Monte Carlo Eigenvalue Simulations - Diagnostics, Acceleration and Benchmarking

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THE NUCLEAR AND RADIOLOGIAL ENGINEERING PROGRAM IN
THE GEORGE W. WOODRUFF SCHOOL

Outline

- Research group
- Research topics
- Topics –today's presentation
- Monte Carlo in reactor physics
- (Hybrid methods for shielding)
- Summary, conclusions and future work

B. Petrovic – Research Group

MSNS - Modeling and Simulations of Nuclear Systems
NFC - Nuclear Fuel Cycle

7 Graduate Students:

2 Undergraduate StudentsResearch:

Research

Methods development
Applications and simulations

Reactor Physics (Monte Carlo eigenvalue simulations)
Shielding (Hybrid methods)
Advanced Systems and Fuel Cycle

Research topics/activities

Methods development

- Criticality Monte Carlo → convergence diagnostics and acceleration
- Fixed source Monte Carlo → investigation of hybrid methodology
- Fuel cycle analysis
- Computational medical physics

Applications

- Advanced fuel and core methods development and simulations
  - Analysis of fuel cycle with reprocessing and P&T
  - MA burn
  - Fast reactors core physics methods
- Monte Carlo 3D (full core) eigenvalue simulations
  - Objective: make MC practical for benchmarking of production methods
  - Current research: international benchmark definition, convergence diagnostics, speed-up for high dominance problems
- Automated variance reduction for shielding applications
  - Using SCALE6/MAVRIC methodology
  - Current research: Application to IRIS shielding studies, NGNP / VHTR studies
- Computational medical physics
  - Proton therapy, development of efficient simulation methodology
- Detection for homeland security, threat reduction
  - Simulations of interrogation systems

Improved methods for reactor analysis (criticality)

- Accurate methods for modeling of nuclear systems
  1) Reclaim margin in analysis of current reactors to reduce COE (uprate and/or operational flexibility)
  2) Facilitate design of advanced systems or novel features, outside of experience database

  Monte Carlo criticality simulations
  Potentially most accurate, but computationally challenging

- Feasibility of MC simulations of large power reactors?

  Focus of today's presentation:
  - Robust convergence diagnostics
  - Speedup of simulations
  - Benchmark representing realistic LWRs

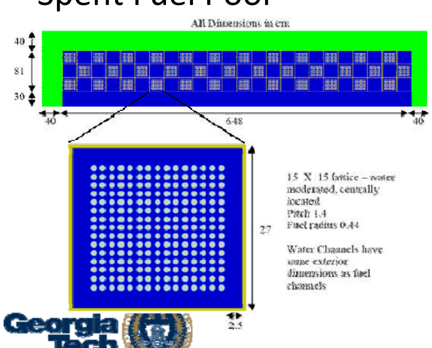
Monte Carlo criticality simulations

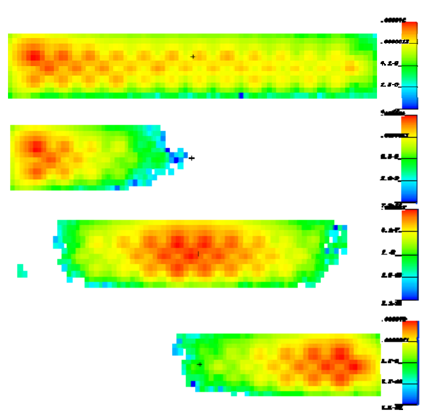
- Slow convergence
- False convergence
- Difficult to establish convergence criteria
- Underestimated statistical uncertainty (correlated histories)
- Under-sampling
- Potentially inaccurate fission source (flux, power) distribution
- Potentially significant reactivity underestimate (NCS)
- Computationally challenging
  (one more implicit level to resolve – eigenvalue/mode)

Monte Carlo Eigenvalue/Criticality Simulations
Source convergence issues

Slow convergence in large, loosely coupled systems. Statistical noise impedes diagnostics.
Large underestimate of uncertainty likely. False convergence detection is difficult.

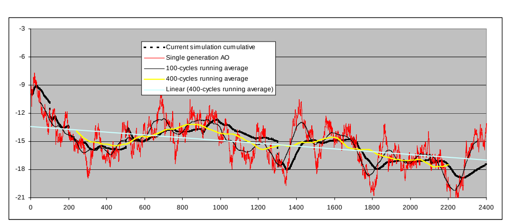
OECD/NEADB
Benchmark Problem#1
Spent Fuel Pool





Initial guess pollutes results for thousands of neutron generations

PWR STUDY
Slow convergence of axial power distribution (top/bottom imbalance shown)



Convergence Diagnostics

MC convergence diagnostics-related issues and challenges

Monte Carlo criticality simulation:

- Slow convergence of large loosely coupled problems
- Robust convergence diagnostics does not exist
- However, accumulation of data should occur only after convergence is ascertained

Entropy-based methods available

Entropy-based convergence diagnostics
Performance and limitations

- Entropy check in MCNP5

$$H(S^B) = -\sum_{i=1}^{B} S^B(i)\log_2(S^B(i))$$

where S denotes the source distribution and *i* is the spatial bin index

[Maximum order or minimum entropy when all source in one mesh]

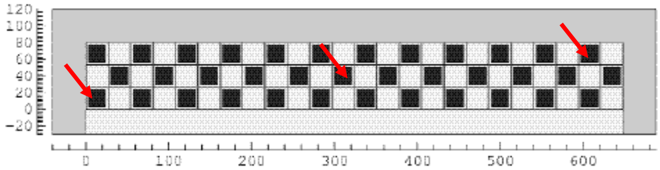
Issues:

- Posterior check: inefficiency
- Loss of local information

OECD Benchmark #1 - Spent fuel pool, checkerboard pattern of assemblies (more loosely coupled than core)

EXAMPLE OF A REAL-LIFE APPLICATION
WITH POTENTIAL FOR UNDERSETIMATING Keff

15x15 FAs, 5%U235
Concrete on 3 sides of the pool
Water on the fourth side
Initial source uniform and at different positions
36 prescribed cases
Almost completely decoupled FAs
Extremely slow source convergence
Somewhat similar to an exaggerated case of a large core, checkerboard pattern, with very low-reactivity twice-burnt fuel



Initial basic results
(Trans. ANS 2002)

Group	Code	Data	Contributor(s)
ANL	VIM	ENDF/B-V	Roger Blomquist
JAERI	MCNP 4B	JENDL3.2	Takeshi Kuroishi
JNC	Keno	SCALE4.4	Shirai Nobutoshi
KFKI	MCNP 4C	ENDF/B-V&VI	Gabor Hordosy
LANL	MCNP 4C	ENDF/B-VI	Forrest Brown
ORNL	KenoV	ENDF/B-V	John Wagner, Lester Petrie
ANSWERS	MONK8A	JEF2	Dave Hanlon

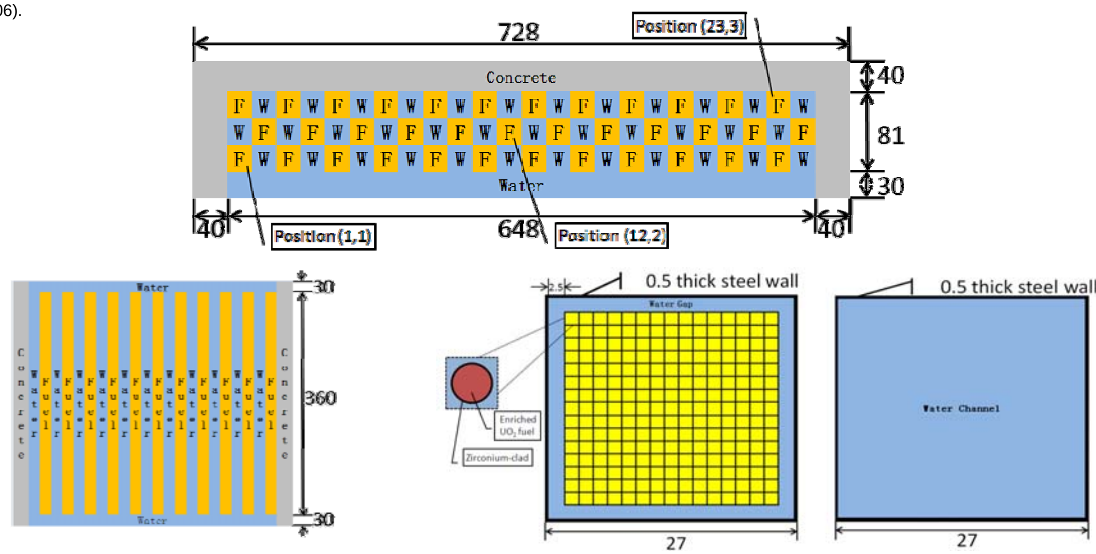
	Min	Max	Case 27
ANL	0.8508 (0.0006)	0.8548 (0.0015)	0.8538 (0.0006)
JAERI	0.8870 (0.0005)	0.8920 (0.0008)	0.8895 (0.0005)
JNC	0.8773 (0.0013)	0.8836 (0.0013)	0.8825 (0.0006)
KFKI	0.8800 (0.0011)	0.8838 (0.0008)	0.8828 (0.0005)
LANL	0.8773 (0.0011)	0.8826 (0.0004)	0.8803 (0.0004)
ORNL	0.8782 (0.0007)	0.8825 (0.0007)	0.8825 (0.0007)
ANSWERS	0.8837 (0.0010)	0.8884 (0.0006)	0.8867 (0.0006)

OECD Benchmark#1 – further analysis (using MCNP5 and entropy diagnostics)

• OECD/NEA benchmark problem

——storage fuel pool

R. N. Blomquist, etc., “Source Convergence in Criticality Safety Analyses,” *NEA Report No. 5431*, Nuclear Energy Agency, Organisation for Economic Co-operation and Development (Nov, 2006).



Benchmark specifications

• Parameters as prescribed:

– Number of skipped generations: 20, 40, and 100.

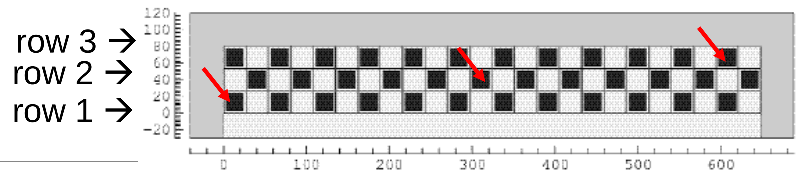
– Number of source neutrons used per generation: 1,000, 2,000, and 5,000

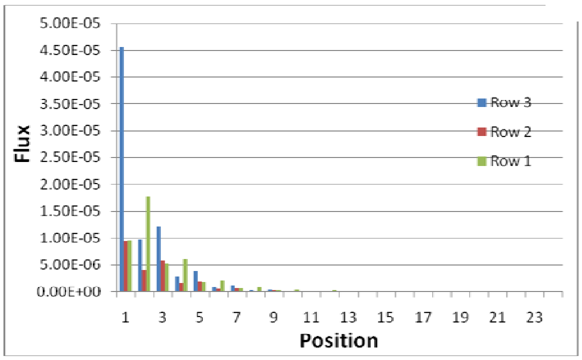
– Distribution of the initial source: all sources in position (1,1), all sources in position (12,2), all sources in position (23,3), and uniform sources over all 36 fuel assemblies

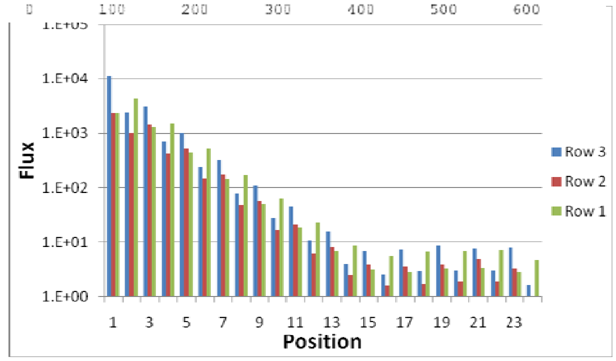
[Note: as prescribed, too few neutrons and generations skipped]

Reference results

- 1,000,000 (10^6) particles per generation
- 1,000 inactive generations, and 1,000 active generations
- Biased source distribution, 20/55







Flux in each assembly position arbitrary units – lin scale

Relative flux to the smallest one in each position with log scale

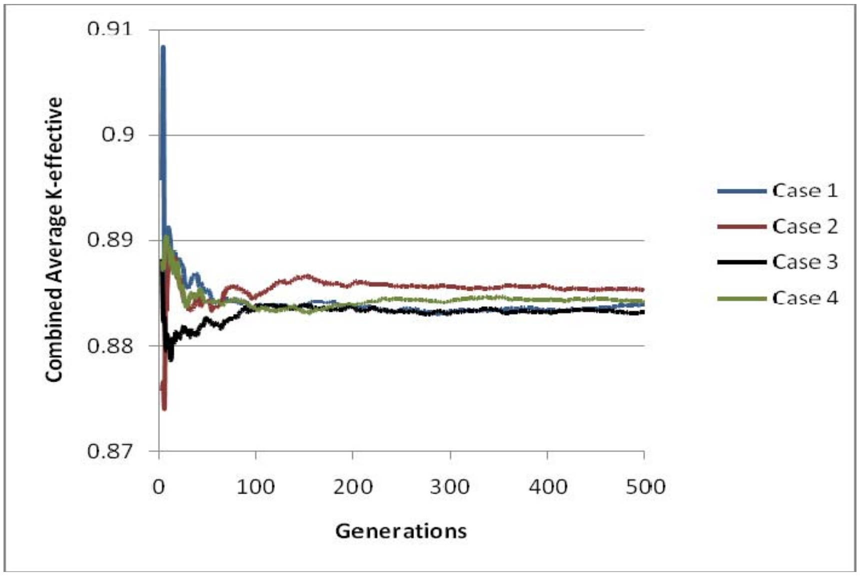
Basic benchmark results — impact of the initial source distribution on k_{eff}

- Four cases with different initial source distributions
  - 5,000 particles per generation
  - 100 inactive generations and 500 active generations

Case	Source	Computing time	keff±σ
1	Uniform in all fuel regions	43.81 min	0.88386±0.00048
2	Uniform in (1,1)	43.51 min	0.88537±0.00051
3	Uniform in (12,2)	44.01 min	0.88310±0.00047
4	Uniform in (23,3)	43.53 min	0.88419±0.00050

Basic benchmark results — impact of the initial source distribution on k_{eff} (cont.)

- k_{eff} convergence with iterations



Each seems flat at 300-500 cycles, but mutually different

Basic benchmark results — impact of the initial source distribution on k_{eff} (cont.)

- Consistency of the k_{eff} from different cases?
- Differences somewhat larger than if normal distribution
- In fact, much larger, but masked by large noise

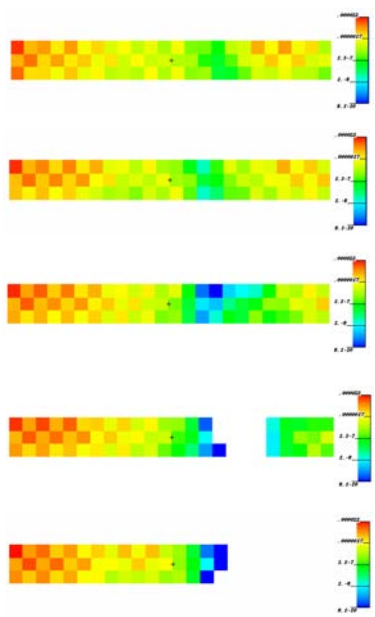
	Case 1	Case 2	Case 3
Case 2	0.00151±0.00070 (2.2σ)	X	X
Case 3	0.00076±0.00067 (1.1σ)	0.00227±0.00069 (3.3σ)	X
Case 4	0.00033±0.00069 (0.5σ)	0.00118±0.00071 (1.7σ)	0.00109±0.00069 (1.6σ)

Evaluation of entropy-based convergence check

Case	First cycle within 1σ with rerun suggestion
1	370, rerun
2	102, rerun
3	141, rerun
4	308, rerun

- For case 1, what if we discard 400 cycles?
- Now (incorrectly) passes the test (393rd skipped cycles required)

Evaluation of entropy-based convergence check

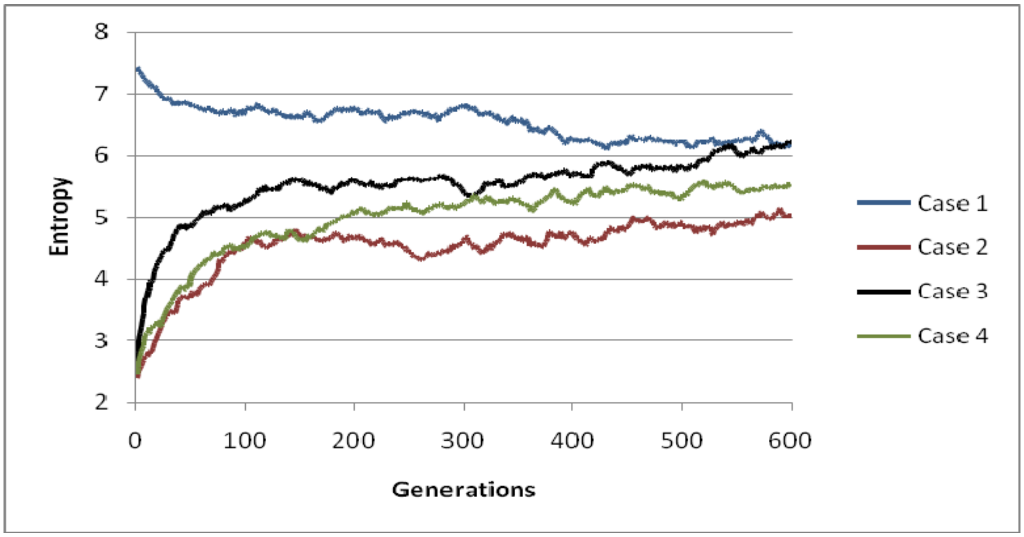


- Flux in position (1,1) for each successive 100 generations (starting with flat in space)

Generations	Flux (arbitrary units)	Estimated σ
401-500	9.896	0.0489
501-600	5.1271	0.0359
601-700	3.9084	0.0315
701-800	6.1409	0.039

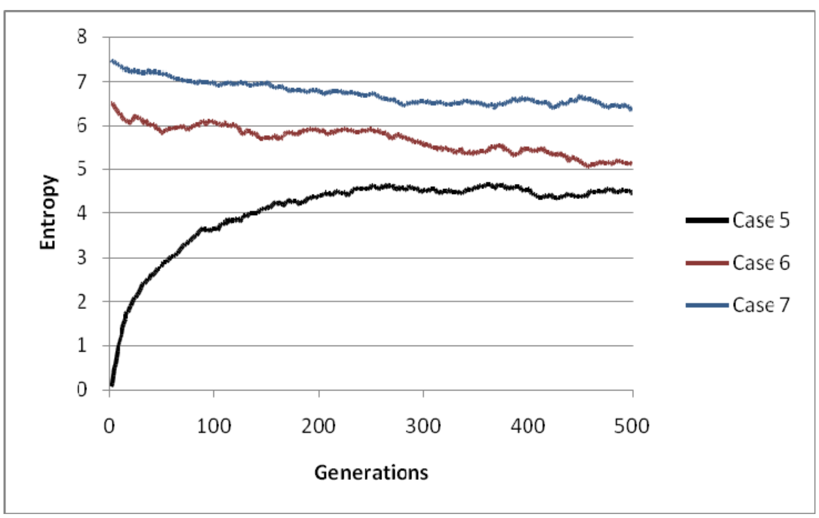
Evaluation of entropy-based convergence check

- Entropy values for the four cases



Evaluation of entropy-based convergence check Entropy-Bounding approach

- Attempt to bound the entropy value by its minimum and maximum.
  - Minimum : All sources in one mesh
  - Maximum : Evenly distributed sources



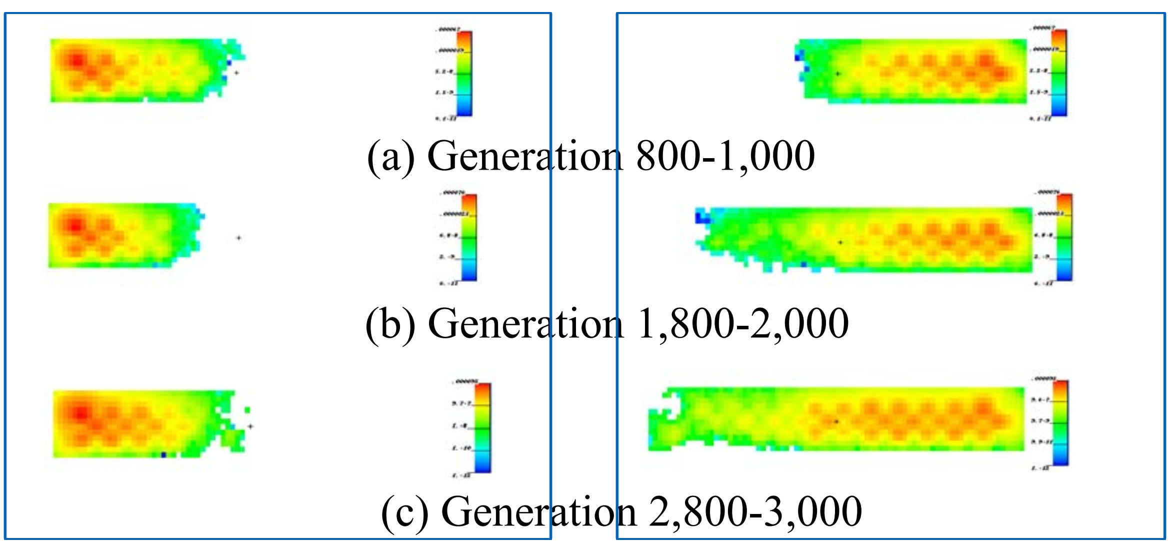
- Potentially useful for idealized problems, not practical/feasible otherwise

Evaluation of entropy-based convergence check
Reference values

- Comparison of the reference entropy values
- Due to tight statistics, inconsistency clear

Case	Average values of entropy (2nd half) with estimated σ	Difference	
		Case 6	Case 7
5 (minimum)	4.50961±0.00516	0.91114±0.01417 64.3σ	2.01757±0.00668 302.0σ
6 (middle)	5.42075±0.01320	X	1.10643±0.01386 79.8σ
7 (maximum)	6.52718±0.00424	X	X

Slow source distribution convergence

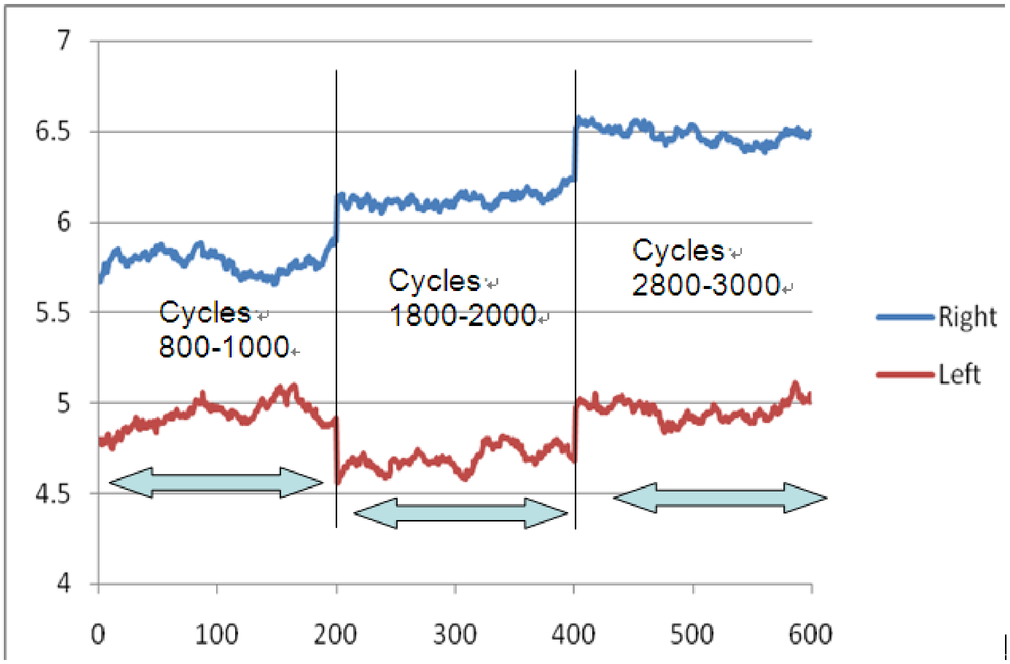


(a) Generation 800-1,000
(b) Generation 1,800-2,000
(c) Generation 2,800-3,000

Initial source on left **Initial source on right**

Examining source distribution rather than entropy clearly demonstrates the need to skip thousands of generations

Slow source distribution convergence (and slow entropy change)

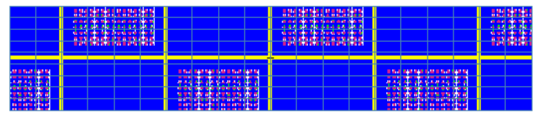


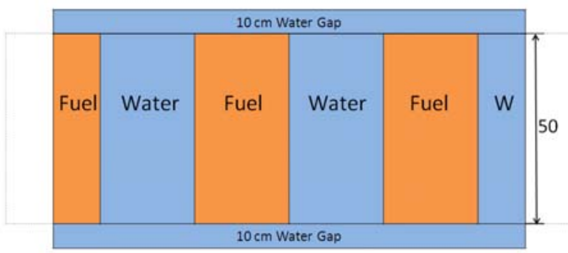
Beyond the entropy-based diagnostics

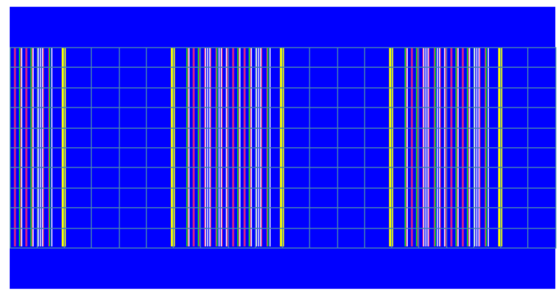
- Use local information

Simplified problem (spent fuel pool – like)

- 20,000 particles per generation
- 100 generations per run
- 1,800 meshes







Statistical consistency analysis

- Compare observed to theoretical normal distribution

$$\left(x_1 - x_2\right) \sim N(0,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

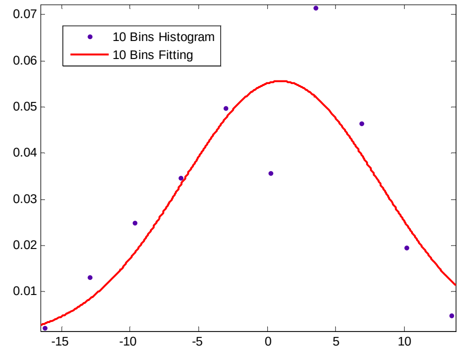
$$\frac{x_1 - x_2}{\hat{\sigma}} \sim N(0,1)$$

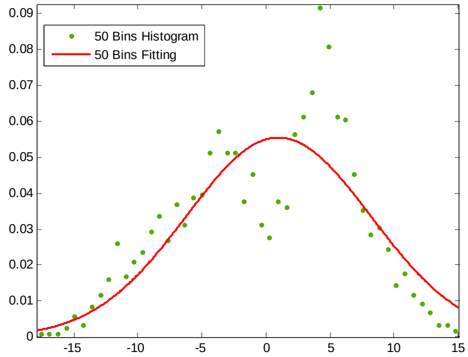
$$\hat{\sigma} = \sqrt{\sigma_1^2 + \sigma_2^2}$$

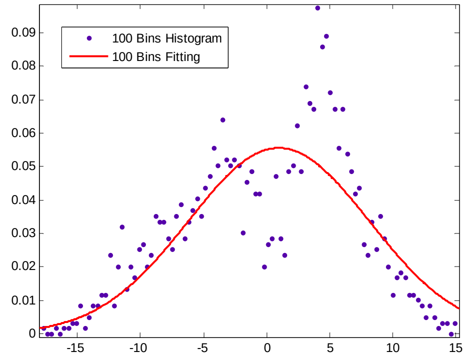
$$\frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Histogram bins and fit to normal

- Compare flux from 501-600 and 601-700
- Histogram with N=10, 50, 100 bins
- Simple normal distribution fit







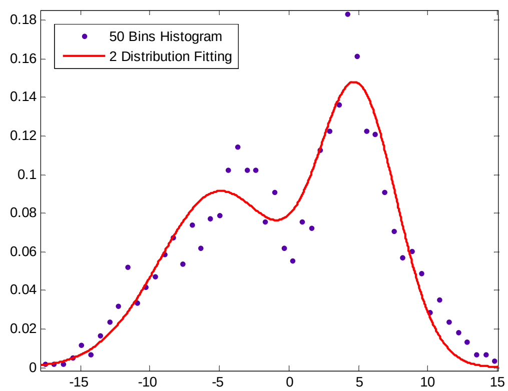
Simple normal distribution fit

Coefficient	10 bins	50 bins	100 bins
μ	0.9916 (-1.382, 3.366)	0.9815 (-0.06596, 2.029)	0.9725 (0.1936, 1.751)
σ	7.174 (5.201, 9.147)	7.187 (6.317, 8.058)	7.174 (6.527, 7.822)

- Compared to “normalized normal” (μ=0, σ=1)
- Clearly not normal distribution
- Underestimate of the variance
- Locally auto-correlation/loose coupling

Fit to multi-normal distribution (sum of two normal)

$$\frac{1}{\sqrt{2\pi\sigma_1}} * \exp\left(-\frac{(x-\mu_1)^2}{2{\sigma_1}^2}\right) + \frac{1}{\sqrt{2\pi\sigma_2}} * \exp\left(-\frac{(x-\mu_2)^2}{2{\sigma_2}^2}\right)$$



Coeff.	Fitting value with 95% confidence interval	Coeff.	Fitting value with 95% confidence interval
μ_1	4.918 (4.581, 5.255)	μ_2	-4.961 (-5.603, -4.318)
σ_1	2.839 (2.576, 3.101)	σ_2	4.377 (3.872, 4.881)

Summary of convergence diagnostics investigation

- The entropy check frequently detects non-convergence, but also produces false-positive convergence indication in some cases.
- The bounding approach may prevent false-positive, but it is not practical.

Work in progress and future work

- Use of local information to evaluate for self-consistency → developing more reliable source convergence diagnostics

Convergence Acceleration

Background

- Monte Carlo criticality simulation
- Typically based on power iteration method
- Convergence to the fundamental eigenmode
- Slow convergence for high dominance ratio problem

Power Iteration Method

Eigenvalue problem:

$$A \ \psi = k\psi$$

With solution:

$$A\psi_i = k_i\psi_i \qquad k_1 > |k_2| > |k_3| > \cdots\cdots$$

$$\psi = \sum_i a_i \psi_i$$

where

$$\lim_{n\to\infty} \frac{1}{k_1^n} A^n \psi = \psi_1 \qquad k_1 = \lim_{n\to\infty} \frac{A^n\psi}{A^{n-1}\psi}$$

Modified Power Iteration Method (T. Booth)

$$\psi = \sum_i (a_i + b_i x)\psi_i$$

$$\lim_{n\to\infty} \frac{1}{k_1^n} A^n \psi = \lim_{n\to\infty} \frac{1}{k_1^n}\left((a_1 + b_1 x)k_1^n \psi_1 + (a_2 + b_2 x)k_2^n \psi_2\right)$$

$$\lim_{n\to\infty} \frac{A^n\psi}{A^{n-1}\psi} = \lim_{n\to\infty} \frac{(a_1 + b_1 x)k_1^n \psi_1 + (a_2 + b_2 x)k_2^n \psi_2}{(a_1 + b_1 x)k_1^{n-1} \psi_1 + (a_2 + b_2 x)k_2^{n-1} \psi_2}$$

Modified Power Iteration Method (T. Booth)

$$k^{R_1} = \frac{A\psi^{R_1}}{\psi^{R_1}} \qquad k^{R_2} = \frac{A\psi^{R_2}}{\psi^{R_2}}$$

$$\psi' = \sum_i a_i \psi_i \qquad \psi'' = \sum_i b_i \psi_i$$

$$\frac{A\psi'_{R_q} + xA\psi''_{R_1}}{\psi'_{R_1} + x\psi''_{R_1}} = \frac{A\psi'_{R_2} + xA\psi''_{R_2}}{\psi'_{R_2} + x\psi''_{R_2}}$$

- Increase in the convergence rate to the fundamental eigenfunction from k_2/k_1 to k_3/k_1

Matrix Problem

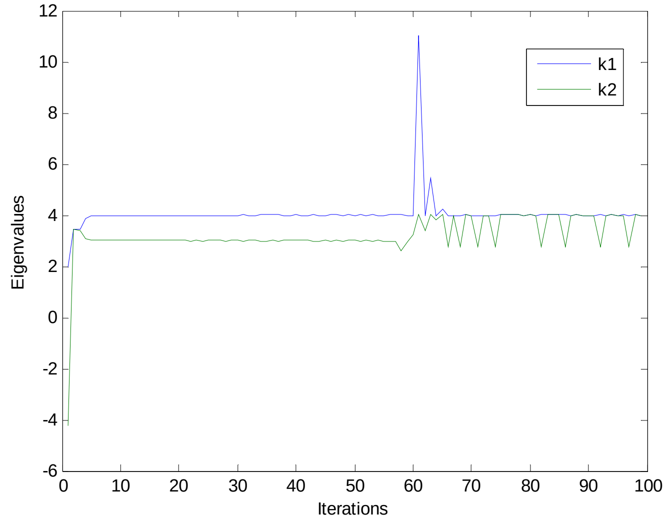
- Test: Apply the modified power iteration method to a "plain" matrix problem

$$A\psi_i = k_i \psi_i \qquad P = \begin{pmatrix} -1.1500 & -0.6250 & -3.0250 & -1.9500 \\ 0.5167 & 1.3750 & 0.6417 & 0.7167 \\ 2.6833 & -0.8750 & 4.0583 & -0.1167 \\ -0.9833 & 2.1250 & 0.3917 & 4.2167 \end{pmatrix}$$

- Eigenvalues: 4, 3, 1, and 0.5
- Initial vectors: a=(1 1 1 1) and b=(1 0 1 1)

Matrix Problem—Test 1

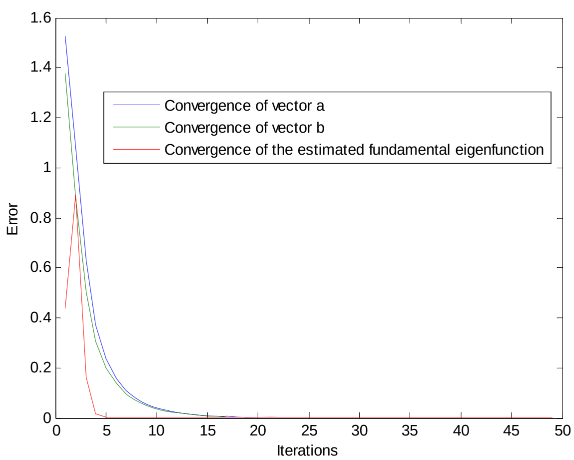
- Evolution of estimated eigenvalues

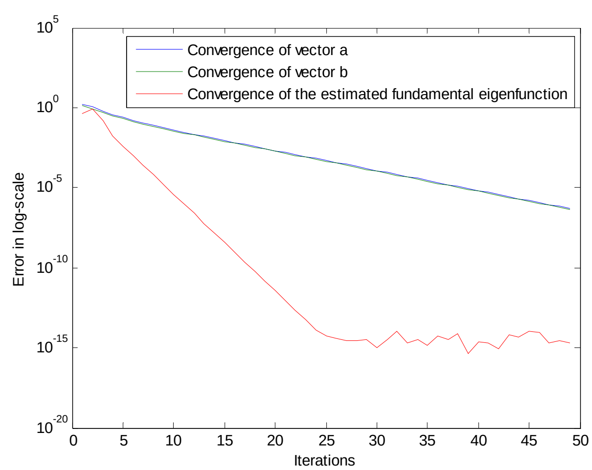


- Round-off error

Convergence Rate

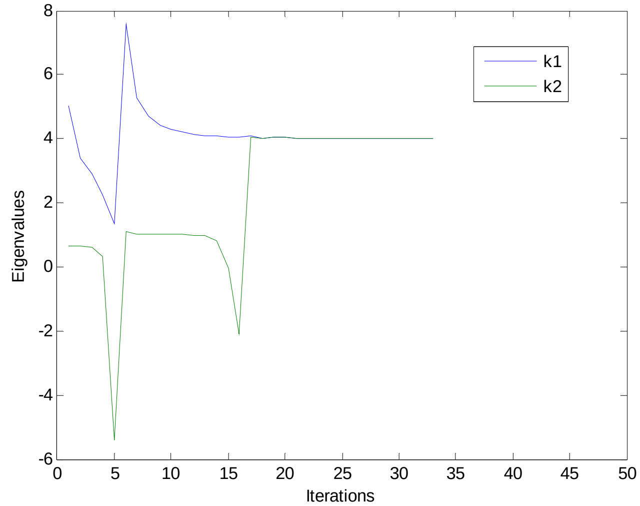
- Error is the L_2 norm of the difference between normalized estimated eigenfunction and known exact eigenfunction,





Matrix Problem—Test 2

- Initial vectors:
  a=(1 1 0 0) and
  b=(0 0 1 1)
- Never converged to k_2
- Collapse of the computation after 35 iterations



Impact of Initial Vectors Selection

- Test 1:

  (1 1 1 1) versus (1 0 1 1)

  (1 1 1 1)=7.1414*ψ_1+10.2794*ψ_2+…
  (1 0 1 1)=5.7131*ψ_1+9.2515*ψ_2+…
  7.1414/10.2794=0.6947, 5.7131/9.2515=0.6175

- Test 2

  (1 1 0 0) versus (0 0 1 1)

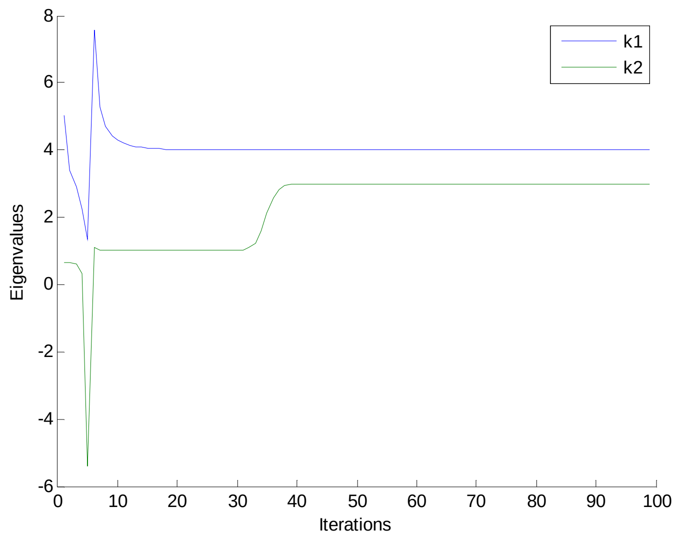
  (1 1 0 0)=2.1424*ψ_1+3.0838*ψ_2+…
  (0 0 1 1)=4.9990*ψ_1+7.1956*ψ_2+…
  2.1424/3.0838=0.6947, 4.9990/7.1956=0.6947

  Difference in ratio $<10^{-4}$ (i.e., nearly proportional vectors)

Caution needed!

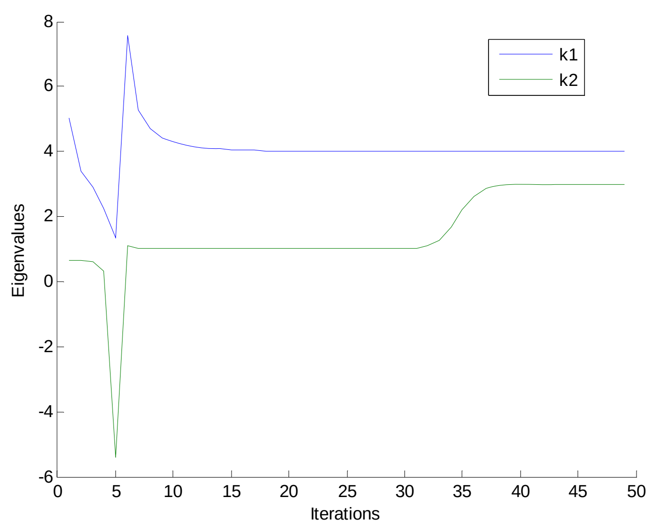
The First Refinement

- Replace P*a with P*a+x_2*P*b.
- Vectors: a=(1 1 0 0) and b=(0 0 1 1)



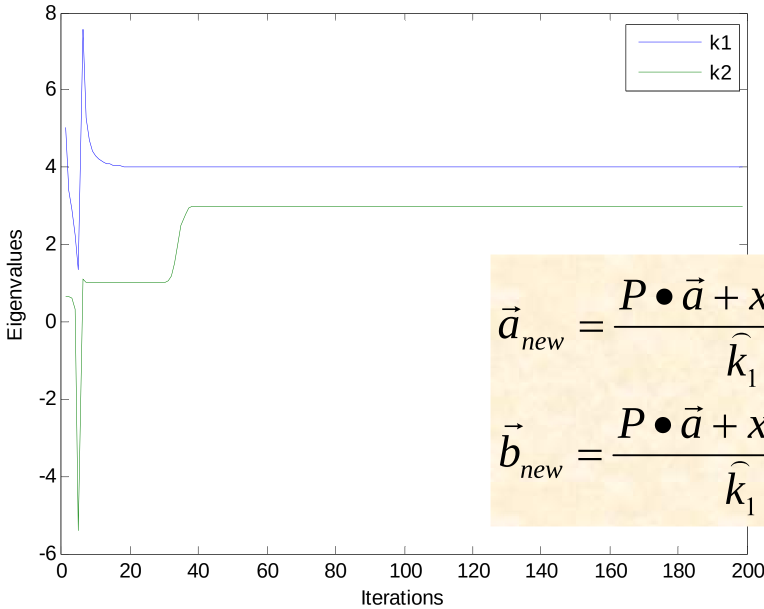
The Second Refinement

- Replace P*b with P*a+x_1*P*b.
- Vectors: a=(1 1 0 0) and b=(0 0 1 1)



New Refinement (GT)

To prevent numerical collapse



$$\vec{a}_{new} = \frac{P \bullet \vec{a} + x_1 P \bullet \vec{b}}{\widehat{k}_1} + \frac{P \bullet \vec{a} + x_2 P \bullet \vec{b}}{\widehat{k}_2}$$

$$\vec{b}_{new} = \frac{P \bullet \vec{a} + x_1 P \bullet \vec{b}}{\widehat{k}_1} - \frac{P \bullet \vec{a} + x_2 P \bullet \vec{b}}{\widehat{k}_2}$$

New refinement within MC simulation
Proof of principle test

- Implemented into in-house MC test code
- One-dimensional, one-group problem
- -4.5 cm to +4.5 cm in the z direction (9 MFP)
- Initial distributions

$$\Sigma_{total} = 1.0cm^{-1}, \Sigma_{scattering} = 0.8cm^{-1}$$

$$\Sigma_{capture} = \Sigma_{fission} = 0.1cm^{-1}, \nu = 3.0$$

$$A = \begin{cases} 0.6 & for \quad z < 0 \\ 1.4 & for \quad z > 0 \end{cases} \qquad B = \begin{cases} 1.6 & for \quad z < 0 \\ 0.4 & for \quad z > 0 \end{cases}$$

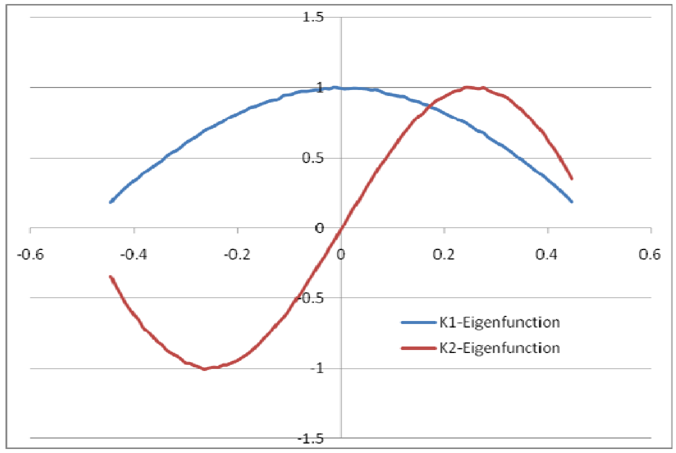
New refinement within MC simulation
Proof of principle test

- Keff results

k_1	k_2
1.30567±0.00042	0.95428±0.00063

- Eigenfunctions

- As theoretically predicted



Weight Cancellation Issue

- Due to the introduction of the negative weight, weight cancellation is needed
  - Exact cancellation
    - » Use point detector mechanism → very expensive
  - Approximate cancellation
    - » Keep the source points
    - » Resample the source points
- An inexpensive yet exact/accurate method is needed

True variance evaluation

- M=50 repetitions, N=50 generations

	Traditional Monte Carlo using resampling	Modified Monte Carlo with new refinement	
		k_1	k_2
$\overline{k}$	**1.30548**	**1.30542**	**0.95499**
$\overline{\sigma}$	**0.00055**	**0.00048**	**0.00090**
σ_{true}	**0.00069**	**0.00053**	**0.00071**

Source convergence improvements - summary

- The modified power iteration method demontraated for both matrix problem and Monte Carlo simulation.
- Possible to compute the first two eigenpairs simultaneously.
- The convergence rate is increased.
- An inexpensive exact weight cancellation method is needed for further application.

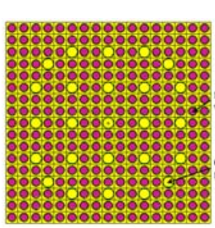
Work in progress and future work:

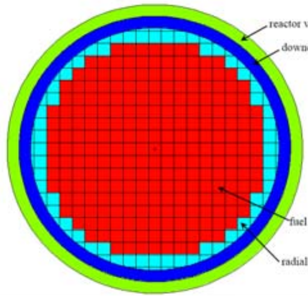
- Extending the test problem to multi-dimension
- Analyzing the behavior of the variance
- Utilizing the dominance ratio for further applications
- Developing an inexpensive exact weight cancellation method

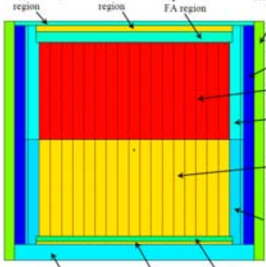
Relevant MC criticality Benchmarks

Monte Carlo Eigenvalue/Criticality Simulations
Feasibility of realistic LWR simulations?

- Need to evaluate feasibility of realistic MC simulations of large power reactors
- 3D benchmark representing a large PWR developed:
  E. Hoogenboom, B. Martin, B. Petrovic
  Available through OECD NEA-DB site
  http://www.nea.fr/dbprog/MonteCarloPerformanceBenchmark.htm
- Determine computational resources needed to achieve acceptable statistical uncertainty; impact of detailed tallies (3D power and isotopics distribution); etc.



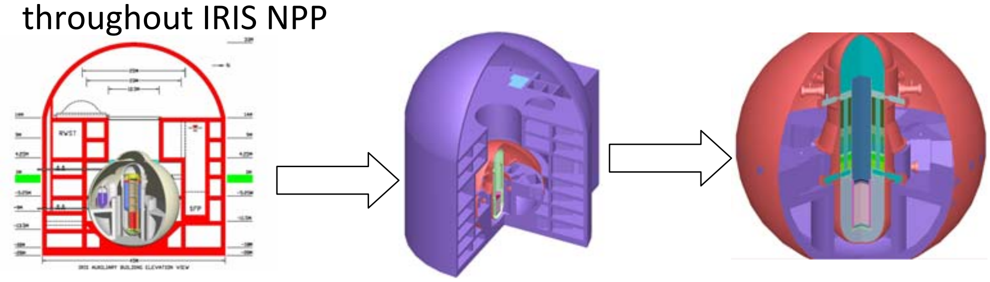




Hybrid MC methods (summary only; presented last year)

Improved Methods for Shielding Analyses
Automated Variance Reduction

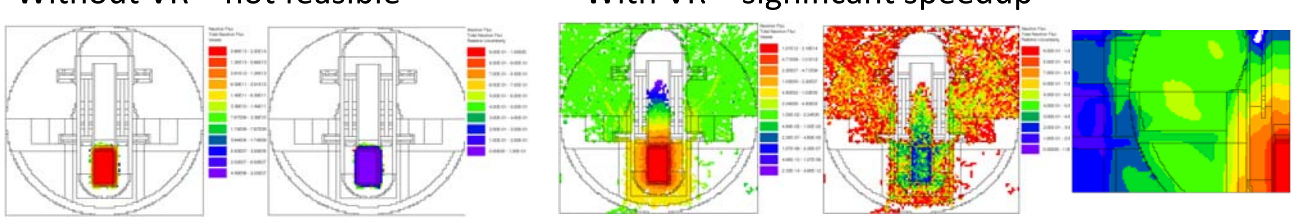
Use of MAVRIC/SCALE code for automated variance reduction (save engineering time!) to determine radiation environment throughout IRIS NPP



Large problem - whole reactor building (50mx57mx60m) modeled
Difficult problem - attenuation over 20 orders of magnitude

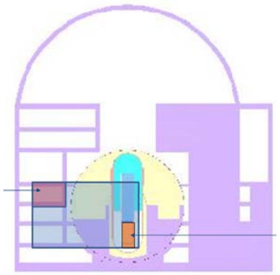
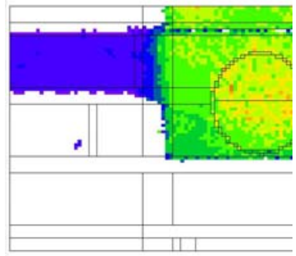
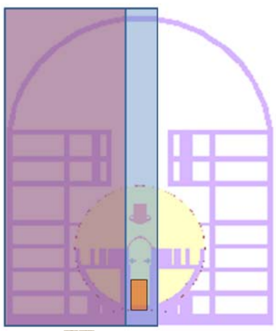
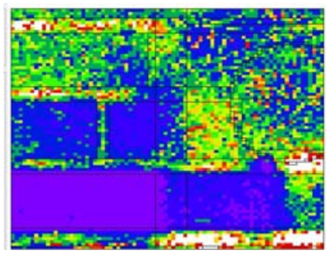
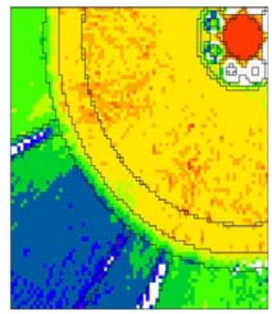
Without VR – not feasible

With VR – significant speedup



Improved Methods for Shielding Analyses
Automated Variance Reduction

1. Dose rate in control room
2. Dose rate throughout the whole building

Summary

- Accurate reactor physics methods needed for design of advanced systems (outside of experience database), enhanced operation of current plants, and validation of production codes and new methods
- Monte Carlo criticality simulations *potentially* provide accurate solution
- Issues of convergence diagnostics, convergence speed and acceleration, and feasibility for simulation of large power systems
- Work in progress….