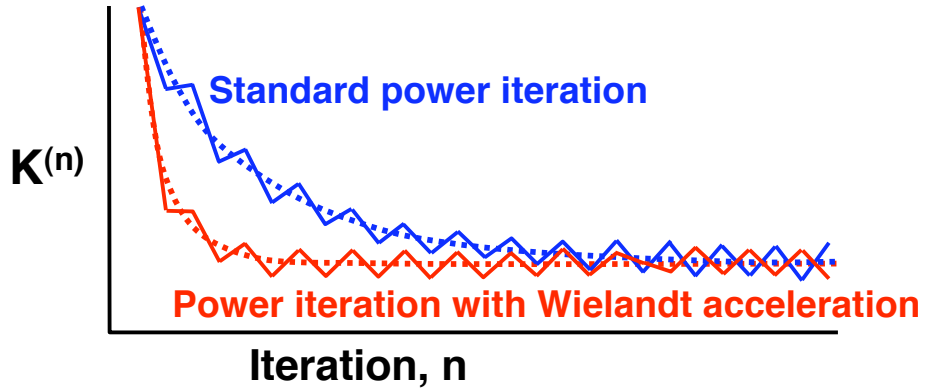
Convergence

- **Eigenfunctions for Wielandt method are same as for basic power iteration, but the eigenvalues are shifted**

- **The dominance ratio for Wielandt method is always smaller than for power iteration**

$$\rho_{Wielandt} = \frac{k_e - k_0}{k_e - k_1} \cdot \rho_{Power} \qquad \rho = \frac{k_1}{k_0} < 1, \qquad k_e > k_0 > k_1 > \ldots$$

$\Rightarrow$ Wielandt method will converge in fewer iterations



Monte Carlo Interpretation

- **Power iteration with Wielandt acceleration**

$$(L + T - S - \frac{1}{k_e} M)\Psi^{(n)} = (\frac{1}{K_{eff}^{(n-1)}} - \frac{1}{k_e})M\Psi^{(n-1)}$$

Fission neutrons to follow in current iteration

Fission neutron source from previous iteration

- **During neutron random walk, at each collision in fissile material:**

Create these neutrons in the current iteration

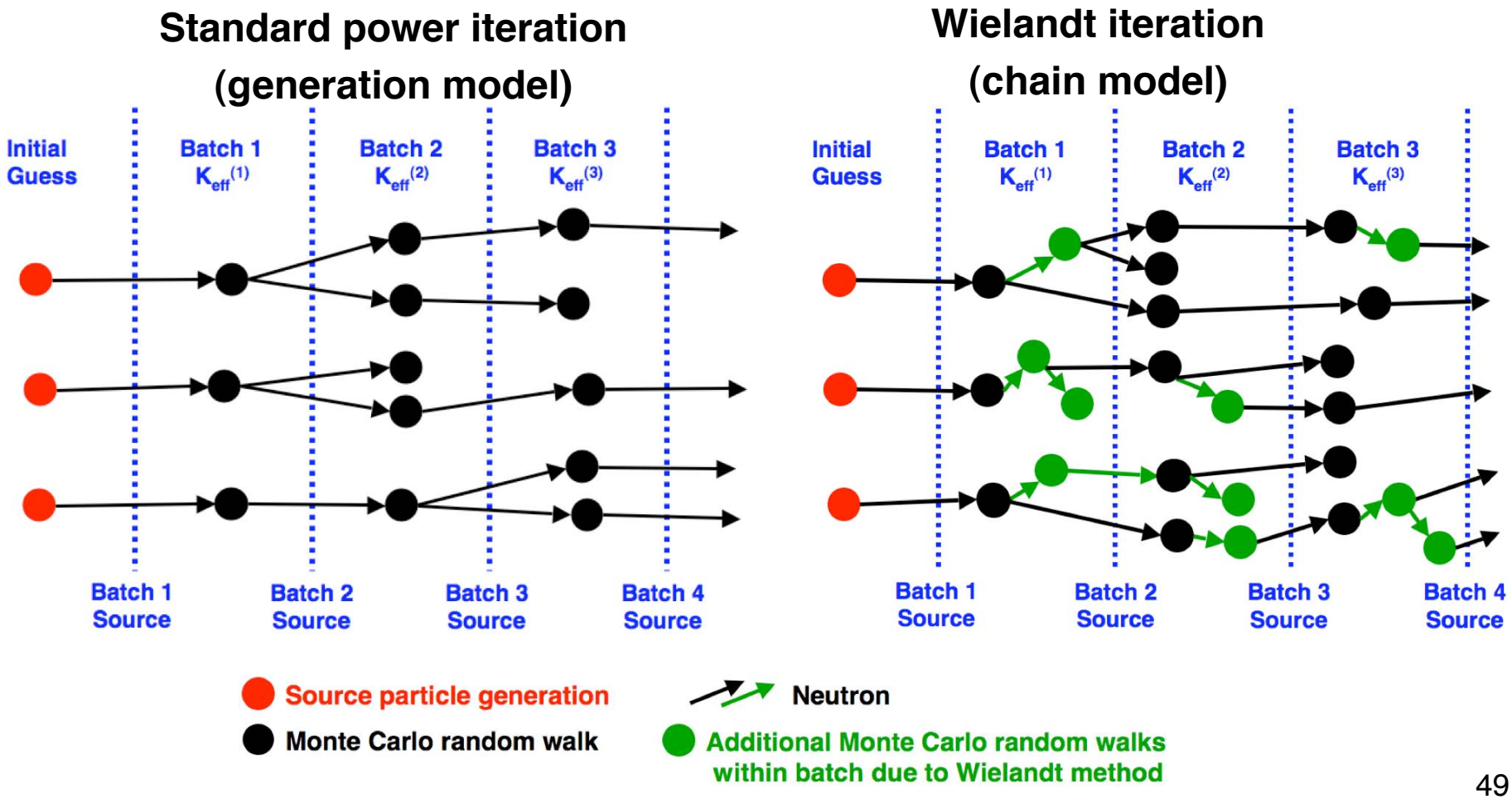
$$n'_e = \left\lfloor wgt \cdot \frac{\nu\Sigma_F}{\Sigma_T} \cdot \frac{1}{k_e} + \xi \right\rfloor$$

Save these neutrons as the source for the next iteration

$$n'_F = \left\lfloor wgt \cdot \frac{\nu\Sigma_F}{\Sigma_T} \cdot \left(\frac{1}{K^{(n-1)}} - \frac{1}{k_e} \right) + \xi \right\rfloor$$

Generations vs Iterations

- **Power method:** one neutron generation per iteration
- **Wielandt method:** multiple neutron generations per iteration, varies for each starting neutron

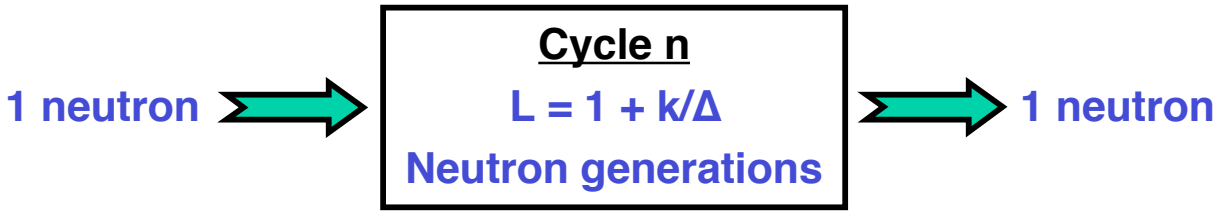


Choosing $k_e = k + \Delta$

- In MCNP, the collision estimator is used for $k_{eff}^{(n-1)}$, so that

$$k_e^{(n)} = k_{col}^{(n-1)} + \Delta$$

- For cycle n, average number of fission generations per source neutron



For k ~ 1: $\Delta = \infty$, L = 1 $\Delta = .5$, L = 3 $\Delta = .05$, L = 21
$\Delta = 1$, L = 2 $\Delta = .1$, L = 11 $\Delta = .01$, L = 101

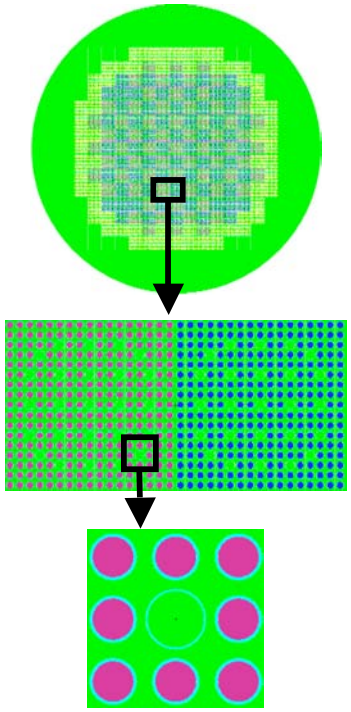
Typical: $\Delta = .1$, .05, or .025

Smaller Δ $\Rightarrow$ larger average chain length, L
$\Rightarrow$ more spread in fission sites each cycle
$\Rightarrow$ faster convergence

Numerical Testing

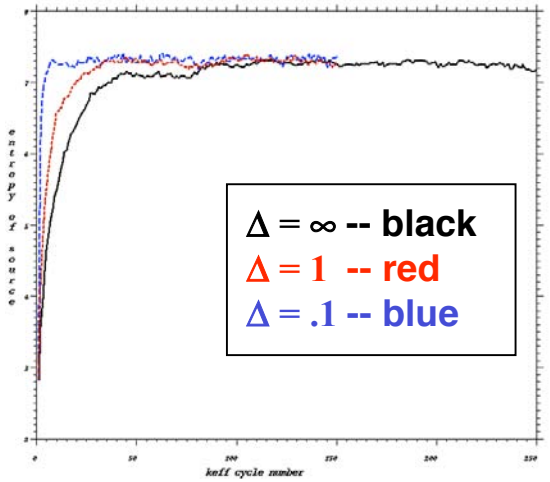
2D PWR test problem

- $K_e^{(n)} = k_C^{(n-1)} + \Delta$
- Repeat calculations with different Δ's
- Plot # iterations to converge H_{src} vs Δ

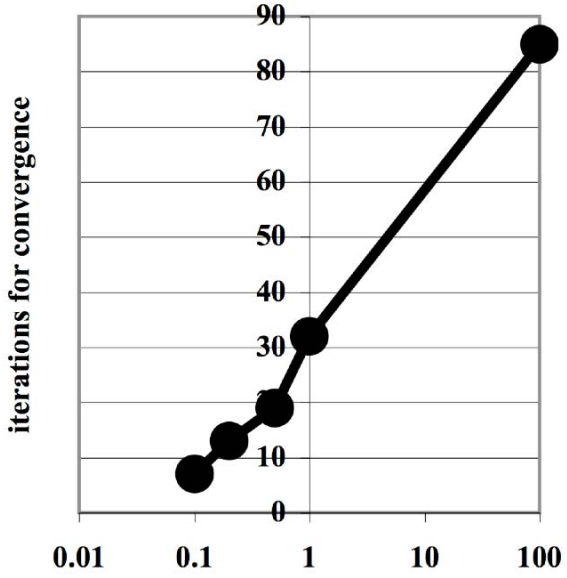


DR = .97

Convergence of H_{src} vs Δ

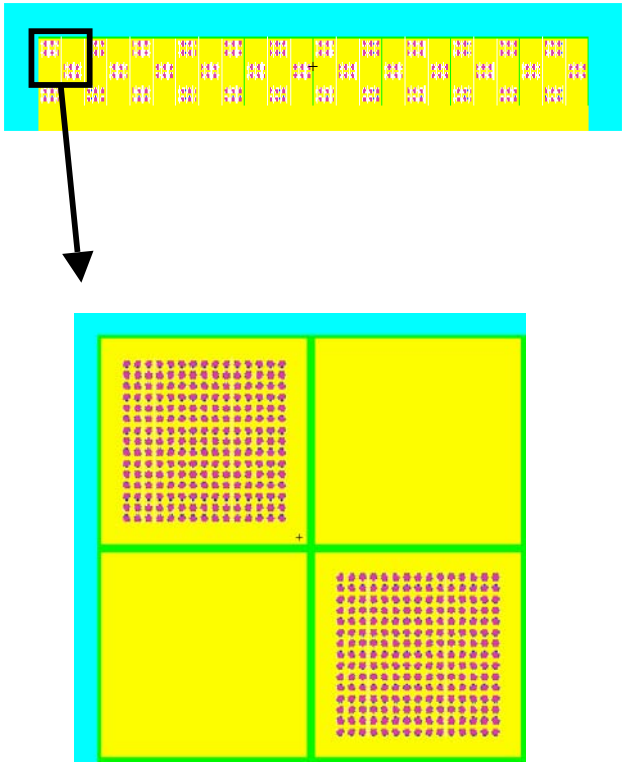


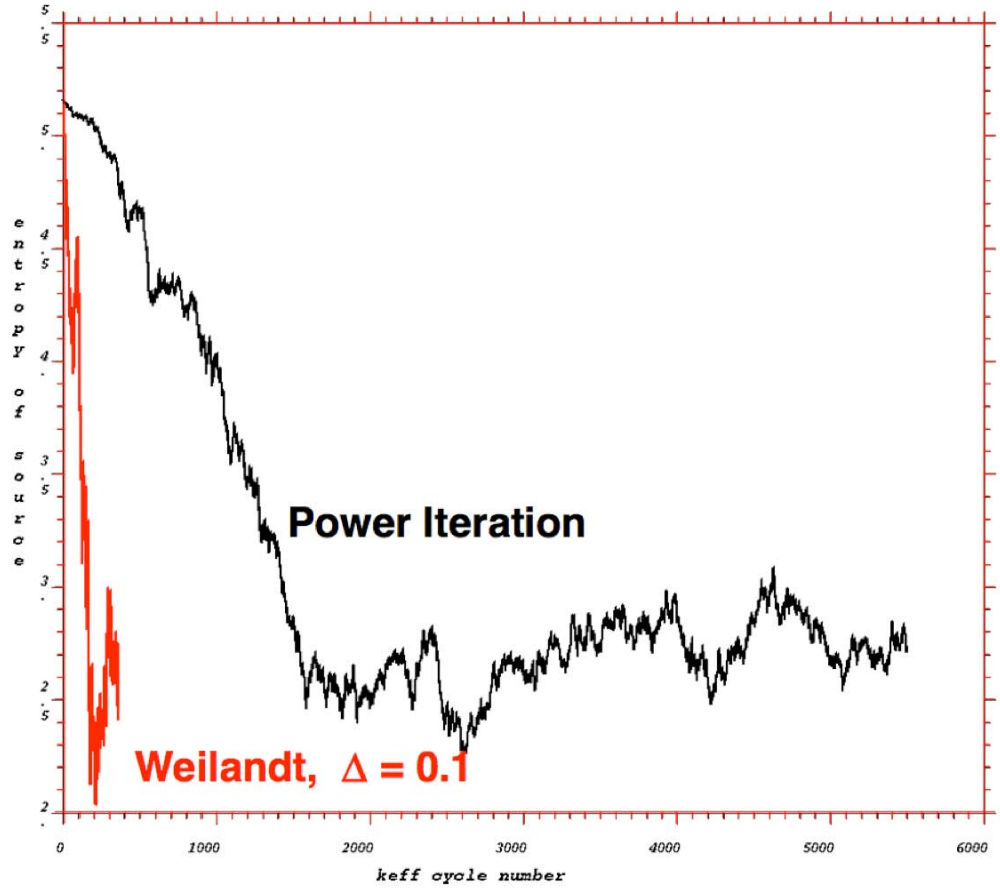
Iterations for convergence vs Δ



Numerical Testing

- **Fuel Storage Vault (Problem OECD_bench1)**





200 2000

DR = .99+

Wielandt Method - Summary

- **Wielandt Method:**
  - **Faster convergence rate than power iteration ⇒ fewer iterations**
  - **Some of the particle random walks are moved from the next generation into the current generation ⇒ more work per iteration**
  - **Same total number of random walks ⇒ no reduction in CPU time**
- **Advantages**
  - **Reduced chance of false convergence for very slowly converging problems**
  - **Reduced inter-generation correlation effects on variance**
  - **Fission source distribution spreads more widely in a generation (due to the additional particle random walks), which should result in more interactions for loosely-coupled problems**

⇒ Wielandt method will be included in future versions of MCNP5

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Iterated Fission Probability

Introduction

- **The need for adjoints**
  - For calculating kinetics parameters, β_{eff} & Λ_{eff}, need tallies for prompt & delayed neutrons that are adjoint-weighted
  - Sensitivity-uncertainty analysis for cross-section data needs adjoints & forward fluxes
- **The difficulty for Monte Carlo**
  - Multigroup adjoint calculations are easy
  - Continuous-energy adjoint calculations involve "running things backwards", and involve some approximations to the physics
- **An alternative**
  - Iterated fission probability

Introduction

- **G. R. Keepin, Physics of Nuclear Kinetics, p. 163, 1965**

The fundamental-mode **adjoint flux** $\Phi_0^*(r,v)$ has the physical significance of being **proportional to the asymptotic power level resulting from the introduction of a neutron of velocity v, at point r in a critical system at zero power**. It is thus a measure of the "**importance**" or "worth" of a neutron as a function of energy and position of the neutron.

Introduction

- **Henry Hurwitz, Jr., "Physical Interpretation of the Adjoint Flux: Iterated Fission Probability", pp 864-869, Naval Reactors Physics Handbook, 1964**

A definition now follows for a function, *F(r,u)*, called the **iterated fission probability**, according to the following occurrences visualized for a reactor which is just critical:

Let a neutron be introduced in the assembly, which is assumed to be just critical, at point *r* and with lethargy *u.* This neutron will, on the average, produce a certain number of fissions with a certain spatial distribution. Neutrons from these fissions will produce further fissions, etc., each succeeding generation having a distribution closer to the actual power distribution in the operating assembly. Furthermore, since the assembly is critical, the number of fissions produced in the nth generation will approach a limit as *n* approaches infinity, and this limit is defined as *F(r,u).*

F(r,*u)* is similar to the probability *P(r,u)* that a neutron introduced at point r with lethargy *u* will produce a fission. … The relation between *F* and *P* can be crudely expressed by saying that ***F* is the infinite order iteration of *P***. … ***F(r,u)* is proportional to the self-consistent adjoint function, $\Phi^*(r,u)$,** … *P(r,u)* is proportional to the constant source adjoint function.

Comments

- **In 2 recent papers, Feghi, Shahriari, & Afarideh have described using a rudimentary implementation of the iterated fission probability to compute adjoints & lifetimes**
  - MCNIC method - Monte Carlo neutron importance calculation
  - Script or program runs a series of MCNP fixed source calculations, to get the total neutron production from entire fission chains; tallied at the corresponding source points
  - This can be considered proof-of-principle (there have been others in the past…)
- **R&D is underway to integrate the iterated fission probability concept into standard Monte Carlo iterations (perhaps with Wielandt's method)**
  - There is the possibility that adjoint-weighted tallies could be performed at very little extra cost, in direct Monte Carlo calculations
  - Look for this at PHYSOR-2010

References

G. R. Keepin, Physics of Nuclear Kinetics, p. 163 (1965)

Henry Hurwitz, Jr., "Physical Interpretation of the Adjoint Flux: Iterated Fission Probability", pp 864-869, Naval Reactors Physics Handbook (1964)

A.F. Henry, Nuclear Reactor Anaylsis, MIT Press (1975)

R.K. Meulekamp & S.C. van der Marck, "Calculating the Effective Delayed Neutron Fraction with Monte Carlo", Nucl. Sci. Eng. 152, 142-148 (2006)

S.A.H. Feghi, M. Shahriari, H. Afarideh, "Calculation of neutron importance function in fissionable assemblies using Monte Carlo method", Ann. Nuc. Energy 34, 514-520 (2007)

S.A.H. Feghi, M. Shahriari, H. Afarideh, " Clalculation of the importance-weighted neutron generation time using MCNIC method", Ann. Nuc. Energy 35, 1397-1402 (2008)

Temperature Dependence

Temperature Dependence

- **Temperature effects on Monte Carlo**
- **Accounting for temperature effects in MCNP**
  - **Generate NJOY libraries during NTH iterations**
  - **Generate NJOY libraries prior to the NTH iterations**
  - **Pseudo-materials approach**
- **Applications**
  - **Explicit coupling of MCNP5 and Star-CD for LWR configurations**
  - **Explicit coupling of MCNP5 and RELAP-Athena for full-core VHTR simulation**

Acknowledgements

- **Results for the STAR-CD/MCNP coupling were provided by Professor Tom Downar at the University of Michigan (UM). Also contributing to this work were Drs. Yunlin Xu and Volkan Seker, who are now at the UM.**

- **The following faculty and students at the UM contributed to the work on pseudo-materials and RELAP5/MCNP coupling:**
  - John C. Lee, Professor
  - Wei Ji, former PhD candidate (now Professor at RPI)
  - Gokhan Yesilyurt, PhD candidate
  - Jeremy Conlin, PhD candidate
  - Kaushik Banerjee, PhD candidate
  - Etienne de Villèle, former exchange student at UM

Temperature Dependence

- **Temperature effects on Monte Carlo calculations**
  - **Thermal expansion: changes in dimensions and densities**
  - **Cross-section data:**
    - Need to Doppler broaden cross sections including resolved and unresolved resonances (probability tables)
    - Need to change S(α,β) thermal scattering kernel

- **For most Monte Carlo codes, temperature effects must be handled explicitly by the code users**
  - **Input changes are required to account for dimension & density changes**
  - **Must use cross-section data generated at the correct problem temperatures**
- **MCNP**
  - Automatically Doppler broadens elastic scattering cross-sections
  - Does NOT adjust:
    - resolved resonance data
    - unresolved resonance data
    - thermal scattering kernels

Approaches to account for temperature changes:

A. Generate explicit temperature – dependent cross section libraries (NJOY)

B. Modify existing libraries (MAKXSF)

C. Approximate approach using pseudo-materials

A. Generate explicit temp-dependent datasets (NJOY)

- **Use NJOY (or similar cross-section processing code) to generate nuclear cross-section datasets**
  - Must generate a separate dataset for each nuclide at each region temperature
  - NJOY routines take care of Doppler broadening (resolved & unresolved) & thermal scattering kernels
- **Two approaches:**
  - **Iterative NJOY updates**: run NJOY **during** the neutronic-thermal/hydraulic (NTH) iterations for each temperature needed for the current T/H calculation.
  - **Pregenerated NJOY libraries**: run NJOY **beforehand** for a range of temperatures that adequately covers the temperatures expected for the NTH calculation, e.g., every 5K from 300K to 1200K for fuel nuclides.

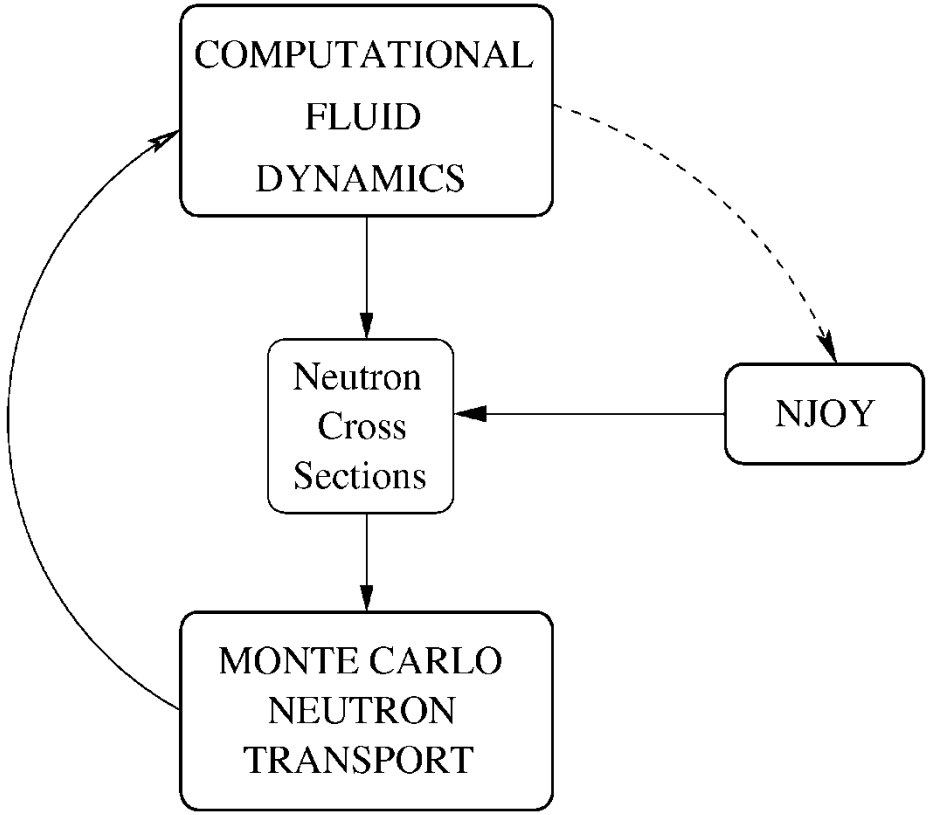
Computational results (Downar, Monterey 2007)

- **Iterative NJOY updating** is very time-consuming
  - 95 s to prepare a dataset for U-235 on 3 Ghz Pentium P4.
  - Not practical for realistic reactor applications.

- **Pregenerated NJOY libraries** is a reasonable approach
  - Used to couple STAR-CD and MCNP
  - NJOY was run at 5K temperature increments over the temperature range. (Temperature increments of 1-2 K cause memory problems with MCNP.)
  - A Perl script was used to manage the NTH iterations.
  - The coupled code system (**McStar**) was applied to a 1/8 pin cell and a 3x3 array of pin cells.
  - Good agreement with DeCart/STAR-CD results

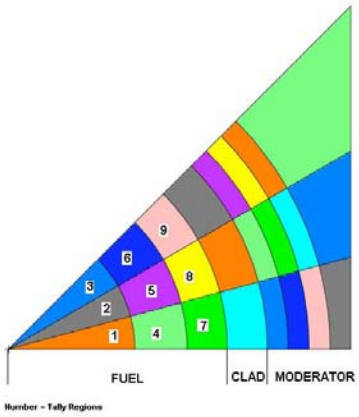
McSTAR

- Monte Carlo Neutron Transport : MCNP5
- Computational Fluid Dynamics : STAR-CD
- Cross Sections: NJOY

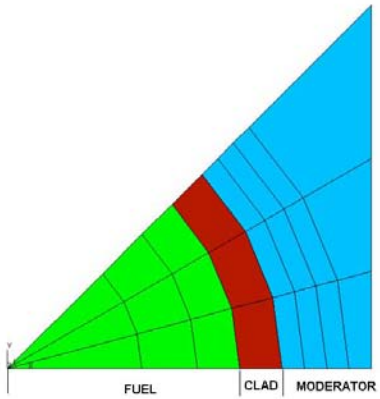


Results: coupled STAR-CD and MCNP results

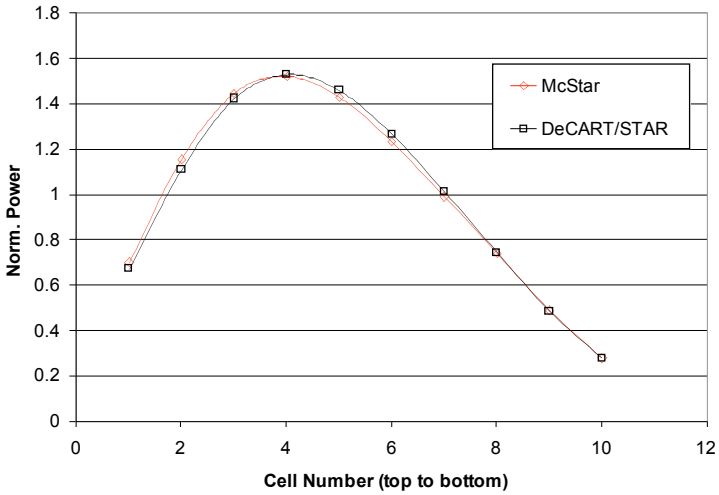
1/8 pin cell



MCNP MODEL

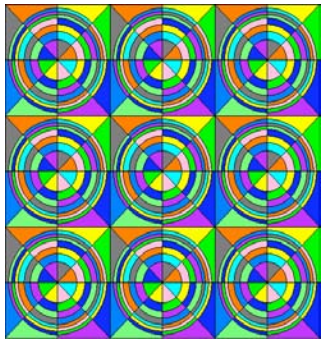


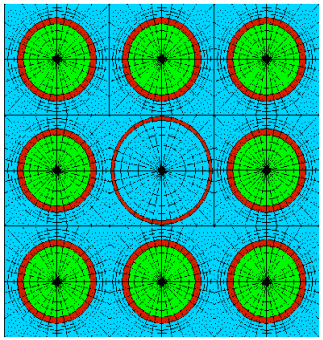
STAR-CD MODEL



keff agrees within 52 pcm with DeCart/STAR-CD

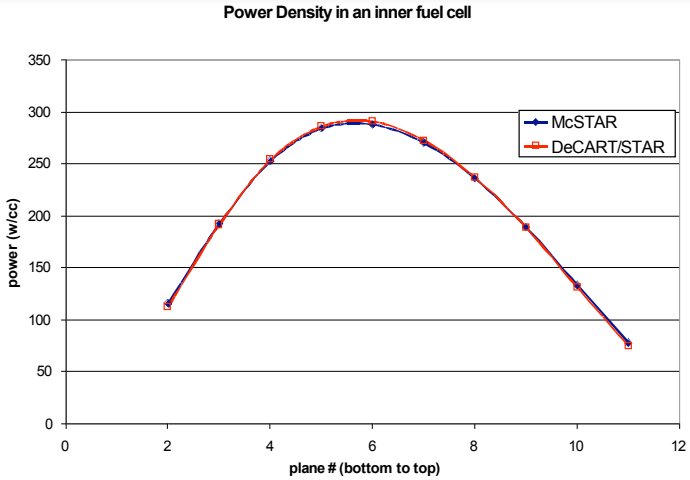
3x3 array of pin cells





•MCNP

•STAR-CD



keff agrees within 66 pcm with DeCart/STAR-CD

Preliminary conclusions for McStar

- The preliminary results for two simple PWR test problems demonstrate the feasibility of coupling Monte Carlo to CFD for a potential audit tool.
- Validation of the cross section update methodology was performed to assess the accuracy of the 5K increment tables for these problems.
- McSTAR is now being applied to advanced BWR fuel assemblies with strong axial heterogeneities to verify the accuracy of the 2D/1D solution methods in DeCART

B. Modify exisiting MCNP library (MAKXSF)

- **New version of MAKXSF**
- **Subset of NJOY routines, easy to use, part of MCNP5/1.50 distribution**
- **For ACE datasets (for MCNP), makxsf performs:**
  - Doppler broadening of resolved resonance data (explicit profiles)
  - Interpolation of unresolved resonance data (probability tables) between ACE datasets at 2 different temperatures
  - Interpolation of thermal scattering kernels (S(α,β) data) between ACE datasets at 2 different temperatures
- **For now, makxsf is run external to MCNP**
- **Long-term plan: put the makxsf routines in-line with the MCNP coding**

C. Approximate method: pseudo-materials

- **"Pseudo-materials" for temperature dependence**
  - Equivalent to **"stochastic interpolation"**
  - To approximate the cross-sections for nuclide X at temperature T, use a **weighted combination of nuclide X at lower temperature T_1 and higher temperature T_2**
  - This weighted combination is input as an MCNP5 material with volume fractions given by the weights

$$w_2 = \frac{\sqrt{T} - \sqrt{T_1}}{\sqrt{T_2} - \sqrt{T_1}}, \quad w_1 = 1 - w_2$$

$$\Sigma_i = \Sigma(T_i)$$

$$\Sigma(T) = w_1 \cdot \Sigma_1 + w_2 \cdot \Sigma_2$$

Pseudo-materials example – MCNP input

Example: ^{235}U at 500 K

Existing datasets for MCNP:

(1) dataset for ^{235}U at **293.6** K: **92235.66c**

(2) dataset for ^{235}U at **3000.1** K: **92235.65c**

Weight the datasets using $T^{1/2}$ interpolation

$$w_2 = \frac{\sqrt{500}-\sqrt{293.6}}{\sqrt{3000.1}-\sqrt{293.6}} = .1389, \qquad w_1 = .8611$$

In the MCNP input:

```
m1      92235.66c   .8611      92235.65c  .1389
```

Application: VHTR geometry*

Normal: explicit NJOY at given temperature
Pseudo: interpolate between closest NJOY libraries (every 100K)

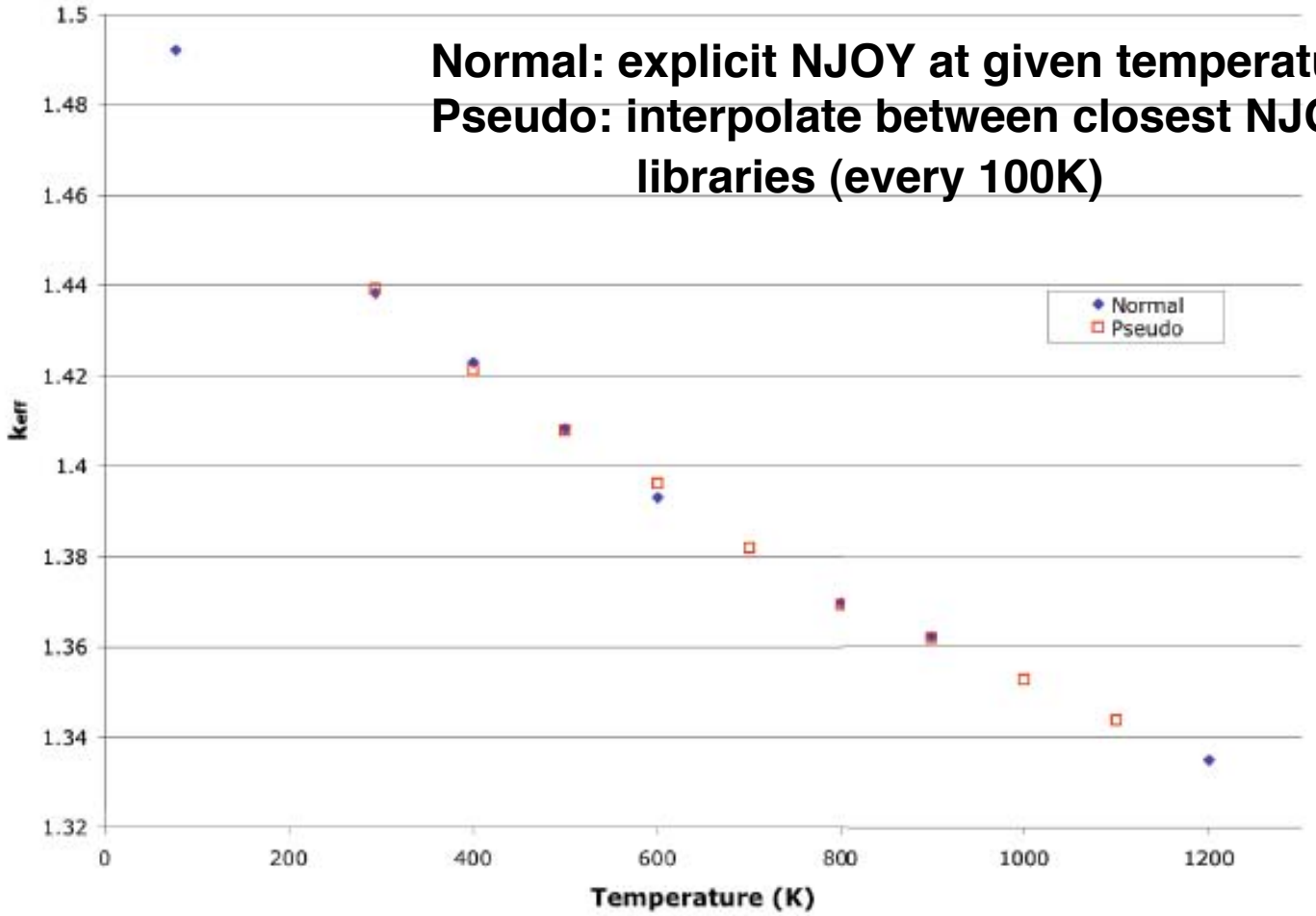


Figure 1. Comparison of k_{eff} between normal and pseudo materials with the VHTGR geometry.

*JL Conlin, W Ji, JC Lee, WR Martin, "Pseudo-Material Construct for Coupled Neutronic-Thermal-Hydraulic Analysis of VHTGR", Trans. ANS 91 (2005)

Application – LWR configuration

Results for LWR configuration with NJOY cross sections at 325K compared to pseudo-material approach using cross sections at 300K and 350K. Most deviations within statistics. (Downar, 2007 Monterey M&C)

	325 K (NJOY)	325 K Interpolated	Deviation
k_{eff}	1.40974 (± 0.00043)	1.41008 (± 0.00044)	34 pcm
ϕ in Fuel	1.37933 (± 0.0003)	1.37929 (± 0.0003)	0.00003
$\sigma_{aF}\phi$	3.67362e-03 (± 0.0006)	3.67648E-03 (± 0.0006)	0.0008
$\sigma_{f}\phi$	5.62964e-03 (± 0.0007)	5.63817E-03 (± 0.0007)	0.0010
$\nu\sigma_{f}\phi$	1.38341e-02 (± 0.0007)	1.38548e-02 (± 0.0007)	0.0010

Application – full core VHTR with T/H feedback

- **MCNP5 code was coupled with the RELAP5-3D/ATHENA code to analyze full core VHTR with temperature feedback (pseudo-materials) including explicit TRISO fuel**

- Utilized a master process supervising independent computing platforms to automate coupled Nuclear-Thermal-Hydraulic (NTH) calculations.

- Axial power fractions determined for 10 axial zones for each of three rings by MCNP5 are input to RELAP5 to determine assembly-average temperature distributions.

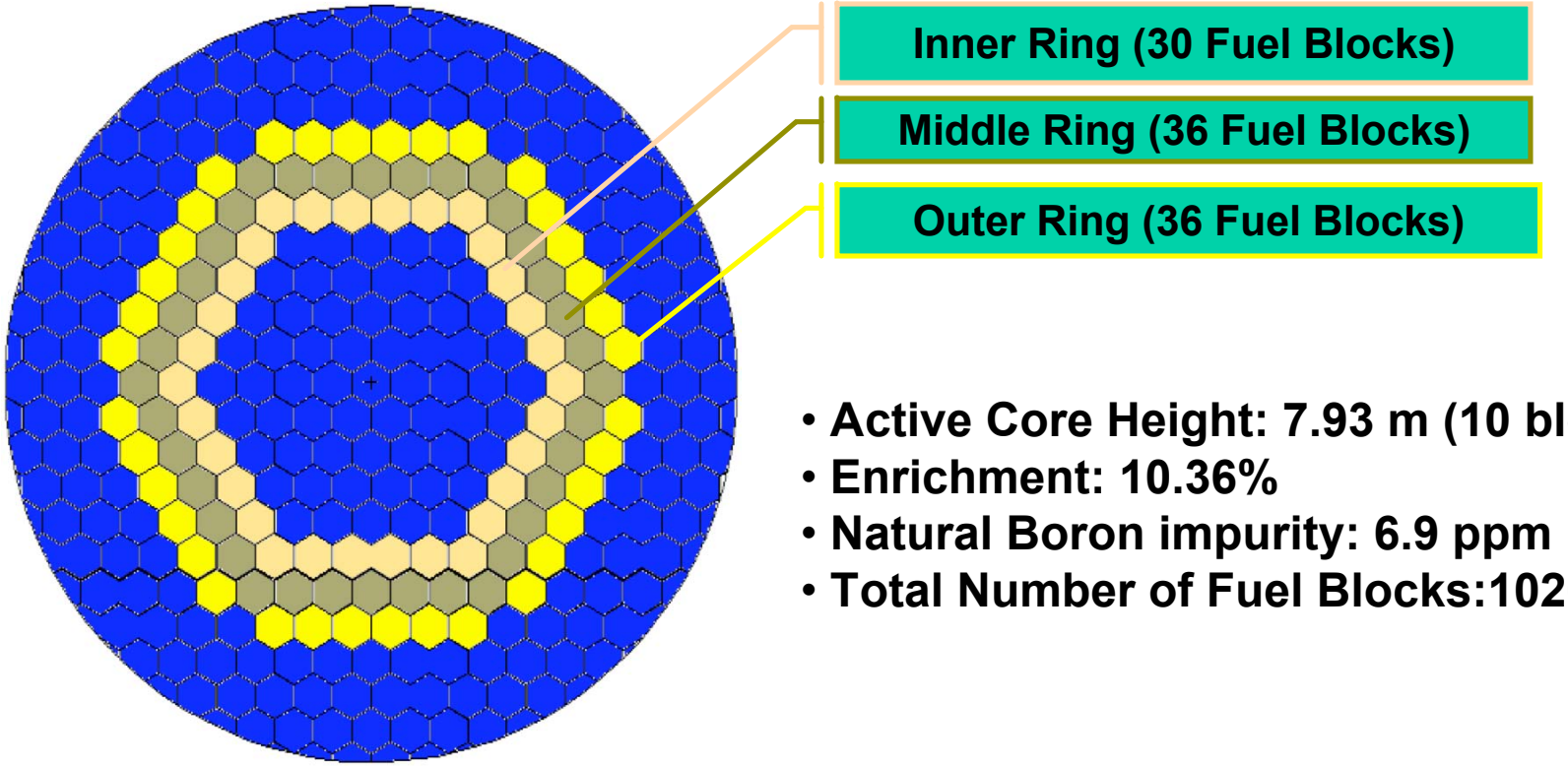
- Updated RELAP5 temperature distributions are used for the next MCNP simulation to obtain updated power fractions. MCNP5 and RELAP5 iterations were performed in a cyclic fashion until convergence in temperature and power distributions were obtained.

- Totally automated with a Perl script that reads output files and generates input files.

Description of VHTR reactor

MCNP5 input decks were set up to represent the VHTR full core with homogeneous and heterogeneous fuel assemblies.

Each ring has 10 axial fuel segments and 30, 36, and 36 fuel assemblies, respectively, for the inner, middle, and outer core rings.



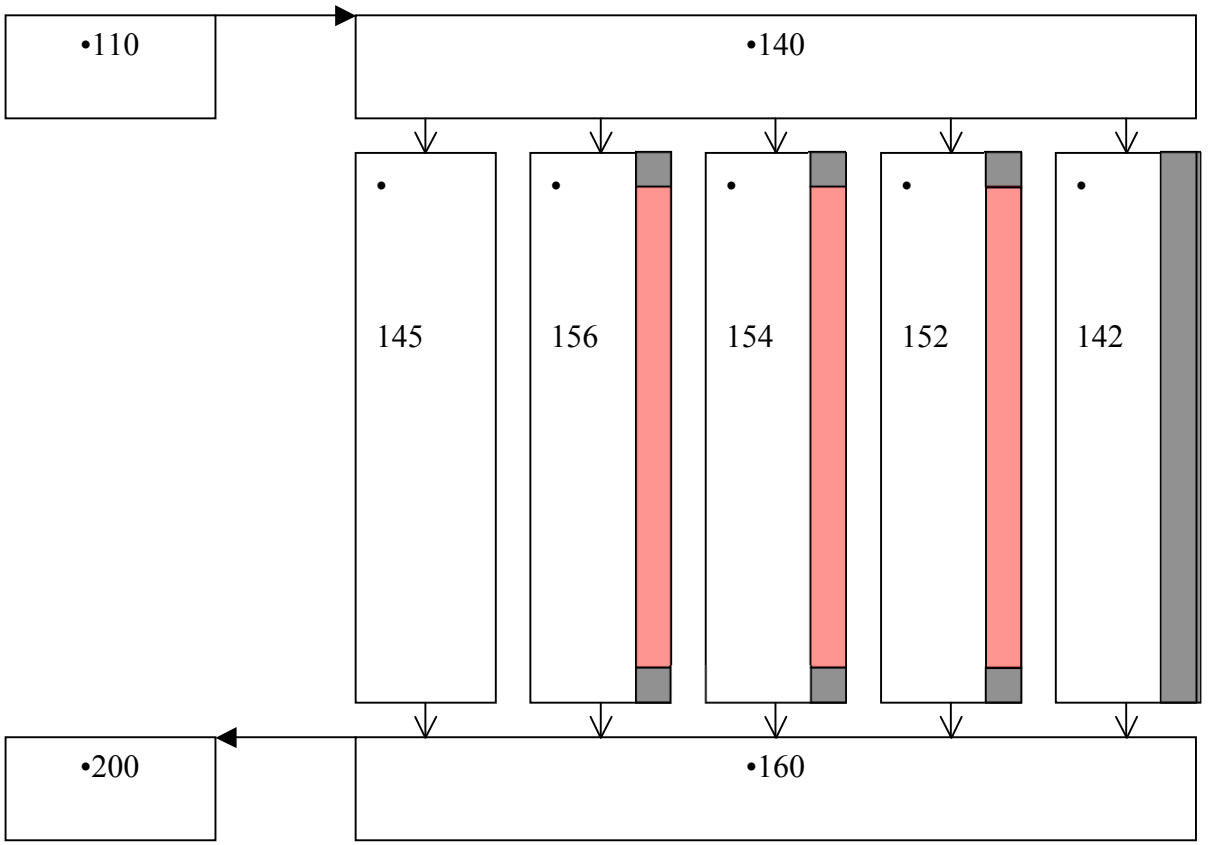
- Active Core Height: 7.93 m (10 blocks)
- Enrichment: 10.36%
- Natural Boron impurity: 6.9 ppm
- Total Number of Fuel Blocks:1020

VHTR simulation - RELAP5 Methodology

- For RELAP5-3D/ATHENA calculations, the core was modeled consistent with the MCNP5 setup.
- Each annular region is axially discretized into ten segments and is represented as a cylindrical coolant channel comprising a central coolant hole, surrounded by three inner graphite rings, four fuel rings, and one outer graphite ring.
- An adiabatic boundary condition is imposed at the outer boundary of the coolant channel.

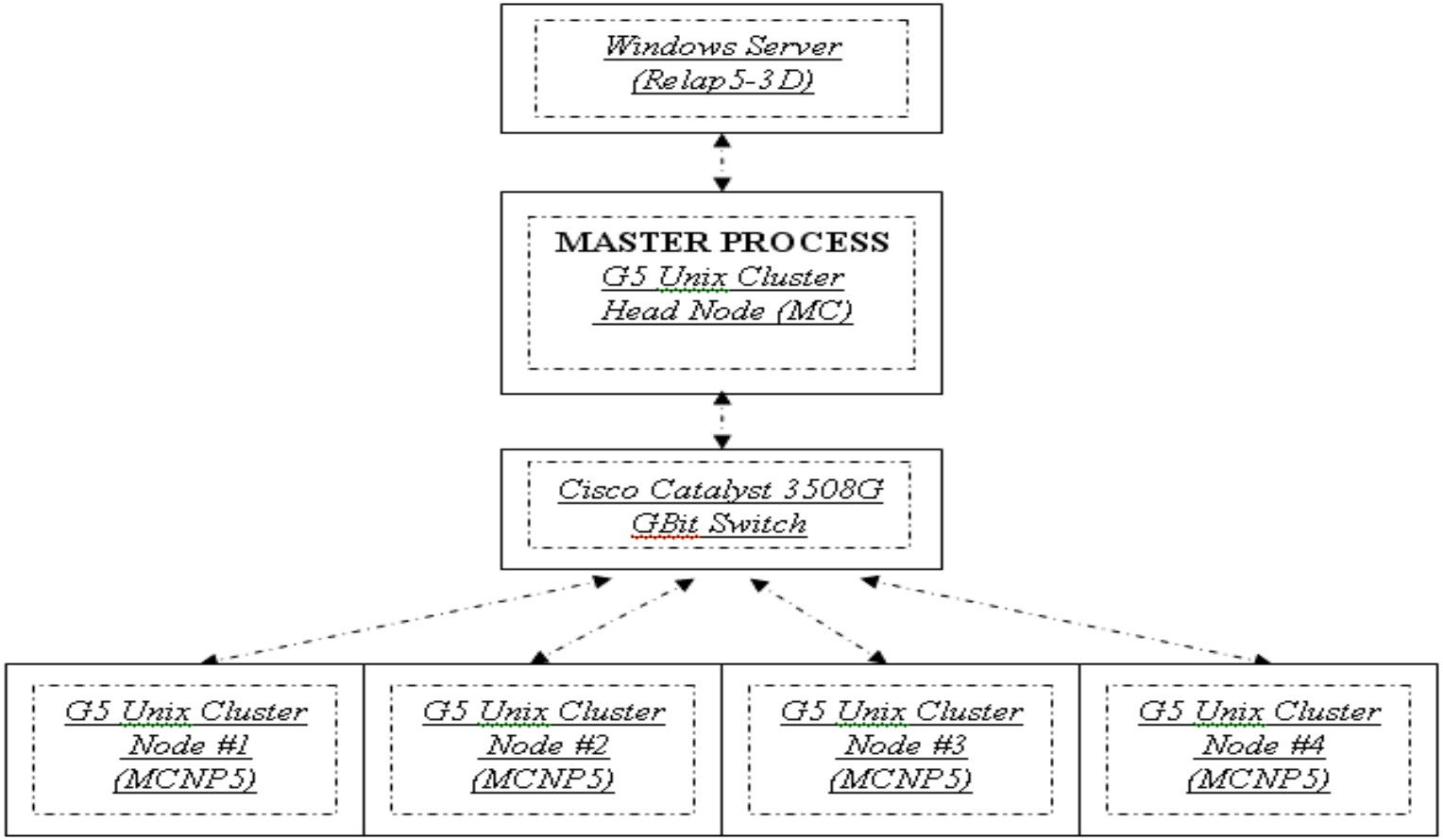
RELAP5 Methodology (cont.)

Based on the NGNP target for the helium outlet temperature of 1273 K, together with the inlet temperature of 763 K, helium mass flow rate was determined as 226 kg/s for rated power output of 600 MWt.



VHTR - Cross Platform NTH Architecture

- MCNP5 was run on a Mac G5 Unix cluster in parallel. 10K particles per cycle were used with a total of 140 active cycles for each MCNP5 calculation.
- RELAP5 was run on a remote Windows server.



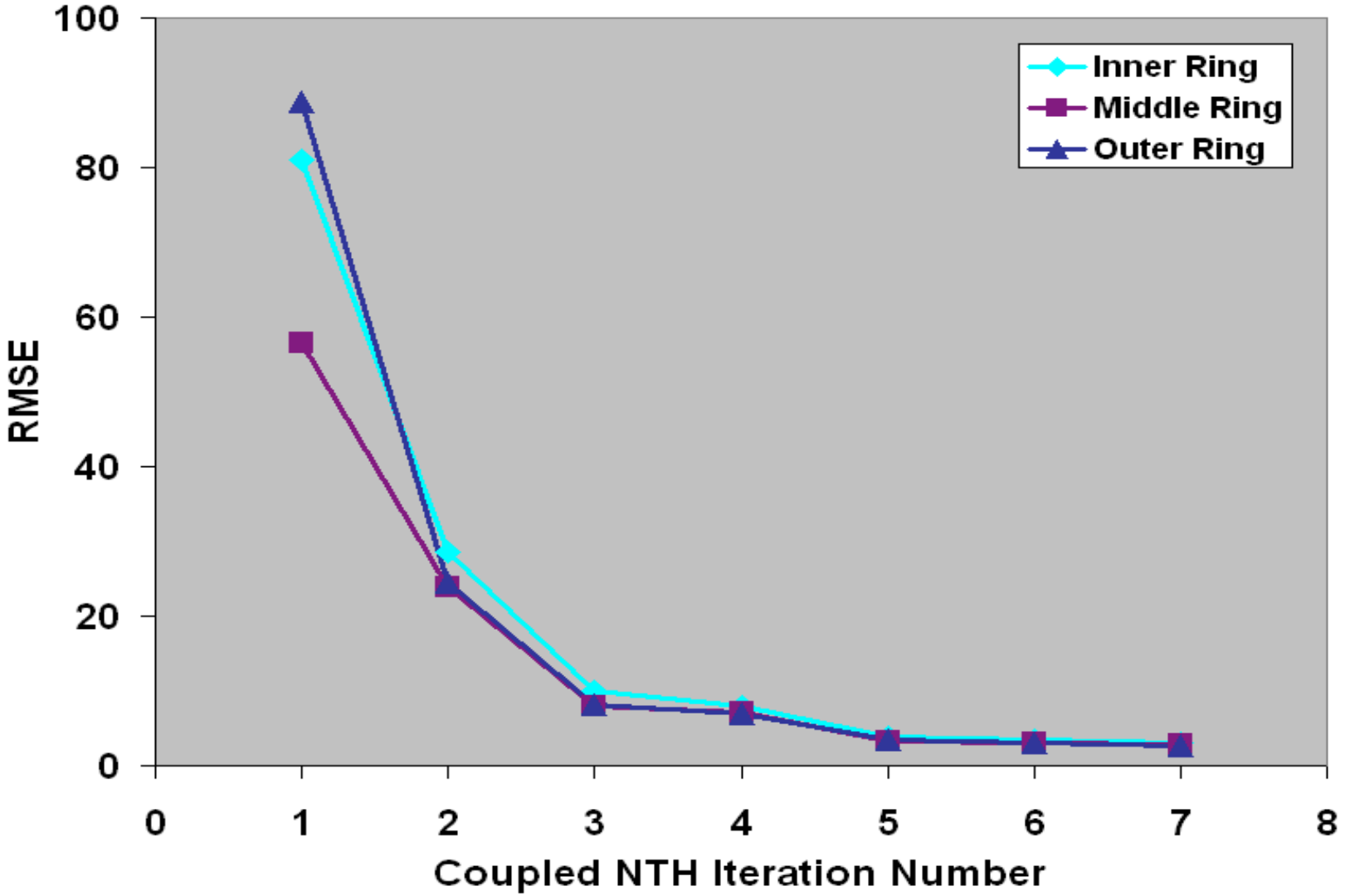
VHTR - NTH Data Communication

- Data was communicated between MCNP5 and RELAP5 codes in a cyclic fashion until convergence in temperature and power distributions were obtained.

- Online monitoring of the RMSE was used to stop the iteration.

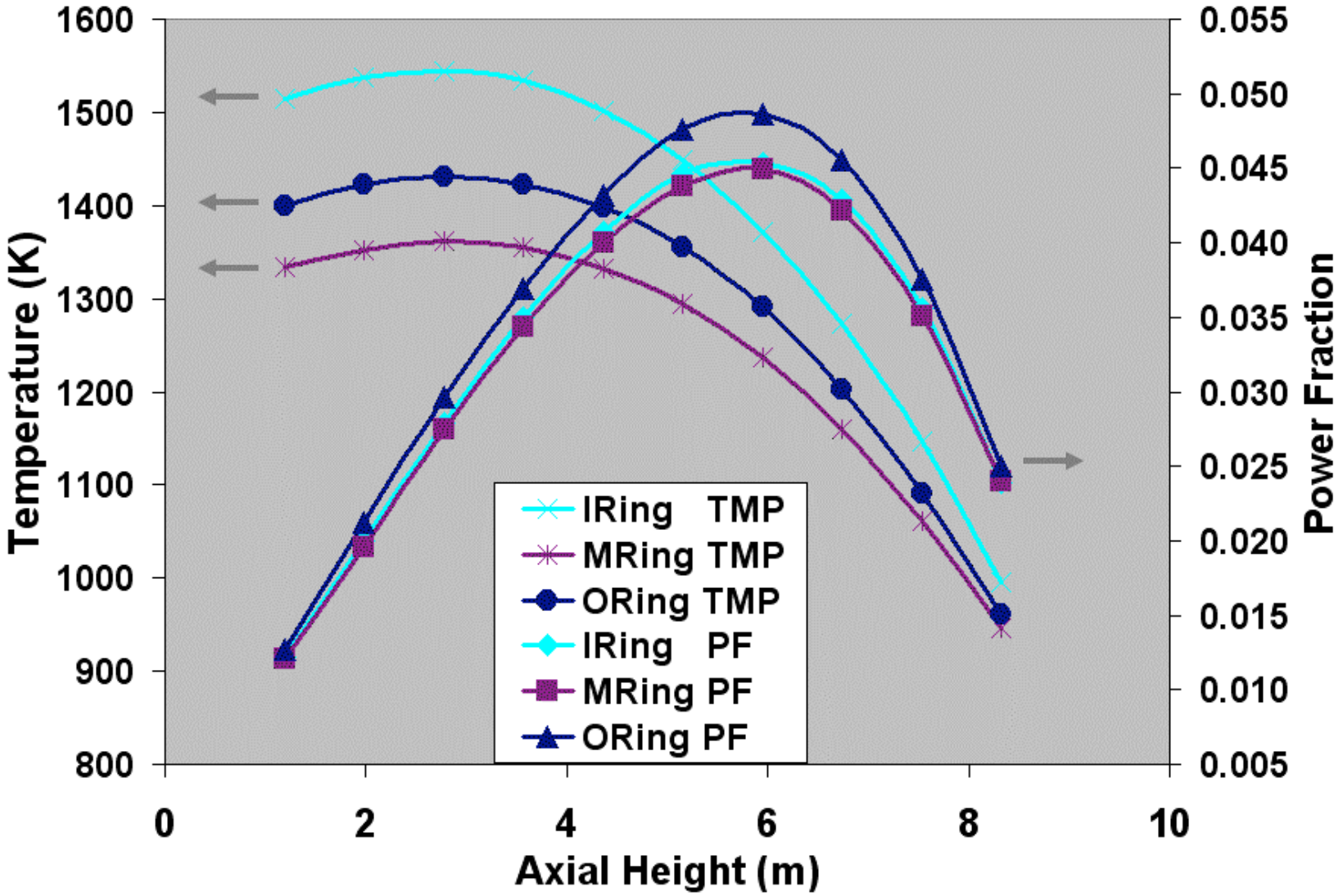
	Power Frac. (MCNP5)		Temp. Dist. (RELAP5)		Power Frac. (MCNP5)		Temp. Dist. (RELAP5)
1	0.016574	→ INPUT TO RELAP5	926.045	→ INPUT TO MCNP5	0.028488	→ INPUT TO RELAP5	1038.256
2	0.026557		1050.207		0.041420		1205.862
3	0.035137		1175.686		0.047680		1333.691
4	0.041325		1293.021		0.047675		1419.931
5	0.045263		1401.488		0.043716		1475.861
6	0.045369		1486.089		0.038116		1513.388
7	0.041935		1543.885		0.031252		1531.816
8	0.035221		1570.742		0.023775		1533.103
9	0.025824		1564.520		0.016720		1523.647
10	0.015604		1533.804		0.010089		1503.648

RMS Error in Temperature vs. NTH Iteration



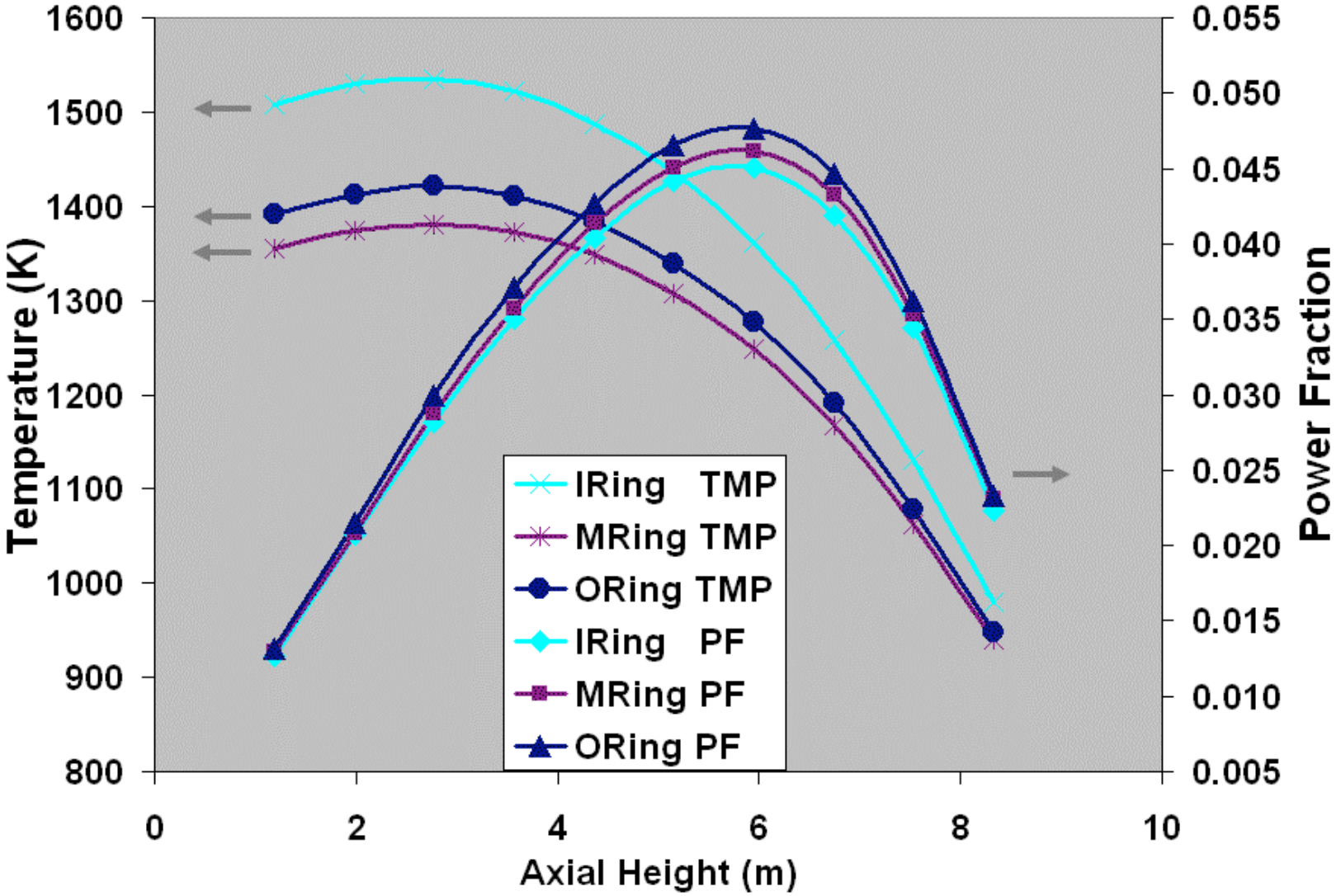
Converged Temperature/Power Distributions

Homogeneous Fuel

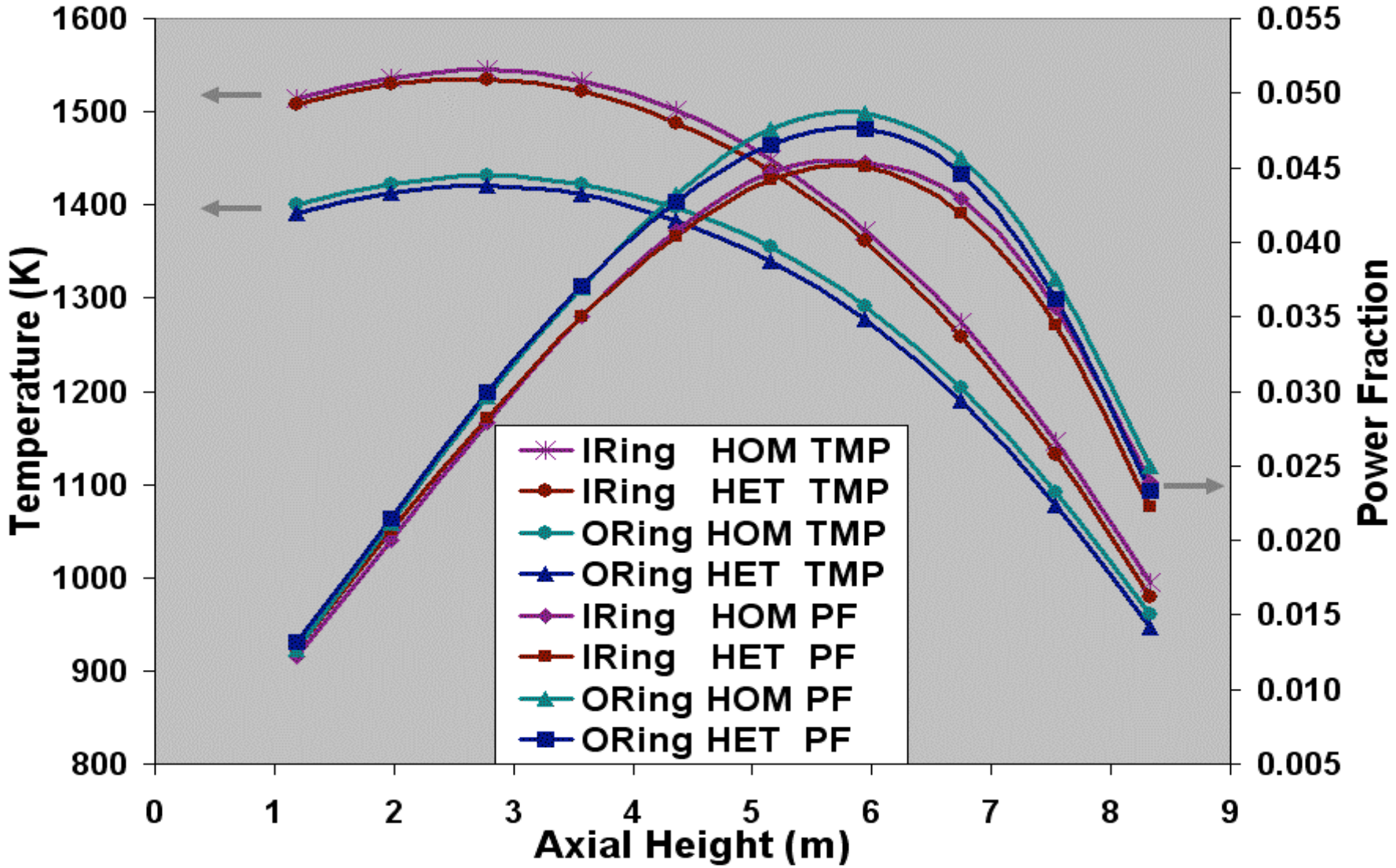


Converged Temperature/Power Distributions

Heterogeneous Fuel



Homogeneous vs Heterogeneous Fuel



VHTR Temperature Feedback - Conclusions

- A cross-platform computer architecture connecting Mac G5 Unix cluster and a Windows server was successfully developed to automate the coupled NTH calculations for the VHTR core.
- Online monitoring of RMSE shows that it converges rapidly (4-7 iterations)
- The converged power distributions are nearly independent of the double heterogeneity accounted for with MCNP5.
- We are now performing more highly resolved MCNP5 calculations with 100,000 histories per cycle and the effect of the heterogeneities appears to be more pronounced.
- The pseudo-material method works very well but the true test will be the above higher resolution cases.

Pseudo-materials – advantages/disadvantages

- **Advantages**
  - **Libraries needed at fewer temperatures (eg, every 100K)**
  - **Can interpolate to any temperature bounded by the library temperatures**
  - **No data preprocessing required**

- **Disadvantages**
  - **Approximate interpolation** - stochastic interpolation is not functional interpolation: one of the two datasets is chosen randomly during the random walk
  - **Finite error due to interpolation – seems to be small**
  - **Cannot be used for S(α,β) thermal scattering kernels**
    - MCNP limitation: does not allow mixture of S(α,β) materials
    - Need to pick S(α,β) dataset at nearest temperature

Fission Energy Deposition

Estimation of the Spatial Distribution of Fission Energy Deposition in a VHTR with (only) MCNP5

How to perform fission energy deposition calculations with standard MCNP tallies with application to a full core VHTR configuration.

Outline

- Acknowledgements
- Motivation and summary
- Fission energy release and deposition
- Capabilities and limitations of MCNP5 fission energy deposition tallies for reactor applications
- Methodology to account for fission energy deposition with MCNP5
- Application to VHTR configurations
- Alternative approach – a simplified methodology

Acknowledgements

- **This work is primarily the work of Etienne de Villèle, an exchange student from France who examined the coupling of MCNP5 and RELAP5 for temperature feedback in a VHTR. This work formed part of his MS thesis for CEA/INSTN.**

- **Other contributors, all from the Department of Nuclear Engineering and Radiological Sciences at the University of Michigan, include:**
  - John C. Lee, Professor
  - Gokhan Yesilyurt, PhD Candidate
  - Wei Ji, former PhD Candidate (now Professor at RPI)

Motivation and summary

- **Motivation** – every few months there are conversations on the MCNP Forum regarding how MCNP handles fission energy deposition and how MCNP can be used to estimate the spatial distribution for a realistic reactor configuration.

- This talk is a summary of the process used at the University of Michigan to estimate the fission energy deposition in VHTR configurations. This is one approach that makes use of standard MCNP tallies and seemed to yield acceptable results. Comments or suggestions are welcome.

Components of energy release in fission

Quantity	Value(eV)	Uncertainty
Kinetic energy of the fragments	1.6912E+08	4.9000E+05
Kinetic energy of the prompt neutrons	4.7900E+06	7.0000E+04
Kinetic energy of the delayed neutrons	7.4000E+03	1.1100E+03
Kinetic energy of the prompt gammas	6.9700E+06	5.0000E+05
Kinetic energy of the delayed gammas	6.3300E+06	5.0000E+04
Total energy released by delayed betas	6.5000E+06	5.0000E+04
Energy carried away by the neutrinos	8.7500E+06	7.0000E+04
Total energy release per fission (sum)	2.0247E+08	1.3000E+05
Total energy less neutrino energy	1.9372E+08	1.5000E+05

Interpreted ENDF file for U-235e (ENDF/B-VI)

F7 tally includes items in red

Sources of Fission Energy (recoverable)

Q_f = kinetic energy of fission fragments

Q_n = kinetic energy of fission neutrons

Q_β = beta decay energy from fission

$Q_{\gamma p}$ = prompt gamma energy from fission

$Q_{\gamma d}$ = delayed gamma energy from fission

$Q_{\gamma c}$ = capture gamma energy from (n,γ) reactions

$$Q = Q_f + Q_n + Q_\beta + Q_{\gamma p} + Q_{\gamma d} + Q_{\gamma c}$$

Energy Released per Fission (ENDF/B-VI)

Particle	Notation	Energy released (MeV)	Deposition site
Fission products	Q_f	169.1	Local
Neutrons	Q_n	4.79	Global
Prompt gammas	$Q_{\gamma p}$	6.97	Global
Betas	Q_β	6.5	Local
Delayed gammas	$Q_{\gamma d}$	6.33	Global
Capture gammas	$Q_{\gamma c}$	~ 6 - 8	Global
Total	Q	**193.69**	

Physical Assumptions

- **Fission fragments and betas deposit their energy locally**
- **Prompt and delayed gammas (from fission product decay) deposit their energy globally and must be transported**
- **Fission neutrons must be transported and heat may be deposited during the neutron trajectory due to:**
  - deposition of kinetic energy during moderation
  - emission of gammas as a result of neutron capture
  - energy release due to fission.
- **Capture gammas are a distributed source of gammas throughout the reactor (including reflector) and they must be transported.**

MCNP5 Capabilities/Limitations

Tally	Accounts for energy deposition due to
F7:n	Fission products, prompt gammas, and neutrons
F6:n	Fission products and neutrons
F6:p	Prompt gammas and capture gammas
F6:np	Fission products, neutrons, prompt gammas, and capture gammas (F6:n + F6:p)

- F7 tally does not account for delayed gammas, betas, or capture gammas.
- No tallies account for betas or delayed gammas which comprise 6-7% of the fission energy release
- This is not a problem if one assumes all fission energy is locally deposited because the power normalization is arbitrary.
- An accurate prediction of the spatial distribution of fission energy deposition, including neutron and gamma transport effects, should include contributions of the betas and delayed gammas.

Overall Approach to Compute Spatial Deposition

- Goal: Compute H(r) where H(r)dr = amount of energy/s deposited in dr about r in a reactor (including reflector) at power P, accounting for all sources of fission energy.

- Use standard F6 / F7 tallies in MCNP5

- Use reasonable models for those quantities that are unknown or not treated by MCNP5

  - Beta energy is deposited locally and can be scaled from the conventional F7 tally.

  - Delayed gamma energy is deposited with the same spatial distribution as the prompt gamma energy

Overall methodology to estimate H(r)

- **Run multiple MCNP runs to get all contributions to the overall fission energy deposition.**
  - **Prompt gammas ($H_{\gamma p}$): F6:p tally with PIKMT card.**
  - **Capture gammas ($H_{\gamma c}$): F6:p tally with PIKMT card.**
  - **Delayed gammas ($H_{\gamma d}$): Scale $H_{\gamma p}$ by $Q_{\gamma d}/Q_{\gamma p}$.**
  - **Fission products + neutrons (H_{fn}): regular F6:n tally.**
  - **Betas (H_{β}): scale regular F7:n tally by Q_{β}/Q_{F7}, where Q_{F7} = 180.88 MeV for U-235 fuel.**

- **Each run, scaled as indicated, yields a spatially dependent contribution to H(r). The total is a simple sum of the individual contributions since they are scaled properly.**

$$H(\underline{r}) = H_{fn} + H_{\gamma p} + H_{\gamma c} + H_{\gamma d} + H_{\beta}$$

- **Scale H(r) to get correct total power P.**

Summary of overall methodology

Particle	Notation	Energy released (MeV)	MCNP Tally	Method
Fission products	Q_f	169.1	F6:n	Normal
Neutrons	Q_n	4.79	F6:n	Normal
Prompt gammas	$Q_{\gamma p}$	6.97	F6:p	PIKMT
Betas	Q_β	6.5	F7:n	Scaled
Delayed gammas	$Q_{\gamma d}$	6.33	F6:p	Scaled
Capture gammas	$Q_{\gamma c}$	~ 6 - 8	F6:p	PIKMT
Total	Q	**193.69**		

Tallied depositions for VHTR Configurations

	ENDF/B-VI	TRISO particle	Hom full core	Het full core
Fission products and neutrons	173.89	171.59	173.45	173.26
Prompt gammas	6.97	6.7	6.71	6.78
Delayed gammas	6.33	6.33	6.44	6.50
Betas	6.5	6.5	6.5	6.5
Subtotal	**193.69**	**191.12**	**193.1**	**193.05**
Capture gammas	-	6.96	4.36	3.70
Total		**198.02**	**197.46**	**196.74**

Power distribution* for full core VHTR (het fuel)

	Inner reflector	Inner core	Middle core	Outer core	Outer reflector	Total
Bottom reflector			-			-
1	0.06	2.72	2.92	2.87	0.08	8.65
2	0.10	4.59	4.89	4.88	0.14	14.59
3	0.13	6.42	6.85	6.82	0.19	20.41
4	0.16	7.81	8.11	8.17	0.24	24.49
5	0.18	8.50	8.97	9.00	0.26	26.91
6	0.19	8.62	9.10	9.06	0.25	27.22
7	0.17	7.97	8.41	8.49	0.24	25.29
8	0.15	6.87	7.33	7.35	0.21	21.92
9	0.11	5.25	5.58	5.57	0.16	16.67
10	0.06	3.23	3.43	3.38	0.09	10.19
Top reflector			-			-
Total	1.31	61.96	65.56	65.57	1.86	196.60

*Error in simulation resulted in zero top and bottom reflector deposition rates

Alternative approach – a simplified methodology

- Multiple MCNP5 runs, especially with PIKMT cards active, are very time-consuming. Not practical for coupled MCNP5/RELAP5 calculations.

- In principle, MCNP5 could be modified to tally these quantities directly. This is probably a low-priority change since work-arounds can yield acceptable results.

- An alternative approach is based on the observation that the F6:n tally accounts for global transport of neutrons and perhaps the spatial distribution of the neutron tally might approximate reasonably well the spatial distribution of the overall fission energy deposition.

Comparison of F6:n with overall heat deposition*

	Inner reflector	Inner core	Middle core	Outer core	Outer reflector
Bottom reflector	-				
1	0.26	0.90	0.89	0.90	0.26
2	0.26	0.90	0.88	0.90	0.26
3	0.26	0.90	0.89	0.90	0.27
4	0.26	0.90	0.88	0.90	0.26
5	0.26	0.89	0.88	0.90	0.25
6	0.25	0.89	0.89	0.90	0.26
7	0.25	0.89	0.88	0.90	0.26
8	0.26	0.89	0.88	0.90	0.26
9	0.26	0.90	0.89	0.90	0.27
10	0.27	0.90	0.89	0.90	0.27
Top reflector	-				

*Ratio of F6:n tally to benchmark fission energy deposition

Simplified methodology – preliminary thoughts

- The F6:n tally (arbitrary normalization) yields fractional energy depositions in the core regions which are 88-90% of the benchmark fission energy fractions and within 25-27% for the reflector regions.

- Although this ratio may change by ~10% in the reflector, only a few % of the fission energy is deposited in the reflector.

- Implication: the F6:n tally, with prior calculations to estimate ratios of the F6:n tally to the true heat deposition tally in the core and reflector regions, may provide a very efficient and reasonably accurate method to estimate the fission power distribution in a realistic reactor configuration.

- These are preliminary results and more work needs to be done to assess the sensitivity of these ratios and to examine the possibility of using other tallies.

Monte Carlo Depletion Tutorial

- Overview
- Timesteps
- Geometry & Depletion
- Materials & Nuclide Setup
- Cross-section Treatment
- Criticality & Depletion
- Concerns - Accuracy
- Error Propagation

Introduction

- **There are now many Monte Carlo depletion systems**
  - MONTEBURNS - MCNP + ORIGEN
  - MCODE - MCNP + ORIGEN
  - MCOR - MCNP + ORIGEN
  - MCNPX - MCNPX with built-in CINDER90
  - MCNP-ACAB - MCNP + ACAB
  - ALEPH - MCNP + ORIGEN
  - BGCore - MCNP + SARAF
  - OCTOPUS - MCNP + ORIGEN or FISPACT
  - SCALE - KENO + ORIGEN
  - PSG - standalone, or with ABURN
  - MVP-BURN
  - McCARD
  - MCB
  - MC21, RCP, RACER
- **This tutorial provides an overview of Monte Carlo depletion, to help researchers & code users interpret the details & differences in the different MC depletion codes**

Introduction

- **Monte Carlo depletion papers at this conference**

Christos Trakas, François Thibout, Sebastien Thareau, Bernard Verboomen, Gert Van den Eynde, **"Benchmark of ALEPH and Monteburns on French post-irradiation experiments"**

Hyung Jin Shim, Ho Jin Park, Han Gyu Joo, Yeong-il Kim, Chang Hyo Kim **"Uncertainty Propagation in Monte Carlo Depletion Analysis"**

Emil Fridman, Eugene Shwageraus, Alex Galperin, **"Implementation of multi-group cross-section methodology in BGCore MC-depletion code"**

Michael Fensin, John Hendricks, Samim Anghaie, **" MCNPX 2.6 depletion method enhancements and testing"**

- **Monte Carlo depletion calculations - basic idea**

1. **Monte Carlo calculation at a fixed time, t_0**
   - All geometry, number densities, temperatures, cross-sections must be constant
   - Keff eigenvalue calculation, normalized to required power level
   - Determine absorption rates, fission rates, fluxes for all depletable regions

2. **Depletion calculation for $\Delta t = t_1 - t_0$**
   - Using number densities, absorption rates, fission rates, fluxes from (1), determine new number densities at time t_1
   - Must account for fission product & actinide buildup/burnout
   - May assume constant flux over Δt, or constant power

$\Rightarrow$ **Repeat (1) & (2) for each time step**

Sounds straightforward, but there are many, many subtleties & complications

Definitions

$\mathbf{N_k = N(t_k)}$

= vector of all the number densities for each isotope of every region in the problem at time $\mathbf{t_k}$

$\mathbf{\Phi_k = \Phi(t_k) = \Phi(N_k)}$

= Monte Carlo Keff calculation of fluxes $\mathbf{\Phi_k}$, absorption rates $\mathbf{A_k}$, fission rates $\mathbf{F_k}$ for all isotopes in all regions of problem at time $\mathbf{t_k}$, normalized to a specified reactor power level

$\mathbf{B_k = B(t_k, \Delta t, N_k, \Phi, A, F, \lambda)}$

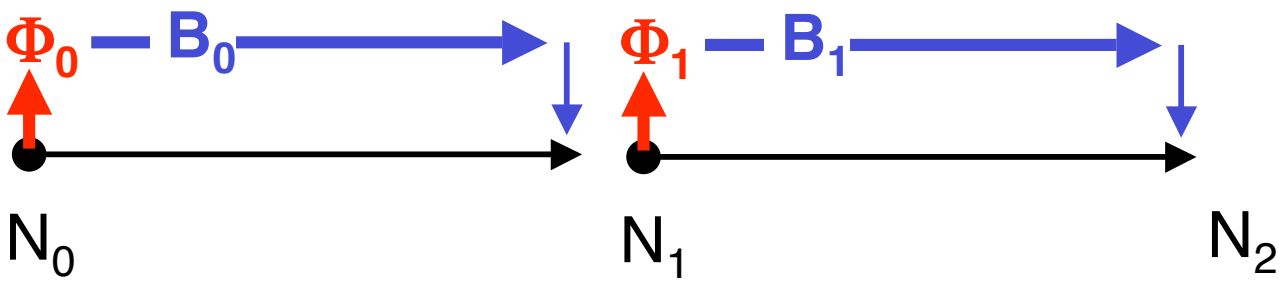
= burnup calculation from time $\mathbf{t_k}$ to $\mathbf{t_k+\Delta t}$, using N_k, $\mathbf{\Phi_k}$, $\mathbf{A_k}$, $\mathbf{F_k}$, λ_k

Solve 1 region at a time, using Φ, A, F for the region from MC

ORIGEN: $\mathbf{N_{k+1}} = \exp\{ -\mathbf{D}_k \Delta t \} \mathbf{N_k}$, where $\mathbf{D_k}$ is a matrix of A, F, λ for each isotope in region at time $\mathbf{t_k}$

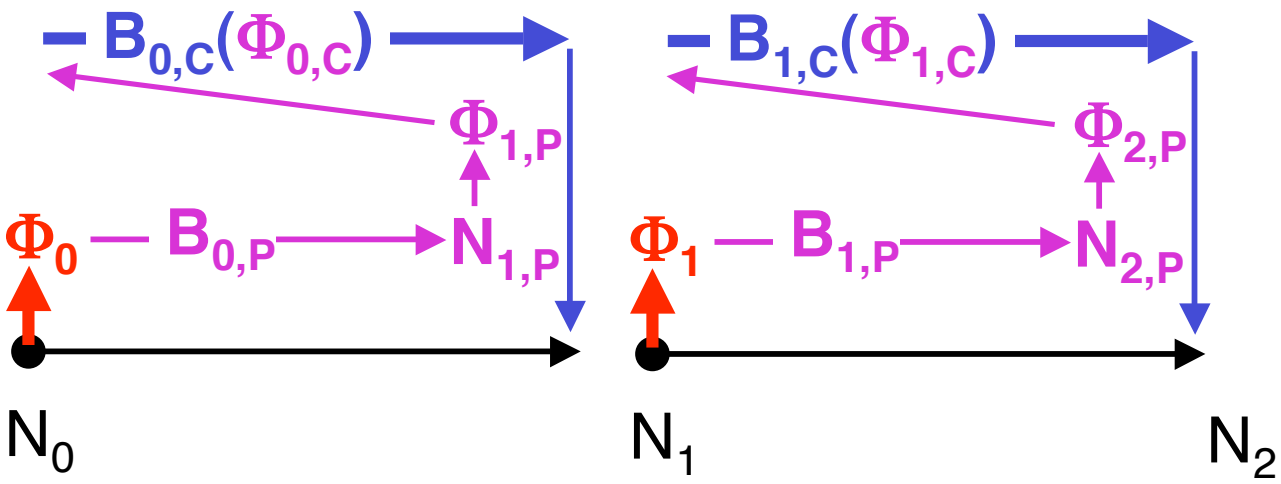
CINDER: Coupled linear chains of ODE's involving A, F, λ for each isotope in region at time $\mathbf{t_k}$

Simple MC Depletion



- During a timestep Δt, if fluxes are constant, then N, A, F change during the step
- Need very small Δt to get accurate results

Predictor-Corrector Scheme for MC Depletion



$\Phi_{0,C} = (\Phi_0 + \Phi_{1,P})/2$ $\Phi_{1,C} = (\Phi_1 + \Phi_{2,P})/2$

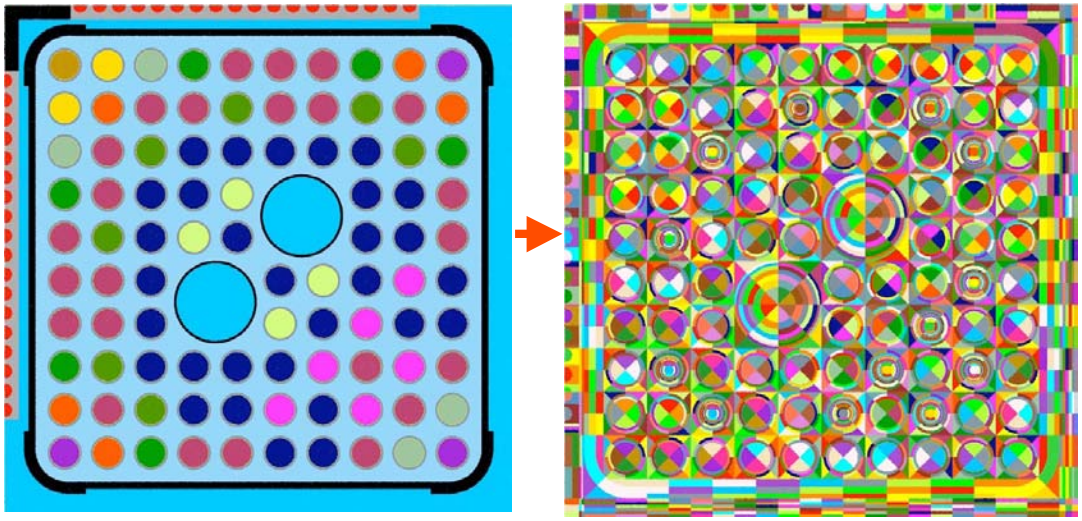
- **Predictor:** MC at start, deplete to end-of-step, MC at end-of-step
- **Corrector:** deplete again, using average beginning- & end- flux

- **Better accuracy, can use much longer time steps**
- **2 MC's & 2 depletions per timestep**
- **Other prescriptions could be used for corrector flux, $\Phi_{J,C}$ (eg, linear, …)**
- **Could iterate until predictor-corrector N's are close**

Note: For some depletion systems, computer time is reduced by ~50% by assuming that $\Phi_J \approx \Phi_{J,P}$

Geometry & Depletion

- **Must choose geometry regions fine enough to represent spatial detail need for accurate depletion**
  - MC fluxes, absorption, fission are tallied for a region (uniform)
  - Material nuclides within a region are depleted uniformly
- **Example - CASMO regions for a fuel assembly**

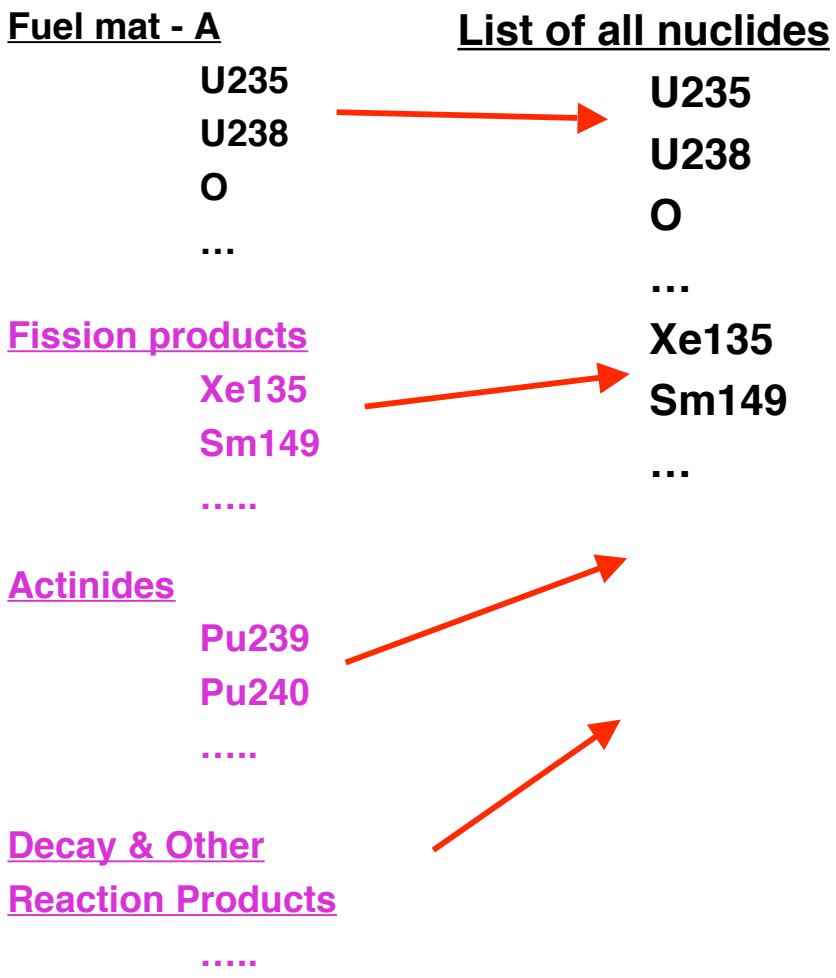


- **Most MC depletion codes can't handle this level of detail (yet) for the entire reactor**
- **If the depletion regions are too large, errors will be introduced**

Materials & Nuclide Setup

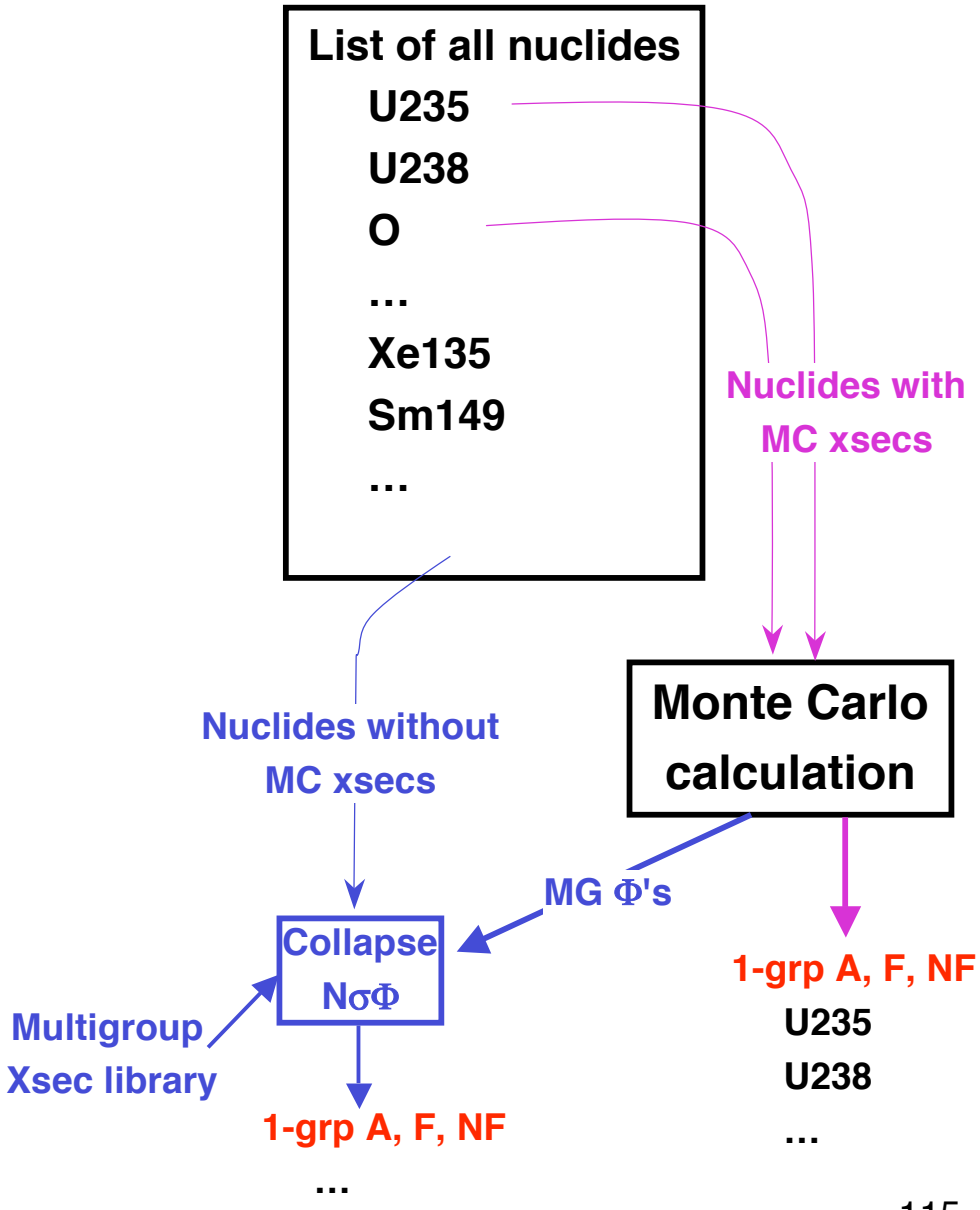
- **Material compositions**
  - At BOL, fission products & actinides are not present
  - Later timesteps must include them
  - Generally, must specify trace amounts of all FPs & actinides at BOL
  - Some MC depletion codes have built-in options, others don't

- **Cross-sections**
  - ENDF/B-VII has yield data for 1325 FPs
  - ENDF/B-VII has datasets for only 390 nuclides
  - Only nuclides with MC cross-sections can be included in the MC simulation
  - All others must be treated outside of the MC



Cross-section Treatment

- **For depletion calculation, just need overall (1-group) absorption & fission in each nuclide**
  - These can be computed directly in the MC, if cross-sections are available
- **For nuclides without MC cross-sections**
  - Can tally multigroup fluxes in each material
  - Outside of the MC - can fold together multigroup MC fluxes & multigroup cross-sections
    - **Cinder90** has its own multigroup library with 3400 nuclides (63-group) & 1325 FP yields
    - **ORIGEN2** has 1-group xsecs for 1700 nuclides & 850 FP yields
    - **ORIGEN-S** has 1-group xsecs for 1946 nuclides & 1119 FP yields



Criticality & Depletion

- **Depletion should be performed with a flux distribution corresponding to a critical system**
  - Real reactors are critical & deplete with a flux distribution corresponding to K_{eff}=1
  - If K_{eff}≠1 in the Monte Carlo, subsequent depletion would use the wrong fluxes
  - Lattice physics codes (eg, CASMO) perform a **buckling search** so that K_{eff}=1, & the depletion is performed with the critical fluxes
  - Not clear what to do for MC depletion

- **Choices**
  - Deplete anyway.
    - For comparisons, **turn off buckling search** in lattice codes for consistency. (wrong, but consistent)
  - For portions of the reactor (eg, assemblies, unit cells), use **albedo boundary conditions** to get the correct leakage (in/out, energy-dependent) so that K_{eff}=1
    - Some MC codes don't allow albedo BCs (eg, MCNP)
    - Getting the albedo BCs is a difficult computational problem

- **This is an area that needs ideas & work …..**

Concerns - Accuracy

- **Timesteps**
  - Should have short 1st timestep (~1 day), to allow Xe135 to build up to equilibrium
  - Should have short 2nd timestep (~4-5 days), to allow SM149 to build up to equilib.
  - Some codes avoid the 2 short steps by automatically handling equilibrium Xe & Sm
  - If timesteps are too long, results will not be accurate
    - Ideally, should run entire depletion lifestudy several times, reducing the timestep sizes until results show convergence
    - This is rarely done.
    - Adequate timestep sizes could be investigated using CASMO/SIMULATE or other codes, rather than with Monte Carlo
- **Geometry & depletion regions**
  - MC materials & tallies are constant within a region
  - Must subdivide depletable regions enough so that step-wise approximation to materials & fluxes is acceptable
  - May require 4-10 regions per fuel pin, or 10-40 regions per poison pin, rather than just 1
  - If the geometry of depletable materials is too coarse, results will not be accurate

Concerns - Accuracy

- **Fission products**
  - Need ~300 FPs in Monte Carlo
  - If that many FPs cannot be used, should consider some sort of **lumped fission product** approach for the "missing" FPs
    - Could assume residual FP xsecs have simple behavior (eg, 1/v in thermal range & constant in fast range) and lump them into 1, 2, or more lumps for the MC
    - Could use a multigroup background FP library, typically generated with a lattice physics code (eg, CASMO)
    - …..

- **Normalization**
  - Need to normalize the MC calculations to the correct power level
  - See other parts of this workshop regarding normalization
  - Difficulties
    - Straight neutron MC doesn't account for gamma transport & heating; must assume local fission energy deposition
    - MCNP only includes **prompt** energy from fission in Q values; need corrections
    - Should normalize total (prompt) fission energy from MC to total (prompt) fission energy of real problem

(note: MCNP manual suggests normalizing neutron source rate, rather than the resulting fission rate)

Concerns - Accuracy

- **Regardless of timesteps, geometry, & fission products**
  - Because of the many materials, nuclides per material, & tallies, the MC part of MC depletion runs much longer than normal, sometimes ~10x longer
  - While it is tempting to compensate by running fewer cycles & fewer neutrons/cycle in the MC, **BEWARE:**
  - Must discard enough initial cycles of each MC calculation to assure fission source distribution has converged before tallies start
  - Must run sufficient cycles after convergence to achieve acceptable statistics
  - Must run enough neutrons/cycle to assure that phase-space is reasonably covered by enough neutrons

Error Propagation

- **Uncertainties in input for MC calcs:**
  - Cross-sections (all calculations)
  - Number densities (depletion calculations)

- **How do uncertainties in input affect results & std-dev's ?**

- **Three basic approaches:**
  - Brute force - sample input params, run calc.; repeat many times
  - Sensitivity/Uncertainty analysis - needs adjoints
  - Perturbation theory approach

- **Outstanding paper on error propagation in MC depletion:**

  N. Garcia-Herranz, O. Cabellos, J. Sanz, J. Juan, J.C. Kuijper, **"Propagation of statistical and nuclear data uncertainties in Monte Carlo burn-up calculations"**, *Annals of Nuclear Energy* 35, 714-730 (2008)

Error Propagation

- **From paper by Garcia-Herranz, et al.**

  To compare the impact of the statistical errors in the calculated flux with respect to the cross uncertainties, a simplified problem is considered, taking a constant neutron flux level and spectrum. It is shown that, **provided that the flux statistical deviations in the Monte Carlo transport calculation do not exceed a given value, the effect of the flux errors in the calculated isotopic inventory are negligible (even at very high burn-up) compared to the effect of the large cross-section uncertainties** available at present in the data files.

- **My experience --**
  - If you run many instances of an entire MC depletion lifestudy, the general trajectories of Keff & number densities are the same, with superimposed noise
  - Overall results & trajectories are not sensitive to the fluctuations in number densities - if something is too low in one step, it will recover in the next
  - Never observed any kind of nonlinear behavior

Impact of ENDF/B-VII Data Libraries

MCNP Verification & Validation Suites

Criticality Validation Suite

Criticality results with modern nuclear data libraries

From work by R. D. Mosteller - see references at end

MCNP Verification & Validation Suites

- **Suite of 42 Regression Tests**
  - Run many times per day
  - Verifies code changes (not physics)
  - ~90% code coverage

- **Criticality Validation Suite**
  - 31 cases from *International Handbook of Evaluated Criticality Benchmark Experiments*
  - Run with ENDF/B-VI & ENDF/B-VII.0 data
  - 31 cases run, 5,000,000 histories each

- **Analytic Benchmarks for Criticality**
  - 10 problems, from Sood/Forster report – exact solutions known
  - 8,000,000 histories each – **all match exact solution within statistics**

- **Radiation Shielding Validation Suite**
  - 8 problems - time-of-flight spectra for neutrons from pulsed spheres
  - 5 problems - neutron & photon spectra at shield walls within simulated fusion reactor
  - 6 problems - photon dose rates
  - 1,000,000 histories for each problem

MCNP Test & Validation Suites

MCNP Installation Test Suite (Regression tests)

- Included with the MCNP5 distribution package
- Cases were constructed to test input options and to execute quickly
- Usually NOT good examples of MCNP input
- Many cases are physically unrealistic
- Results are not well converged
- Suitable for making sure that the code executes as designed, but NOT suitable for verification/validation purposes

MCNP Validation Suites

- Defined and tested for specific types of applications
- Objectives:
  - Provide true validation of the MCNP package (including nuclear data)
  - Establish a basis for assessing the impact of improvements to MCNP and changes to its associated nuclear data libraries
- All of the cases in the suites are based on well-documented benchmark experiments
- Currently, validation suites exist for:
  - **Criticality**
  - **Radiation Shielding**

MCNP Criticality Validation Suite

Cases were selected to encompass a wide variety of parameters:

- **Fissile isotopes:** ^{233}U, ^{235}U, ^{239}Pu
- **Spectra:** Fast, intermediate, thermal
- **Compositions:** Metals, oxides, solutions
- **Configurations:** Bare and reflected spheres and cylinders,
  2-D and 3-D lattices,
  Infinite homogeneous & heterogeneous regions
- **^{235}U enrichment:** HEU, IEU, LEU
- **Input specifications for all 31 cases are taken from the International Handbook of Evaluated Criticality Safety Benchmark Experiments**

Int. Crit. Safety Benchmark Eval. Project

HEU-MET-THERM-003

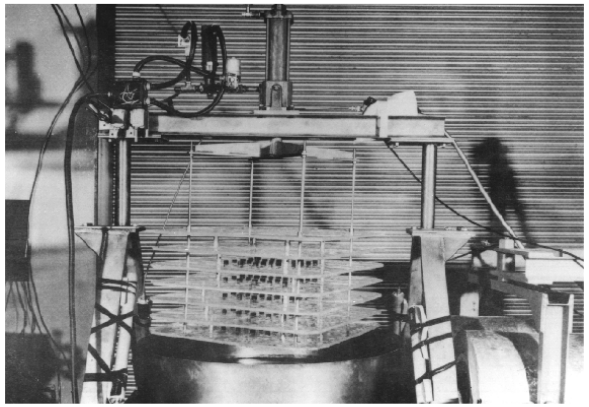
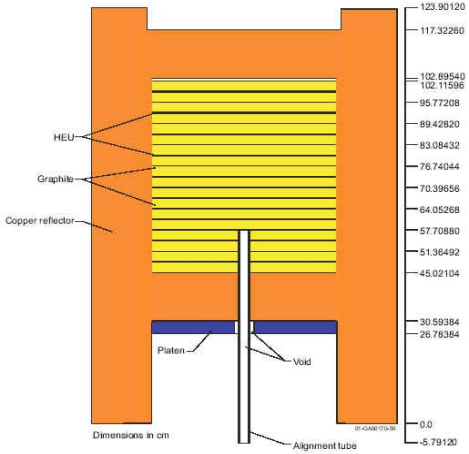
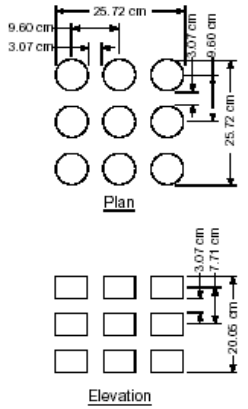


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

Zeus-2, HEU-MET-INTER-006, case 2



PU-MET-FAST-003, case 3



Case 103
3 x 3 x 3 array
3-kg Pu part
V_{cell} = 710.1 cm^3

IEU-COMP-THERM-002, case 3

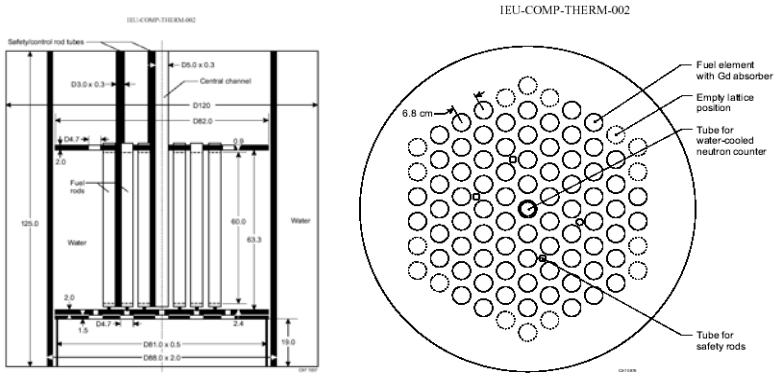


Figure 6. Lattice Plate Loading Chart for Assemblies with Gd Absorber (Case 3 and Case 4).

PNL-33 - MIX-COMP-THERM-002

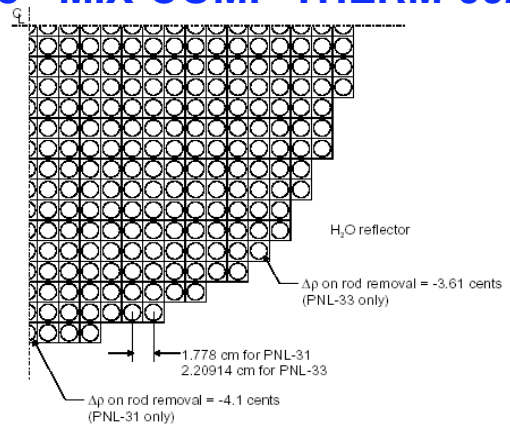


Figure 7. Fuel Loading for PNL-31 and PNL-33.

Cases in the MCNP Criticality Validation Suite

Spectrum	Fast			Intermed	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05	Falstaff-1*	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2	Flattop-25	Godiver	Zeus-2 UH_3	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H†	IEU-CT-02	STACY-36
LEU					B&W XI-2	LEU-ST-02
Pu	Jezebel Jezebel-240 Pu Buttons	Flattop-Pu THOR	Pu-MF-11	HISS/HPG†	PNL-33	PNL-2

* Extrapolated to critical

† k_∞ measurement

Criticality Validation Suite

Name	Spectrum	Handbook ID	Description
Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
Flattop-23	Fast	U233-MET-FAST-006	Sphere of ^{233}U reflected by normal U
U233-MF-05	Fast	U233-MET-FAST-005, case 2	Sphere of ^{233}U reflected by beryllium
Falstaff-1	Intermediate	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in ^{233}U
SB-2½	Thermal	U233-COMP-THERM-001, case 3	Lattice of ^{233}U fuel pins in water
ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate solution enriched in ^{233}U
Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
Tinkertoy-2	Fast	HEU-MET-FAST-026, case C-11	3 x 3 x 3 array of HEU cylinders in paraffin box
Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
Godiver	Fast	HEU-MET-FAST-004	HEU sphere reflected by water
Zeus-2	Intermediate	HEU-MET-INTER-006, case 2	HEU platters moderated by graphite and reflected by copper
UH_3	Intermediate	HEU-COMP-INTER-003, case 6	UH_3 cylinders reflected by depleted uranium
SB-5	Thermal	U233-COMP-THERM-001, case 6	Lattice of HEU fuel pins in water, with blanket of ThO_2 pins
ORNL-10	Thermal	HEU-SOL-THERM-032	Large sphere of HEU nitrate solution
IEU-MF-03	Fast	IEU-MET-FAST-003	Bare sphere of IEU (36 wt.%)
BIG TEN	Fast	IEU-MET-FAST-007	Cylinder of IEU (10 wt.%) reflected by normal uranium
IEU-MF-04	Fast	IEU-MET-FAST-004	Sphere of IEU (36 wt.%) reflected by graphite
Zebra-8H	Intermediate	MIX-MET-FAST-008, case 7	IEU (37.5 wt.%) reflected by normal U and steel
IEU-CT-02	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
STACY-36	Thermal	LEU-SOL-THERM-007, case 36	Cylinder of IEU (9.97 wt.%) uranyl nitrate solution
B&W XI-2	Thermal	LEU-COMP-THERM-008, case 2	Large lattice of LEU (2.46 wt.%) fuel pins in borated water
LEU-ST-02	Thermal	LEU-SOL-THERM-002, case 2	Sphere of LEU (4.9 wt.%) uranyl fluoride solution
Jezebel	Fast	PU-MET-FAST-001	Bare sphere of plutonium
Jezebel-240	Fast	PU-MET-FAST-002	Bare sphere of plutonium (20.1 at.% ^{240}Pu)
Pu Buttons	Fast	PU-MET-FAST-003, case 103	3 x 3 x 3 array of small cylinders of plutonium
Flattop-Pu	Fast	PU-MET-FAST-006	Plutonium sphere reflected by normal U
THOR	Fast	PU-MET-FAST-006	Plutonium sphere reflected by thorium
PU-MF-11	Fast	PU-MET-FAST-011	Plutonium sphere reflected by water
HISS/HPG	Intermediate	PU-COMP-INTER-001	Infinite, homog. mixture of plutonium, hydrogen, & graphite
PNL-33	Thermal	MIX-COMP-THERM-002, case 4	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Thermal	PU-SOL-THERM-021, case 3	Sphere of plutonium nitrate solution

Purpose & Use of the MCNP Criticality Validation Suite

- **The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries**
- **Suite is *not* an absolute indicator of the accuracy or reliability of a given nuclear data library, nor is it intended to be**
- **Suite can provide a general indication of the overall performance of a nuclear data library**
- **Suite can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data**

Modern Nuclear Data Libraries for MCNP

- **ENDF/B-VI (Final)**
  - ACTI (.62c, ENDF/B-VI.8) and ENDF66 (.66c, ENDF/B-VI.6) are included in the MCNP5 distribution
- **JENDL-3.3**
  - FSXLib-J33 (available from RSICC)
- **JEFF-3.1**
  - ZZ-MCJEFF 3.1 (available from NEA Data Bank)
- **ENDF/B-VII.0**
  - Results presented herein were obtained with data libraries prepared by the LANL X-1-NAD data team for the MCNP5-1.50 release to RSICC (2008)
- **MCNP5 Calculations for Criticality Validation Suite**
  - Each calculation employed 550 generations with 10,000 neutrons per generation (SB-5 and Zebra-8H employed 350 generations)
  - Results from first 50 generations were excluded from the statistics
  - Results therefore are based on 5,000,000 active histories for each case (3,000,000 for SB-5 and Zebra-8H)
  - JENDL-3.3 calculations for thermal cases used ENDF/B-VI scattering laws (SAB-2002), because none are included in the JENDL-3.3 library

Results for ^{233}U Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
Jezebel-233	1.0000 ± 0.0010	0.9995 ± 0.0003	0.9926 ± 0.0003	1.0038 ± 0.0003	1.0041 ± 0.0003
Flattop-23	1.0000 ± 0.0014	0.9994 ± 0.0003	1.0003 ± 0.0003	1.0062 ± 0.0003	0.9985 ± 0.0003
U233-MF-05	1.0000 ± 0.0030	0.9929 ± 0.0003	0.9972 ± 0.0003	1.0004 ± 0.0003	1.0019 ± 0.0003
Falstaff-1	1.0000 ± 0.0083	0.9843 ± 0.0005	0.9895 ± 0.0005	0.9841 ± 0.0005	0.9879 ± 0.0005
SB-2½	1.0000 ± 0.0024	1.0042 ± 0.0005	0.9964 ± 0.0005	0.9971 ± 0.0004	0.9979 ± 0.0005
ORNL-11	1.0006 ± 0.0029	1.0015 ± 0.0002	0.9974 ± 0.0002	0.9975 ± 0.0002	0.9989 ± 0.0002

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

- Relative to ENDF/B-VI, ENDF/B-VII dramatically improves k_{eff} for Jezebel-233 and eliminates reactivity swing from Jezebel-233 to Flattop-23
- ENDF/B-VII.0 k_{eff} is higher than ENDF/B-VI for SB-2½ but lower for U233-MF-05 and Falstaff-1, both of which include Be
- Overall, JENDL-3.3 produces best results

Results for HEU Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
Godiva	1.0000 ± 0.0010	0.9994 ± 0.0003	0.9963 ± 0.0003	0.9965 ± 0.0003	1.0033 ± 0.0003
Tinkertoy-2	1.0000 ± 0.0038	1.0003 ± 0.0003	0.9973 ± 0.0003	0.9977 ± 0.0003	1.0042 ± 0.0003
Flattop-25	1.0000 ± 0.0030	1.0030 ± 0.0003	1.0021 ± 0.0003	1.0020 ± 0.0003	0.9974 ± 0.0003
Godiver	0.9985 ± 0.0011	1.0003 ± 0.0003	0.9948 ± 0.0003	0.9946 ± 0.0003	1.0019 ± 0.0004
UH_3	1.0000 ± 0.0047	0.9951 ± 0.0004	0.9914 ± 0.0003	0.9942 ± 0.0004	0.9967 ± 0.0004
Zeus-2	0.9997 ± 0.0008	0.9961 ± 0.0003	0.9942 ± 0.0003	0.9950 ± 0.0003	0.9956 ± 0.0003
SB-5	1.0015 ± 0.0028	0.9995 ± 0.0005	0.9965 ± 0.0005	0.9968 ± 0.0005	0.9990 ± 0.0006
ORNL-10	1.0015 ± 0.0026	0.9992 ± 0.0002	0.9992 ± 0.0002	0.9988 ± 0.0002	0.9999 ± 0.0002

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

- Relative to ENDF/B-VI, ENDF/B-VII.0 substantially improves k_{eff} for Godiva, UH_3, and SB-5 and also improves it for Godiver and Zeus-2
- ENDF/B-VII.0 k_{eff} for Flattop-25 deteriorates relative to ENDF/B-VI
- Reactivity swing from Godiva to Flattop-25 is reduced significantly

Results for IEU Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
IEU-MF-03	1.0000 ± 0.0017	1.0025 ± 0.0003	0.9987 ± 0.0003	0.9985 ± 0.0003	0.9969 ± 0.0002
BIG TEN	0.9948 ± 0.0013	0.9948 ± 0.0002	1.0071 ± 0.0003	0.9876 ± 0.0002	0.9851 ± 0.0002
IEU-MF-04	1.0000 ± 0.0030	1.0074 ± 0.0003	1.0036 ± 0.0003	1.0037 ± 0.0003	1.0024 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	1.0191 ± 0.0002	1.0406 ± 0.0002	1.0156 ± 0.0002	1.0152 ± 0.0002
IEU-CT-02	1.0017 ± 0.0044	1.0037 ± 0.0003	1.0004 ± 0.0003	1.0001 ± 0.0003	1.0014 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9989 ± 0.0003	0.9986 ± 0.0003	0.9991 ± 0.0003	0.9999 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

- ENDF/B-VII.0 produces dramatic improvement in k_{eff} for BIG TEN
- Relative to ENDF/B-VI, k_{eff} is worse for IEU-MF-03 and IEU-MF-04 and drops substantially for Zebra-8H
- For IEU-CT-02 and STACY-36, changes to resonance parameters partially offset reactivity effects of other changes for uranium isotopes

Results for LEU Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
B&W XI-2	1.0007 ± 0.0012	1.0010 ± 0.0003	0.9968 ± 0.0003	1.0004 ± 0.0003	0.9991 ± 0.0003
LEU-ST-02	1.0024 ± 0.0037	0.9958 ± 0.0003	0.9953 ± 0.0003	0.9963 ± 0.0003	0.9963 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

- Relative to ENDF/B-VI, ENDF/B-VII.0 substantially improves k_{eff} for B&W XI-2, which eliminates need for *ad hoc* adjustment to ^{238}U resonance integral (used in many nuclear data libraries since early 1970s)

- For LEU-ST-02, changes to resonance parameters for ^{235}U and ^{238}U offset reactivity effects of other changes

Results for Pu Benchmarks

Case	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
Jezebel	1.0000 ± 0.0020	1.0002 ± 0.0003	0.9971 ± 0.0003	1.0000 ± 0.0003	0.9966 ± 0.0004
Jezebel-240	1.0000 ± 0.0020	0.9998 ± 0.0003	0.9980 ± 0.0003	1.0043 ± 0.0003	1.0009 ± 0.0004
Pu Buttons	1.0000 ± 0.0030	0.9984 ± 0.0003	0.9962 ± 0.0003	0.9996 ± 0.0003	0.9958 ± 0.0004
Flattop-Pu	1.0000 ± 0.0030	1.0003 ± 0.0003	1.0016 ± 0.0003	1.0019 ± 0.0003	0.9904 ± 0.0003
THOR	1.0000 ± 0.0006	0.9977 ± 0.0003	1.0057 ± 0.0003	1.0020 ± 0.0003	1.0066 ± 0.0003
Pu-MF-11	1.0000 ± 0.0010	1.0005 ± 0.0003	0.9966 ± 0.0004	0.9970 ± 0.0003	0.9982 ± 0.0003
HISS/HPG	1.0000 ± 0.0110	1.0120 ± 0.0002	1.0106 ± 0.0003	1.0073 ± 0.0002	1.0134 ± 0.0003
PNL-33	1.0024 ± 0.0021	1.0068 ± 0.0003	1.0029 ± 0.0003	1.0072 ± 0.0003	1.0069 ± 0.0003
PNL-2	1.0000 ± 0.0065	1.0044 ± 0.0005	1.0033 ± 0.0005	1.0045 ± 0.0004	1.0062 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

- Relative to ENDF/B-VI, ENDF/B-VII.0 produces striking improvement in k_{eff} for fast cases but k_{eff} for PNL-33 gets worse
- Reactivity increases for HISS/HPG, PNL-33, and PNL-2 but decreases substantially for THOR

Summary for MCNP Criticality Validation Suite

Range	ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDL-3.3
$\|\Delta k\| \leq \sigma$	18	13	12	13
$\sigma < \|\Delta k\| \leq 2\sigma$	7	9	7	9
$\|\Delta k\| > 2\sigma$	6	9	12	9

- ENDF/B-VII.0 produces best overall results
  - significantly more results within 1 standard deviation of benchmark values
  - significantly fewer results beyond 2 standard deviations from benchmark values

- ENDF/B-VII.0 produces substantial improvements for bare metal spheres (Jezebel-233, Godiva, and Jezebel), BIG TEN, UH_3, Pu metal sphere in water (Pu-MF-011), and LEU lattice (B&W XI-2)

- It also improves the results for Godiver, ORNL-10, IEU-CT-03, STACY-36, B&W XI-2, and LEU-ST-02

Conclusions

- **Overall, ENDF/B-VII.0 produces major reactivity improvements relative to ENDF/B-VI, JEFF-3.1, and JENDL-3.3**
- **ENDF/B-VII.0 produces dramatic improvements for bare metal spheres, BIG TEN, UH3, THOR, and Pu sphere in water**
- **Reactivity swings from bare spheres to corresponding systems reflected by normal uranium are eliminated or substantially reduced**
- **Need for ad hoc adjustment to ^{238}U resonance integral may be eliminated**

- **Some Remaining Areas of Concern**
  - Unresolved resonance region for ^{235}U
  - Fast cross sections for ^{237}Np
  - Fast cross sections for Cu
  - Thermal cross sections for ^{239}Pu
  - Angular scattering distribution for ^{2}H
- **Already resolved**
  - Thermal ^{113}Cd cross sections
  - New cross sections for ^{113}Cd will be included in the next interim distribution, ENDF/B-VII.1

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The "Kord Smith Challenge"

Monte Carlo will not be accepted as a realistic tool for routine reactor design and analysis until a full core calculation can be performed within a reasonable amount of time. Kord Smith proposed a simple measure to estimate when Monte Carlo may achieve this standard of performance. This talk will review the "Kord Smith Challenge" and update the prediction of when this goal will be achieved. This talk is based on a review talk given by Bill Martin at the Monterey M&C Conference in April 2007.

Whither Monte Carlo?

In principle

Monte Carlo can analyze neutronic configurations of arbitrary geometrical complexity, arbitrary physics complexity, and is known to perform efficiently (parallelization efficiency) on all known (production) computer architectures

In practice

Substantial limitations on Monte Carlo performance due to:

- Sheer size of the problem to be solved
- Slow convergence for global reactor problems
- May be painful to adapt Monte Carlo algorithms to some architectures that are being offered or proposed by computer vendors

Kord Smith's challenge .....

The Challenge for Monte Carlo (Kord Smith, Gatlinburg M&C, 2003)

- **The problem may be huge:**
  - # of fuel assemblies 200
  - # of axial planes 100
  - # of pins/assembly 300
  - # of depletion regions/pin 10
  - # isotopes to be tracked 100
  - Total number of tallies 6 billion

- **But the method is slow ….**
  - Need 1% statistics on peak powers
  - For a 2D assembly calculation, ~ 1M histories needed to achieve 1% statistics ⇒ ~ 20B histories for 1% for full core (100 axial planes)
  - But DR = .75 for assembly vs .995 (or worse!) for full core ⇒ ~ 50x longer to converge

5000 h to complete full-core calculation on a 2 GHz PC

Prohibitive run time is the overriding issue against Monte Carlo

- **Smith's conclusion:** Assuming Moore's Law holds, it would be 2030 before a full core Monte Carlo could be done in less than an hour on a single CPU
- One can glean from Kord's talk that a deterministic calculation will take 1/4 second in 2030!
- However, we don't just do one calculation:
  - 10,000s of 3D steady state calculations
  - 100s of 3D transient calculations
  - 1000s of operational support calculations
- Is there any hope for routine global analysis with Monte Carlo?
- Is the situation that bad? …..

Independent Check

Independent check on Kord's estimate may be obtained from a talk that was given at Monterey on 4/16/07 ……

HIGH ACCURACY LARGE SCALE MONTE CARLO AND DETERMINISTIC TRANSPORT CALCULATIONS FOR CRITICAL SYSTEMS, S. Langenbuch, A. Seubert, and W. Zwermann

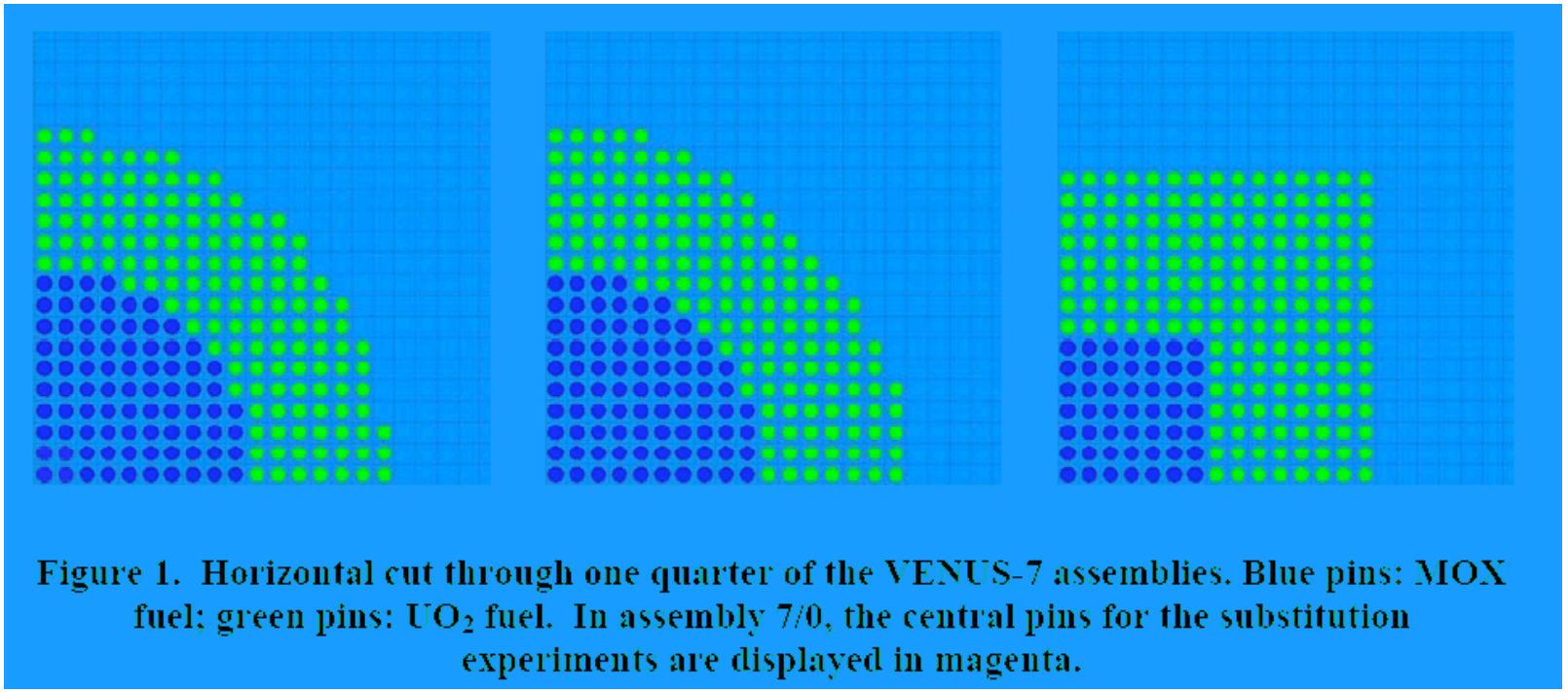

Figure 1. Horizontal cut through one quarter of the VENUS-7 assemblies. Blue pins: MOX fuel; green pins: UO_2 fuel. In assembly 7/0, the central pins for the substitution experiments are displayed in magenta.

Independent estimate of time for full core simulation

- Performed 3D simulation of Venus critical to within .1% pin power statistics (axial average)
  - 20,000 active cycles and 10,000 neutrons/cycle
  - 200M histories
- ~ 32 h on single processor of Cray XD1 (MCNP4C)

- Scaling to commercial core:
  - ~ 45x for 40,000 fuel pins
  - 100x for axial depletion regions vs average
  - .01x due to .1% vs 1% statistics
  - $\Rightarrow$ 9B histories or ~ 1500 h on Cray XD1 single processor

~1500 h to complete full-core calculation on a Cray XD1

Look more carefully at the 2030 challenge

- Key assumption: single CPU
- Since 2003, vendors have been offering multicore processors
  - Essentially an SMP on a chip
  - Apple – now offers dual quad core
  - Intel – working on a 80 core processor
  - By 2030, how many cores? 1000? 10,000?
  - Monte Carlo can easily take advantage of threads
- Assuming perfect speedup, we need a 1500 core processor to get the execution time to one hour.
- Assuming Moore's Law manifests itself as ONLY more cores starting with a dual quad core today (April 2007), then a 1500 core processor will occur in log2(1500/8)*1.5 years ~ 11 years or 2018 Q2!
- So we are now at 2018 vs 2030! Progress.

Meeting the challenge

- Monte Carlo will always be ceded the role of the benchmark methodology because of its capability to handle complex geometry and complex physics with minimal approximation

- For Monte Carlo to go beyond a "benchmark only" role and become a routine tool for reactor designers and analysts, improvements need to be made in several areas.

- Monte Carlo's key advantage – no "operator split" step in energy to create MGD cross section libraries.
  - This step may degrade the high fidelity simulation of resonance absorption and anisotropic energy transfer
  - This may be important for high fidelity simulation with thermal-hydraulic feedback, especially transients.

Meeting the challenge: MC algorithm & methods development

- Accelerate Monte Carlo fission source convergence
- Couple Monte Carlo with deterministic transport methods
- Accommodate large number of spatial zones and a huge number of tallies (due to depletion)
- Coupled physics with Monte Carlo

  this does not speed up Monte Carlo but is important for making Monte Carlo a useful tool for reactor analysis
- Global variance reduction techniques to speed up criticality problems
- Take advantage of new computer architectures

Fission source convergence

- The key impediment to routine use of Monte Carlo for global reactor analysis
- Assumption: Monte Carlo depletion will require 1% statistics on converged power distribution, otherwise propagated errors may be too large. This needs to be quantified and is only assumed here.
- Entropy: recent advance that is key to assessing fission source convergence. This was covered earlier in this workshop.

Coupled Monte Carlo and Deterministic Transport

- Monte Carlo does very well with complex physics and complex geometry and very poorly with global (keff) calculations where the global distribution is needed (e.g., to deplete)

- Deterministic methods are challenged by complex physics (e.g., due to multigroup approx) and complex geometry (e.g., TRISO fuel) but handle global calculations very efficiently (relative to MC)

- One approach – use deterministic methods for the overall calculation but use Monte Carlo as a "subgrid" method for specific regions of phase space where the deterministic methods don't perform as well. The Monte Carlo simulation could be a source problem.
  - End result: each method does what it does best.
  - Michigan: coupling MCNP5 and CPM3 for VHTR analysis

Accommodate huge demand on memory

- 6 billion tallies ⇒ 48 GB memory

  (other estimates: 128 GB!)

- Today's Monte Carlo codes would be hard pressed to deplete an assembly with only 1 depletion region per pin and 100 isotopes, as this would require 30k tallies and this may exceed the current limits of many production Monte Carlo codes. Full core analysis with pinwise depletion is out of the question.

- MC21, the next generation Monte Carlo code for Naval Reactors, will accommodate 100s of millions of tallies, as will Mercury, the LLNL next generation Monte Carlo code.

Domain decomposition may help memory demand

- The Mercury Monte Carlo code from LLNL utilizes domain decomposition with the ability to replicate domains that have too many particles. This additional flexibility can help with load balance.
- Saving grace for keff calculations – the load balance is reasonably uniform and can be estimated a priori if needed.
- Need to use batch statistics to calculate variance if domain decomposition is used.

Coupled physics with Monte Carlo

- High fidelity neutronic analysis for GNEP applications will require consistent physics due to thermal-hydraulic feedback and structural response such as rod bowing for fast reactors.
- For steady-state design, specific physics modules coupled at the I/O level may be sufficient. Then it is a matter of having a script (or a very patient human) that interrogates output files and writes input files and manages the sequence of simulations.
- For transient analysis, coupling at the I/O level is probably not going to work. Work is needed to examine coupling of time-dependent feedback with Monte Carlo.
- **Issue** – how to communicate information between a Monte Carlo code that predicts histogram quantities and a physics code that may have a continuous representation of the field quantities. This difficulty is compounded by the uncertainty (variance) of the Monte Carlo predictions.
  - **Potential solution**: use functional expansion tallies (FET) (Griesheimer et al) to allow the Monte Carlo module to read or write continuous representations of the solution or other field quantities. This does not help the uncertainty issue.

Global variance reduction methods

- Conventional wisdom – variance reduction does not work for criticality problems because there are no preferred places to "guide" the neutrons
- Recent work by Larsen and Yang (Functional Monte Carlo) is very promising*:
  - Monte Carlo is used to solve the transport equation
  - A second "low-order" equation is derived that is on a grid and which has no truncation errors by construction.
    - This equation has unknown coefficients that are functionals of the transport solution.
    - The eigenfunction ψ and eigenvalue k_{eff} satisfy this equation exactly.
  - The Monte Carlo solution is used to estimate these functionals, which are not real sensitive to the solution.
  - The "low-order" equations are solved for the eigenfunction ψ and eigenvalue k_{eff} .

*E.W. Larsen and J. Yang, NSE 159, 107–126 (2008).

Adapting to new computer architectures

- To stay on the performance curve promised by Moore's Law, Monte Carlo codes must be adapted to run efficiently on new architectures.
- Monte Carlo scales well on parallel architectures:
  - Random walks are inherently parallel within a fission source cycle or within a timestep.
  - Parallelizing across particles is natural and allows efficient load balancing without a priori knowledge of the solution.
    - MCNP5 – history-based parallelization with MPI and OpenMP
- Monte Carlo can scale well on vector architectures:
  - The history-based random walk algorithm can be turned inside out to yield an event-based (or its stack-driven variant) algorithm that results in excellent speedups on vector and parallel-vector architectures
    - RACER – KAPL (event-based)
    - MVP – JAERI (stack-driven)

Architectural trends

- **HPC hardware advances are dependent on advances in "consumer" processors and "server" processors.**
  - **Consumer processors are driven by the game industry and is trending in the direction of cell processors.**
  - **Server processors are driven by transaction processing and web applications and is moving in the direction of increasing N-core processors.**

- **Monte Carlo can take advantage of either but it would be very painful for most production Monte Carlo codes to adapt efficiently to cell processors.**
  - **Notable exceptions – RACER and MVP (already vectorized)**

What about multi-core processors?

- Dual core and quad core processors are in wide use today. The trend by the chip manufacturers is N-core where N is increasing rapidly.
  - Quad cores are here (Apple and Intel dual quad core nodes)
  - Intel is developing an 80-core processor
- Monte Carlo codes which use OpenMP, or "threaded" across histories, can take immediate advantage of multi-core processors.
- MCNP5 is threaded and uses MPI, so it can take full advantage of multiple N-core processors.

What about cell processors?

- The cell processors are essentially attached SIMD processors that function like vector processors.
- The IBM Roadrunner, installed at LANL, consists of conventional multi-core processors with attached cell processors.
- Monte Carlo will scale well on cell processors **if the code has already been "vectorized."** Only RACER and MVP among well-known production Monte Carlo codes are vectorized (to my knowledge).
- **Estimate**: many tens (if not 100s!) of person-years to vectorize a conventional Monte Carlo code such as MCNP. By the time it was done, the architects would have moved on to another design. Sigh.
- **If HPC architectures move exclusively** down the cell processor path (seems unlikely), this could be a limiting factor for using Monte Carlo for routine design/analysis of global reactor configurations.

Conclusions

- Monte Carlo is likely to remain a benchmark analysis tool for the foreseeable future.
- Enabling Monte Carlo to become a production tool will require:
  - Substantial advances to accelerate fission source convergence
  - Ned to enable huge numbers of tallies
  - Need to allow convenient coupling of stochastic transport with deterministic transport as well as deterministic physics modules.
  - Could also require substantial effort to port to new architectures although this seems unlikely given current architectural trends

Monte Carlo will always complement deterministic methods; it will not replace them, at least not before 2018!