Title: Monte Carlo Techniques for Nuclear Systems - Theory Lectures

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Web

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Monte Carlo Techniques for Nuclear Systems –

Theory Lectures

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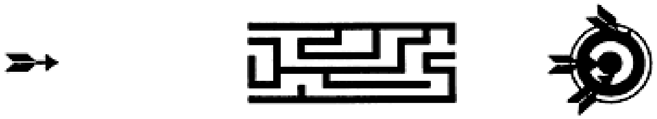
Lecture Topics

Principal lectures
Supplemental

Nuclear Engineering 462

Monte Carlo Techniques for Nuclear Systems



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Course Information (1)

NE 462 - Monte Carlo Techniques for Nuclear Systems - Description

Theory: Solving particle transport problems with the Monte Carlo method is simple - just simulate the particle behavior. The devil is in the details, however. These lectures provide a balanced approach to the theory and practice of Monte Carlo simulation codes. The first lectures provide an overview of Monte Carlo simulation methods, covering the transport equation, random sampling, computational geometry, collision physics, and statistics. The next lectures focus on the state-of-the-art in Monte Carlo criticality simulations, covering the theory of eigenvalue calculations, convergence analysis, dominance ratio calculations, bias in Keff and tallies, bias in uncertainties, a case study of a realistic calculation, and Wielandt acceleration techniques. The remaining lectures cover advanced topics, including HTGR modeling and stochastic geometry, temperature dependence, fission energy deposition, depletion calculations, parallel calculations, and parameter studies.

Practice: This portion of the class focuses on using MCNP to perform criticality calculations for reactor physics and criticality safety applications. It is an intermediate level class, intended for those with at least some familiarity with MCNP. Class examples provide hands-on experience at running the code, plotting both geometry and results, and understanding the code output. The class includes lectures & hands-on computer use for a variety of Monte Carlo calculations. Beginning MCNP users are encouraged to review LA-UR-09-00380, "Criticality Calculations with MCNP: A Primer (3nd Edition)" (available at http://mcnp.lanl.gov under "Reference Collection") prior to the class.

Computing: No Monte Carlo class can be complete without having students write their own simple Monte Carlo routines for basic random sampling, use of the random number generator, and simplified particle transport simulation.

Course Information (2)

NE 462 - Monte Carlo Techniques for Nuclear Systems - Description

- **Three Credit Hours; One 170-minute lecture per week.**

- **Textbook: None**

  Supplemental materials: a DVD provided to all students, containing:

  Lecture notes for 17 lectures on the theory of Monte Carlo methods

  Lecture notes for 19 lectures on the practical use of Monte Carlo methods

  Lecture notes for 16 lectures on computing methods related to Monte Carlo

  186 example problems for practical use of MCNP

  737 technical reports on Monte Carlo methods, including tutorials, a complete introductory book, technical workshops, and references

  Supplemental materials: MCNP6 Monte Carlo code package. Students are required to obtain this (at no cost) from the US DOE computer code center, RSICC. The code is used for the practical part of the course in learning to apply Monte Carlo methods to nuclear engineering problems.

- **Specific Course Information**

  Catalog description: Monte Carlo methods for nuclear criticality and reactor analysis and radiation shielding calculation using production Monte Carlo codes, understand basics of probability and statistics and of particle transport in the context of Monte Carlo methods.

  Corequisite: NE 410.

  Restriction: admitted to School of Engineering.

  Required course in the program

Course Information (3)

NE 462 - Monte Carlo Techniques for Nuclear Systems - Specific Goals

- **Students should develop a basic understanding of Monte Carlo simulation techniques and be able to explain and discuss the following topics:**
  - Random number generation and random sampling methods used in the Monte Carlo simulation of radiation transport
  - Basic statistical concepts including mean, variance, probability density function, cumulative distribution function
  - 3-dimensional computational geometry used to represent physical systems
  - Simulation of the basics physics interactions for particle collisions with the nuclides in problem materials
  - Obtaining engineering results from tallies performed during the Monte Carlo simulation
- **Students should develop a basic understanding of how Monte Carlo methods are applied to realistic nuclear systems and be able to explain and discuss the following topics:**
  - How Monte Carlo methods can be used to determine basic physical quantities including scalar flux, nuclear cross-sections, material reaction rates with radiation
  - How Monte Carlo methods can simulate basic aspects of nuclear systems, including the production of neutrons from fission, the slowing down process due to collisions with moderator material, and the capture and fission of neutrons in the thermal and resonance energy ranges
  - General principles for applying Monte Carlo methods to realistic models of nuclear reactor systems and criticality safety analyses
- **Students should develop a basic understanding of how Monte Carlo methods are implemented into computer codes:**
  - Demonstrate the ability to write simple Monte Carlo programs using a programming language they know (e.g., Matlab, C++, Fortran, etc.)
  - Demonstrate the ability to perform realistic Monte Carlo calculations using an industry-standard Monte Carlo code (e.g., MCNP6)

Course Information (4)

NE 462 - Monte Carlo Techniques for Nuclear Systems - Topics to be covered

- **Overview of Monte Carlo methods**
- **Theory:**
  - Basics - Nuclear Engineering & Monte Carlo
  - Random Numbers & Random Sampling
  - Computational Geometry
  - Collision Physics
  - Tallies & Statistics
  - Eigenvalue Calculations – Parts I, II
  - Variance Reduction
- **Practical:**
  - Introduction to MCNP
  - MCNP Basics
  - Criticality Calculations
  - Advanced Geometry
  - Sources
  - Tallies
  - Physics & Nuclear Data
  - Point Kinetics Parameters
  - Sensitivity-Uncertainty Analysis
- **General:**
  - Eigenvalue Calculations – Part III
  - Parallel Monte Carlo
  - Parameter Studies
  - Doppler Broadening
  - Monte Carlo Depletion

Preliminaries (1)

- **Monte Carlo Techniques for Nuclear Systems**
  - **Introduction to Monte Carlo methods for particle transport simulation**
  - **Limited to neutrons & photons**
  - **Roughly 2/3 theory & 1/3 practical**
    - **Understand basic MC simulation techniques**
      - Random number generation, random sampling
      - 3D computational geometry
      - Basic physics simulation & collisions
      - Tallies
    - **Application to nuclear systems**
      - Flux, cross-sections, reaction rates
      - Simple models
      - Reactor models
      - Criticality safety
    - **Computing**
      - Simple DIY MC programs
      - Using MCNP for realistic models

Preliminaries (2)

- **Useful references & websites**

– **MCNP6 User Manual,**	**part of MCNP6 distribution**
– **MCNP5 Theory Manual (Volume I),**	**on class DVD & MCNP website**
– **Carter & Cashwell book,**	**on class DVD & MCNP website**

  - **MCNP website - mcnp.lanl.gov**
  - **RSICC website - rsicc.ornl.gov**

    For ordering MCNP, SCALE, …..
  - **MCNP Forum email-list - see MCNP website**

  - **National Nuclear Data Center, Brookhaven National Lab. - nndc.bnl.gov**

    ENDF nuclear cross-sections & plotting

    Chart of the Nuclides
  - **Wikipedia ???** **Maybe for class, not for work or papers**

- **Note**
  - **In class or at work, you should always cite the sources for any physical data you use - cross-sections (ENDF/B-VI, -VII.0, VII.1, …), masses, isotopic abundances, etc.**

Nuclear Engineering Review
&
Monte Carlo Basics

Outline

- Introduction
- Review of Nuclear Engineering basics
  - Flux
  - Cross-sections
  - Reaction rates
- Monte Carlo – intro
  - Linear Boltzmann Transport Equation
  - Monte Carlo Simulation
  - Criticality Calculations
- Review of statistics
  - Basic Random Sampling
  - Probability Density (PDF)
  - Cumulative Distribution (CDF)
  - Statistics

Introduction

- **John Von Neumann invented scientific computing in the 1940s**
  - Stored programs, "software"
  - Algorithms & flowcharts
  - Assisted with hardware design as well
  - "Ordinary" computers today are called "Von Neumann machines"

- **Von Neumann invented Monte Carlo methods for particle transport in the 1940s (with Ulam, Fermi, Metropolis, & others at LANL)**
  - Highly accurate - no essential approximations
  - Expensive - typically the "method of last resort"
  - First MC code for ENIAC in 1947
  - Monte Carlo codes for particle transport have been proven to work effectively on all types of computer architectures:

SIMD, MIMD, vector, parallel, supercomputers, clusters,
workstations, PCs, netbooks, tablets,
CPUs, GPUs, MICs, …

Introduction

- **Two basic ways to approach the use of Monte Carlo methods for solving the transport equation:**
  - **Mathematical technique for numerical integration**
  - **Computer simulation of a physical process**

  ➜ Each is "correct"

  - **Mathematical approach is useful for:**

    Importance sampling, convergence, variance reduction, random sampling techniques, eigenvalue calculation schemes, …..

  - **Simulation approach is useful for:**

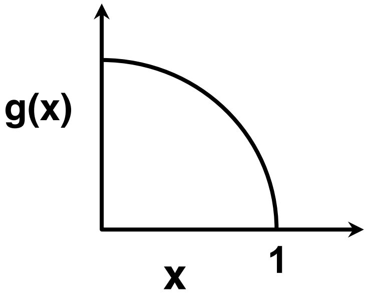
    collision physics, tracking, tallying, …..

- **Monte Carlo methods solve integral problems, so consider the integral form of the Boltzmann equation**

Introduction

Simple Monte Carlo Example

Evaluate $G = \int_0^1 g(x)dx, \quad \text{with} \quad g(x) = \sqrt{1-x^2}$



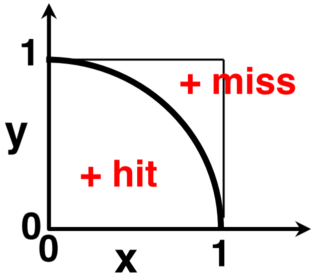
- **Mathematical approach:**

For k = 1, …, N: **choose** $\hat{x}_k$ **randomly in (0,1)**

$$G \approx \tfrac{1}{N} \cdot \sum_{k=1}^{N} g(\hat{x}_k) = \tfrac{1}{N} \cdot \sum_{k=1}^{N} \sqrt{1-\hat{x}_k^2}$$

- **Simulation approach, "darts game":**

For k = 1, …, N: **choose** $\hat{x}_k, \hat{y}_k$ **randomly in (0,1),**
if $\hat{x}_k^2 + \hat{y}_k^2 \le 1$, **tally a "hit"**



$$G \approx \frac{\text{number of hits}}{N}$$

Review of NE Basics

- **Flux**

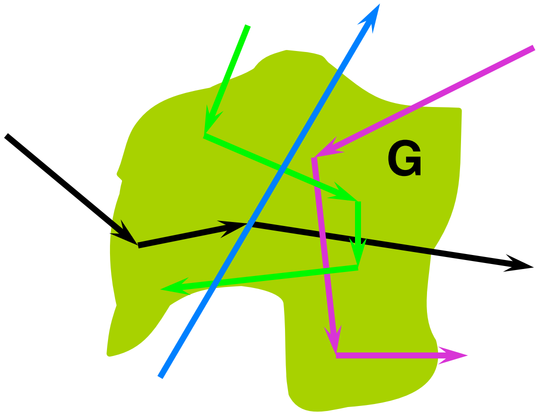
$$\Phi = n\ v$$

– n = particle density,	particles/cm^3	function of position
– v = particle speed,	cm/sec	
– Φ = scalar flux,	particles/cm^2-sec	function of position & energy (but not direction)

– **Most textbooks:**

Scalar flux is the total distance traveled by all particles, per cm^3, per sec

- **Thought experiment:**
  - **Suppose we could watch all particles as they fly around & have collisions**



- **Keep track of all the portions of flight distances within a region G, for all the particles, for a second**

- The **total distance traveled** divided by the volume & 1 second **is the scalar flux** in the region

⇒ This is how MC estimates the flux in a region.

This is the basis for a “pathlength estimator”

Mean Free Path & Macroscopic Cross-section

- **Mean Free Path, λ**
  - λ = average distance to collision

- **Macroscopic Cross-section, Σ**

$$\Sigma = 1/\lambda = N\sigma$$

  - Probability of interaction with a material, per unit distance traveled
  - N = nuclide density, atoms/barn-cm, $N = \frac{N_{av} \cdot m}{A \cdot V} = \frac{N_{av} \cdot \rho}{A}$
  - σ = microscopic cross-section, target area per nuclide
    units: barns, 1 barn = 10^{-24} cm^2
  - Σ = [nuclides/barn-cm] * [barns/nuclide] = 1 / cm
  - For a mixture of nuclides, add Σ's for each nuclide

$$\Sigma_T^{UO2} = N^{U235}\sigma_T^{U235} + N^{U238}\sigma_T^{U238} + N^{O16}\sigma_T^{O16} + \ldots$$

Macroscopic Cross-sections

- **Material Cross-section**

  - **Add Nσ for each nuclide, for a particular reaction x (x: T,A,F,S,C,N-2N, …..)**

$$\Sigma_x^{mat} = \sum_i^{\text{nuclides in material}} N^i \cdot \sigma_x^i$$

$$\Sigma_T^{UO2} = \Sigma_T^{U235} + \Sigma_T^{U238} + \Sigma_T^{O16} + \ldots$$

$$= N^{U235}\sigma_T^{U235} + N^{U238}\sigma_T^{U238} + N^{O16}\sigma_T^{O16} + \ldots$$

  - **Given that a collision occurs in a material, the probability that it will involve nuclide J is:**

$$p_J^{mat} = \frac{\Sigma_T^J}{\Sigma_T^{mat}}$$

⇒ This is how MC selects a particular nuclide, given that a collision occurs in a material

Macroscopic Cross-sections

- **If a neutron collision occurs in UO_2 fuel, find the probability that the collision is with U^{235}, U^{238}, or O^{16}**

$$\Sigma_T^{fuel} = N^{U235}\sigma_T^{U235} + N^{U238}\sigma_T^{U238} + N^{O16}\sigma_T^{O16} = \Sigma_T^{U235} + \Sigma_T^{U238} + \Sigma_T^{O16}$$

Probability that collison is with

$$\text{U235:} \quad P = \frac{\Sigma_T^{U235}}{\Sigma_T^{fuel}}, \qquad \text{U238:} \quad P = \frac{\Sigma_T^{U238}}{\Sigma_T^{fuel}}, \qquad O16: \quad P = \frac{\Sigma_T^{O16}}{\Sigma_T^{fuel}},$$

- **If a neutron collision occurs in UO_2 fuel, find the probability that the neutron is absorbed**

$$\Sigma_A^{fuel} = N^{U235}\sigma_A^{U235} + N^{U238}\sigma_A^{U238} + N^{O16}\sigma_A^{O16} = \Sigma_A^{U235} + \Sigma_A^{U238} + \Sigma_A^{O16}$$

$$\Sigma_S^{fuel} = N^{U235}\sigma_S^{U235} + N^{U238}\sigma_S^{U238} + N^{O16}\sigma_S^{O16} = \Sigma_S^{U235} + \Sigma_S^{U238} + \Sigma_S^{O16}$$

$$\Sigma_T^{fuel} = \Sigma_A^{fuel} + \Sigma_S^{fuel}$$

Probability that neutron is

$$\text{Absorbed:} \quad P_A = \frac{\Sigma_A^{fuel}}{\Sigma_T^{fuel}}, \qquad \text{Scattered:} \quad P_S = \frac{\Sigma_S^{fuel}}{\Sigma_T^{fuel}}, \qquad P_A + P_S = 1$$

Microscopic Cross-sections

- **Microscopic Cross-section, σ**
  - **σ = Target area of <u>single nuclide</u> for an interaction**
  - **Units: barns** **1 barn = 10^{-24} cm²**
  - **Examples:** σ_A^{U235}, σ_S^{H}, $\sigma_{N\text{-}2N}^{U238}$ Isotope Type of reaction
  - **Microscopic cross-section data:**
    - Measured in experiments
    - Determined from theory (eg, quantum mechanics)
    - Experiment + theory + judgement used by CSWEG to produce ENDF/B datasets

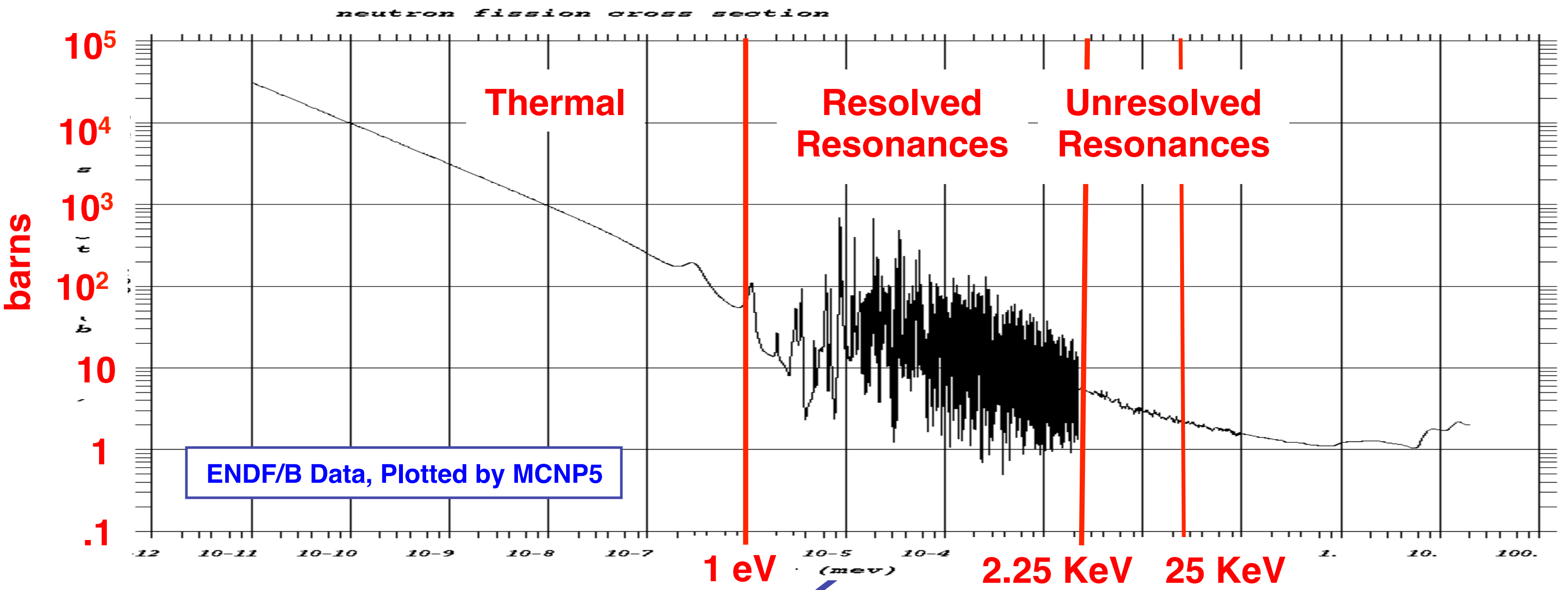
- **Absorption vs Capture**
  - **For NE's and this class:**

$$\sigma_A = \sigma_C + \sigma_F$$

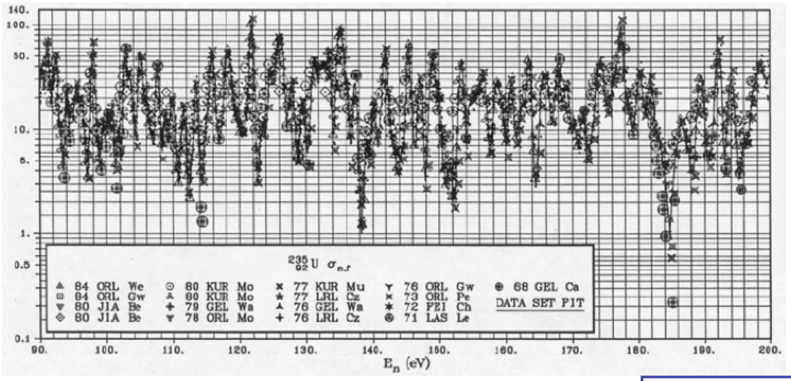
$$\sigma_T = \sigma_C + \sigma_F + \sigma_S = \sigma_A + \sigma_S$$

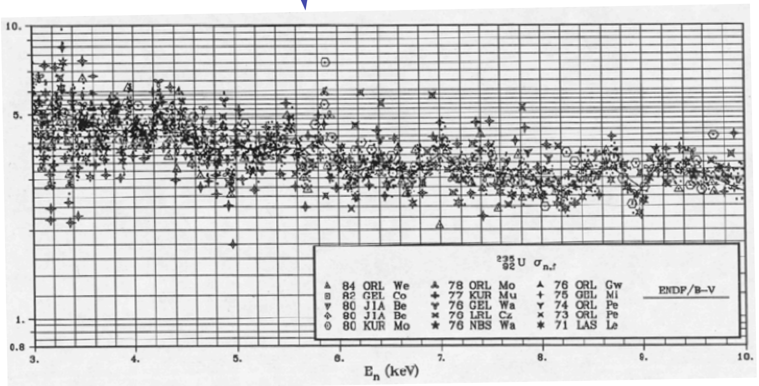
  - **Absorption = fission + capture**
  - **Physicists often interchange “capture” & “absorption”**

U^{235} Fission Cross-section, σ_F^{U235}



ENDF/B Data, Plotted by MCNP5





Experimental Data used by CSWEG

Nuclear Data - Where to Find It

- Use the MCNP built-in cross-section plotter
  - Generally, MCNP uses latest ENDF/B-VII.0 nuclear data
  - Can plot any isotope & reaction (if available) in a problem
  - Will be covered in Practical Lecture on Nuclear Data
- LANL T-2 Nuclear Information Service
  - t2.lanl.gov
  - Nuclear Data Viewer & ENDF data
- National Nuclear Data Center, Brookhaven National Lab.
  - nndc.bnl.gov - has ENDF data & plotting utilities
  - Isotopic abundances - AMDC
  - Chart of the Nuclides

Microscopic Cross-sections

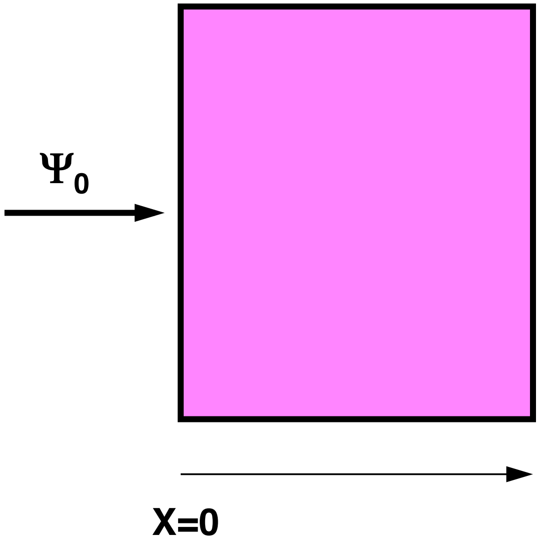
- **Thought experiments:**
  - **Given that a collision occurs with nuclide J, what is the probability of the incoming particle surviving the collision?**
    - Note that $\sigma_T^J = \sigma_A^J + \sigma_S^J$

      Absorption ⇒ particle disappears
      Scatter ⇒ particle survives
    - Probability of surviving the collision $= \sigma_S^J / \sigma_T^J$
  - **Given that a collision occurs with nuclide J, what is the probability of fission?**
    - Note that $\sigma_T^J = \sigma_F^J + \sigma_C^J + \sigma_S^J$
    - Probability of fission $= \sigma_F^J / \sigma_T^J$

⇒ In MC codes, "given that a collision occurs with nuclide J", probabilities based on ratios of partial σ' s for nuclide J are used in sampling what reaction takes place with that nuclide

Beam Attenuation

- For a beam of particles
  - Ψ(r, E, Ω) = angular flux at r, direction Ω
    - Directional quantity
    - Integrate over all Ω to get scalar flux Φ
  - If a beam of particles is directed at a purely-absorbing infinite slab,
    what is the beam strength at penetration x?



$$\psi(x) = \psi_0 \cdot e^{-\Sigma_T x}$$

  - Probability of traveling distance x <u>without</u> collision is $e^{-\Sigma_T x}$
  - Probability of <u>colliding at distance x</u> is

[prob of colliding at x per-unit-dist] * [prob of reaching x w/o collision]

$$f(x) \;=\; \Sigma_T \cdot e^{-\Sigma_T x}$$

⇒ MC codes use this relation to sample the distance to the next collision

Reaction Rates

- Most of the time, nuclear engineers don't care about flux. The important & useful quantities desired include:

  absorption in a region, fission in a region, heating in a region,
  absorption in U^{235} U^{238} Pu^{239} B^{10} Hf Xe^{135} Zr ….., etc.

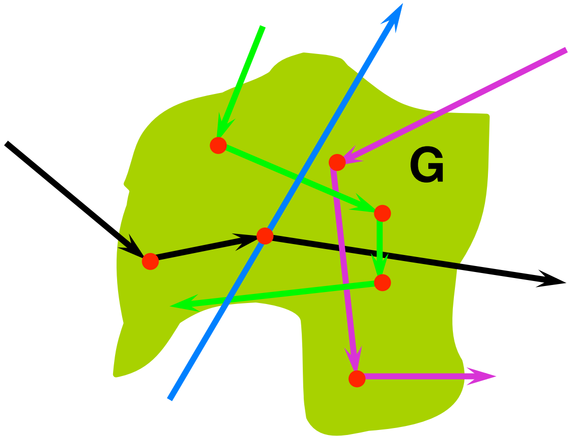
- Reaction rates
  - Collision rate = $\Sigma_T \Phi$
  - Fission rate = $\Sigma_F \Phi$
  - Neutron production rate = $\nu\Sigma_F \Phi$
  - Absorption rate in U^{235} = $\Sigma_A^{U235} \Phi$

  - Reaction rate = [reactions / cm] * [total cm traveled / cm^{3}sec]
    = reactions / cm^{3}sec
  - To get total reactions/sec for a region, integrate over the region volume

  - For reaction rates in a material, use Σ for the material
  - For reaction rates for a nuclide, use Σ for the nuclide (in the material)

Another Flux Estimator

- **Thought experiment:**
  - **Suppose we could watch all particles as they fly around & have collisions**



- **Keep track of all the collisions within a region G, for all the particles, for a second**
- **[collision rate]** = $\Sigma_T\Phi$
- Solve for flux: Φ = [collision rate] / Σ_T

⇒ **MC uses this to estimate the flux in a region.**
This is the basis for a "collision estimator"

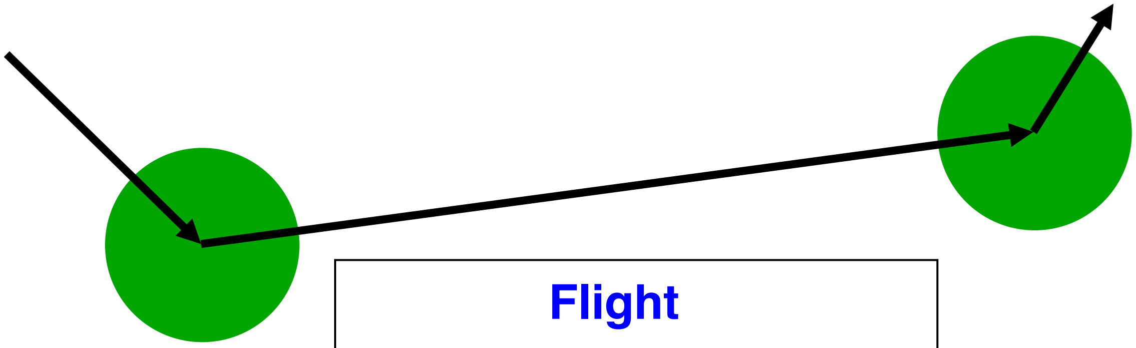
- **We have seen that MC can estimate the flux in a region in several ways:**
  - Pathlength estimator - [total distance traveled in region] / (Volume x time)
  - Collision estimator - [total collisions in region] / Σ_T / (Volume x time)

• Which is correct?	Both
• Which is better?	Depends on physics & geometry of problem
• Are there other flux estimators?	Yes (flux at point, flux on surface, …..)
• Which one should be used?	If available, all (statistically combined)

- MCNP only provides pathlength flux estimators for a region.
  Some MC codes only provide collision estimators; some provide both.

Monte Carlo - Introduction

- Goal: Simulate nature,
  particles moving through physical objects



Flight

Random sampling using Σ_T & exponential PDF:

- Free-flight distance to next collision, s

Ray-tracing in 3D computational geometry

Collision

Simulate absorption:

- absorb, or
- reduce weight

Random sampling using nuclear data:

- Collision isotope
- Reaction type
- Exit E' & Ω'
- Secondary particles

During analysis of both flights & collisions, tally information about distances, collisions, etc. to use later in statistical analysis for results

Monte Carlo Simulation - Assumptions

Assume:

- Neutrons & photons are particles, not waves
- Particles move in a straight line between collisions (neutrons, photons)
- Collisions occur instantaneously, at a point in space
- Particle speeds are small enough to neglect relativistic effects
- Particle speeds are high enough to neglect quantum effects
- Particle collisions do not change the properties of a material
  (ie, no feedback, no material heating, no depletion)
- Material properties are fixed for the duration of the simulation
  (geometry, densities, temperatures, material compositions, …..)

Why?

- Want to solve the linear Boltzmann transport equation
- Want to apply the superposition principle
- Want the Central Limit Theorem to apply for computing statistics
  - Statisticians love the term "IID" - Independent, Identically Distributed

(Any or all of the above assumptions can be relaxed, with careful analysis & extra computing cost.)

Linear Boltzmann Transport Equation

- **Time-dependent linear Boltzmann transport equation for neutrons, with prompt fission source & external source**

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = \overset{\text{External source}}{Q(\vec{r},E,\vec{\Omega},t)} + \overset{\text{Scattering}}{\iint \psi(\vec{r},E',\vec{\Omega}',t)\,\Sigma_S(\vec{r},E' \to E,\vec{\Omega}\cdot\vec{\Omega}')\,d\vec{\Omega}'dE'}$$

$$+ \overset{\text{Multiplication}}{\frac{\chi(\vec{r},E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\,\psi(\vec{r},E',\vec{\Omega}',t)\,d\vec{\Omega}'dE'}$$

$$-\left[\,\overset{\text{Leakage}}{\vec{\Omega}\cdot\nabla} + \overset{\text{Collisions}}{\Sigma_T(\vec{r},E)}\,\right]\cdot\psi(\vec{r},E,\vec{\Omega},t)$$

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = \underset{\text{Gains}}{Q + [S+M]\cdot\psi} - \underset{\text{Losses}}{[L+T]\cdot\psi}$$

- **This equation can be solved directly by Monte Carlo, assuming:**
  - **Each neutron history is an IID trial (independent, identically distributed)**
  - **All neutrons must see same probability densities in all of phase space**
  - **Usual method: geometry & materials fixed over solution interval Δt**

Time-dependent Diffusion

- **Monte Carlo codes solve the transport equation**

- **For comparison, the multigroup diffusion equation is an approximation used by many codes & taught to undergrads:**

$$\frac{1}{v}\frac{\partial\Phi_G(\vec{r},t)}{\partial t} = \overset{\text{External source}}{Q_G(\vec{r},t)} + \overset{\text{Scattering}}{\sum_{G'\neq G}\Sigma_{S,G'\to G}(\vec{r})\cdot\Phi_{G'}(\vec{r},t)} + \overset{\text{Multiplication}}{\frac{\chi_G(\vec{r})}{4\pi}\sum_{G'}\nu\Sigma_{F,G'}(\vec{r})\cdot\Phi_{G'}(\vec{r},t)}$$

$$-\left[\ \overset{\text{Absorption}}{\Sigma_{A,G}(\vec{r})} - \overset{\text{Leakage}}{\nabla\cdot D_G\nabla}\ \right]\cdot\Phi_G(\vec{r},t)$$

$$\frac{1}{v}\frac{\partial\Phi(\vec{r},t)}{\partial t} = Q_G + \underset{\text{Gains}}{[S+M]\cdot\Phi} - \underset{\text{Losses}}{[L+T]\cdot\Phi}$$

- **Many approximations - angle, energy, D, …..**

Monte Carlo & Transport Equation

- **Derive integral equation, in kernel form**
  - Start with integro-differential equation
  - Use integrating factor $\exp\left[-\int_0^R \Sigma_T(\vec{r}-R\hat{\Omega},E)\,dR'\right]$, where $R\hat{\Omega}=\vec{r}-\vec{r}\,'$
  - Define

$$\vec{E}=E\cdot\hat{\Omega}$$

Collision density: $\Psi(\vec{r},\vec{E})=\Sigma_T(\vec{r},E)\cdot\psi(\vec{r},\vec{E})$

Transport kernel: $T(\vec{r}\,'\to\vec{r},\vec{E})=\Sigma_T(\vec{r},E)\cdot\exp\left[-\int_0^{|\vec{r}-\vec{r}\,'|}\Sigma_T(\vec{r}\,'+s\hat{\Omega},E)\,ds\right]\cdot\frac{\delta\left(\hat{\Omega}\bullet\frac{\vec{r}-\vec{r}\,'}{|\vec{r}-\vec{r}\,'|}-1\right)}{|\vec{r}-\vec{r}\,'|^2}$

Collision kernel: $C(\vec{E}\,'\to\vec{E},\vec{r})=\frac{\Sigma_S(\vec{r},\vec{E}\,'\to\vec{E})}{\Sigma_T(\vec{r},E')}+\frac{\chi(\vec{r},E)\nu\Sigma_F(\vec{r},E')}{4\pi\cdot\Sigma_T(\vec{r},E')}$

  - Then

$$\Psi(\vec{r},\vec{E})=\int\left[\int\Psi(\vec{r}\,',\vec{E}\,')\cdot C(\vec{E}\,'\to\vec{E},\vec{r}\,')\,d\vec{E}\,'+Q(\vec{r}\,',\vec{E}\,')\right]\cdot T(\vec{r}\,'\to\vec{r},\vec{E})\,d\vec{r}\,'$$

Reference: D.C. Irving, "The Adjoint Boltzmann Equation and Its Simulation by Monte Carlo" *Nuclear Engineering & Design* 15, 273-292 (1971)

Monte Carlo & Transport Equation

Basis for the Monte Carlo Solution Method

$$\Psi(\vec{r},\vec{E}) = \int \left[\int \Psi(\vec{r}',\vec{E}') \cdot C(\vec{E}' \rightarrow \vec{E},\vec{r}') d\vec{E}' + Q(\vec{r}',\vec{E}') \right] \cdot T(\vec{r}' \rightarrow \vec{r}, \vec{E}) d\vec{r}'$$

Let $\mathrm{p} = (\vec{\mathrm{r}},\vec{\mathrm{E}})$ and $\mathrm{R}(\mathrm{p}' \rightarrow \mathrm{p}) = \mathrm{C}(\vec{\mathrm{E}}' \rightarrow \vec{\mathrm{E}},\vec{\mathrm{r}}') \cdot \mathrm{T}(\vec{\mathrm{r}}' \rightarrow \vec{\mathrm{r}},\vec{\mathrm{E}})$

Expand Ψ into components having 0,1,2,...,k collisions

$$\Psi(\mathrm{p}) = \sum_{\mathrm{k}=0}^{\infty} \Psi_{\mathrm{k}}(\mathrm{p}), \qquad \text{with} \quad \Psi_0(\mathrm{p}) = \int \mathrm{Q}(\vec{\mathrm{r}}',\vec{\mathrm{E}}) \cdot \mathrm{T}(\vec{\mathrm{r}}' \rightarrow \vec{\mathrm{r}},\vec{\mathrm{E}}) \mathrm{d}\vec{\mathrm{r}}'$$

By definition,

$$\Psi_{\mathrm{k}}(\mathrm{p}) = \int \Psi_{\mathrm{k}-1}(\mathrm{p}') \cdot \mathrm{R}(\mathrm{p}' \rightarrow \mathrm{p}) \mathrm{d}\mathrm{p}'$$

Markovian: collision k depends only on the results of collision k-1, and not on any prior collisions k-2, k-3, ...

Monte Carlo & Transport Equation

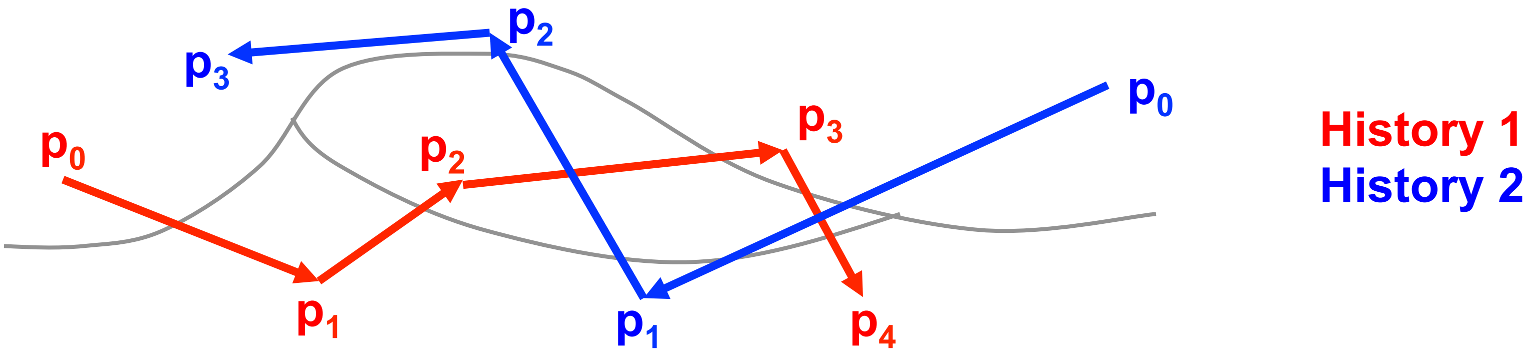
Histories

- After repeated substitution for Ψ_k

$$\Psi_k(p) = \int \Psi_{k-1}(p') \cdot R(p' \rightarrow p)dp'$$

$$= \int \ldots \int \Psi_0(p_0) \cdot R(p_0 \rightarrow p_1) \cdot R(p_1 \rightarrow p_2) \ldots R(p_{k-1} \rightarrow p)dp_0 \ldots dp_{k-1}$$

- A "history" is a sequence of states $(p_0, p_1, p_2, p_3, \ldots..)$



- For estimates in a given region, tally the occurrences for each collision of each "history" within a region

Monte Carlo & Transport Equation

$$\Psi_k(p) = \int \ldots \int \Psi_0(p_0) \cdot R(p_0 \to p_1) \cdot R(p_1 \to p_2) \ldots R(p_{k-1} \to p) dp_0 \ldots dp_{k-1}$$

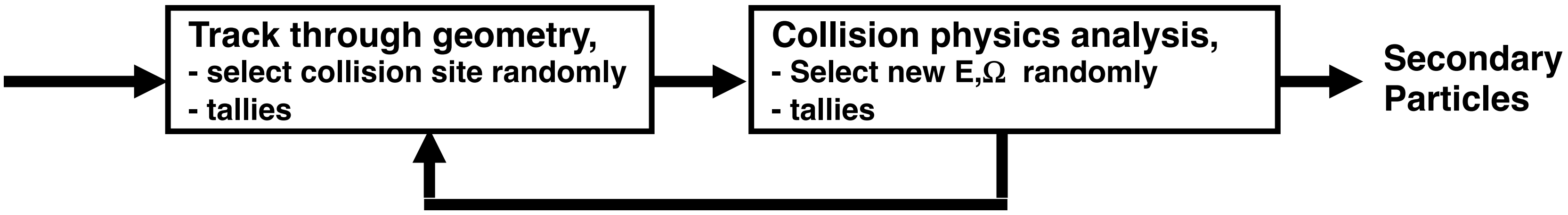
Monte Carlo approach:

- **Generate a sequence of states (p_0, p_1, p_2, p_3, …..) [i.e., a history] by:**
  - **Randomly sample from PDF for source: $\Psi_0(p_0)$**
  - **Randomly sample from PDF for kth transition: $R(p_{k-1} \to p_k)$**
- **Generate estimates of results by averaging over states for M histories:**

$$A = \int A(p) \cdot \Psi(p) dp \approx \frac{1}{M} \cdot \sum_{m=1}^{M} \left(\sum_{k=1}^{\infty} A(p_{k,m}) \right)$$

Fixed-source Monte Carlo Calculation

Random Walk for a particle

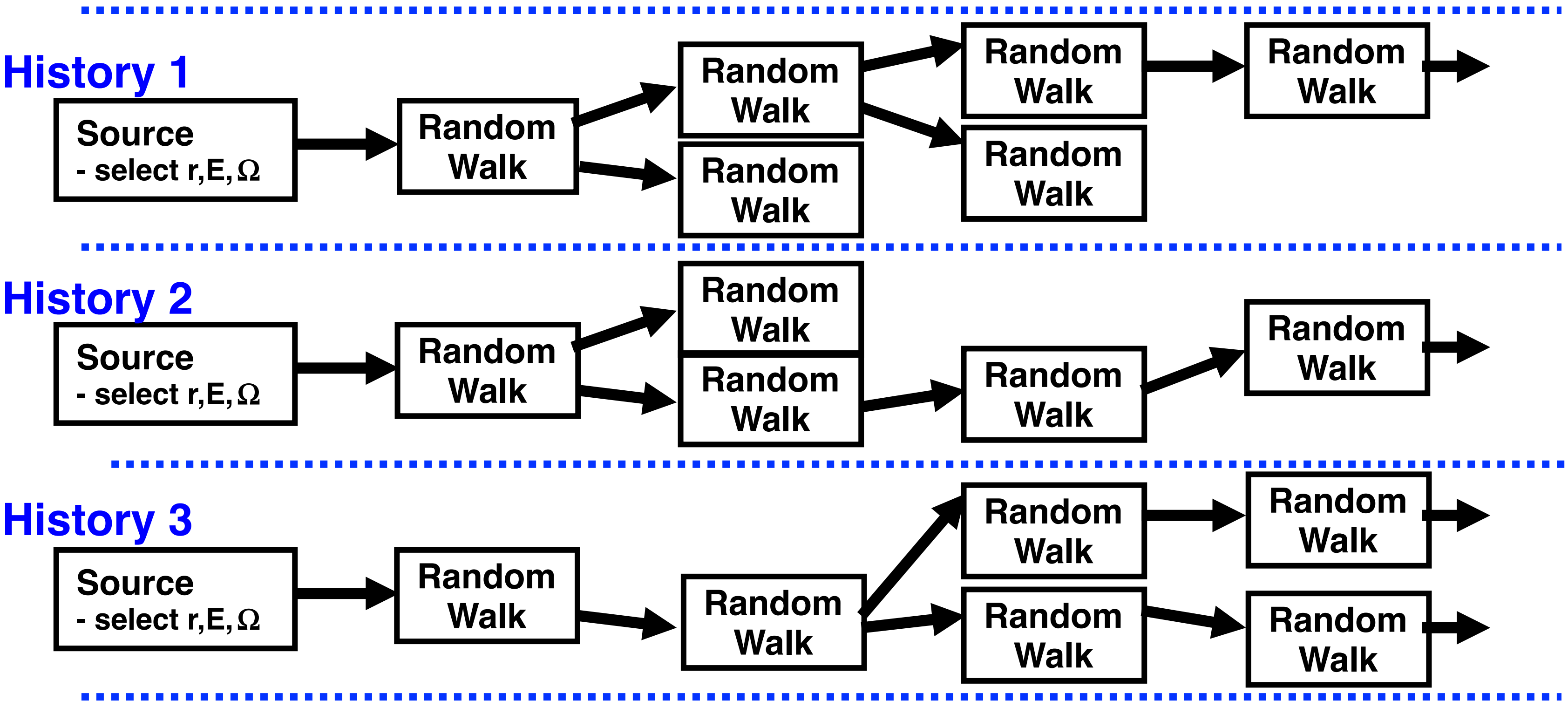


Track through geometry,
- select collision site randomly
- tallies

Collision physics analysis,
- Select new E,Ω randomly
- tallies

Secondary Particles

Particle Histories



History 1

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

History 2

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

History 3

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

K_{eff} Eigenvalue Equation

- For problems with fission multiplication, another approach is to create a static eigenvalue problem from the time-dependent transport equation (the asymptotic or steady-state solution)

- Introduce K_{eff}, a scaling factor on the multiplication (ν)

- Assume:
  1. Fixed geometry & materials
  2. No external source: $Q(r,E,\Omega,t) = 0$
  3. $\partial\Psi/\partial t = 0$: $\nu \Rightarrow \nu / k_{eff}$

- Setting $\partial\Psi/\partial t = 0$ and introducing the K_{eff} eigenvalue gives

$$\left[L + T\right]\Psi_k(\vec{r},E,\vec{\Omega}) = \left[S + \frac{1}{K_{eff}} M\right]\Psi_k$$

  – Steady-state equation, a static eigenvalue problem for K_{eff} and Ψ_k
  – K_{eff} = effective multiplication factor
  – Critical: K=1, subcritical: k<1, supercritical: k >1
  – K_{eff} and Ψ_k should never be used to model time-dependent problems.

K_{eff} Eigenvalue Equation

Leakage Collisions Scattering

$$\left[\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E)\right]\cdot\psi(\vec{r},E,\vec{\Omega}) = \iint \psi(\vec{r},E',\vec{\Omega}')\Sigma_S(\vec{r},E'\to E,\vec{\Omega}\cdot\vec{\Omega}')\,d\vec{\Omega}'dE'$$

Multiplication

$$+ \frac{1}{k_{eff}}\frac{\chi(\vec{r},E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E',t)\,\psi(\vec{r},E',\vec{\Omega}')\,d\vec{\Omega}'dE'$$

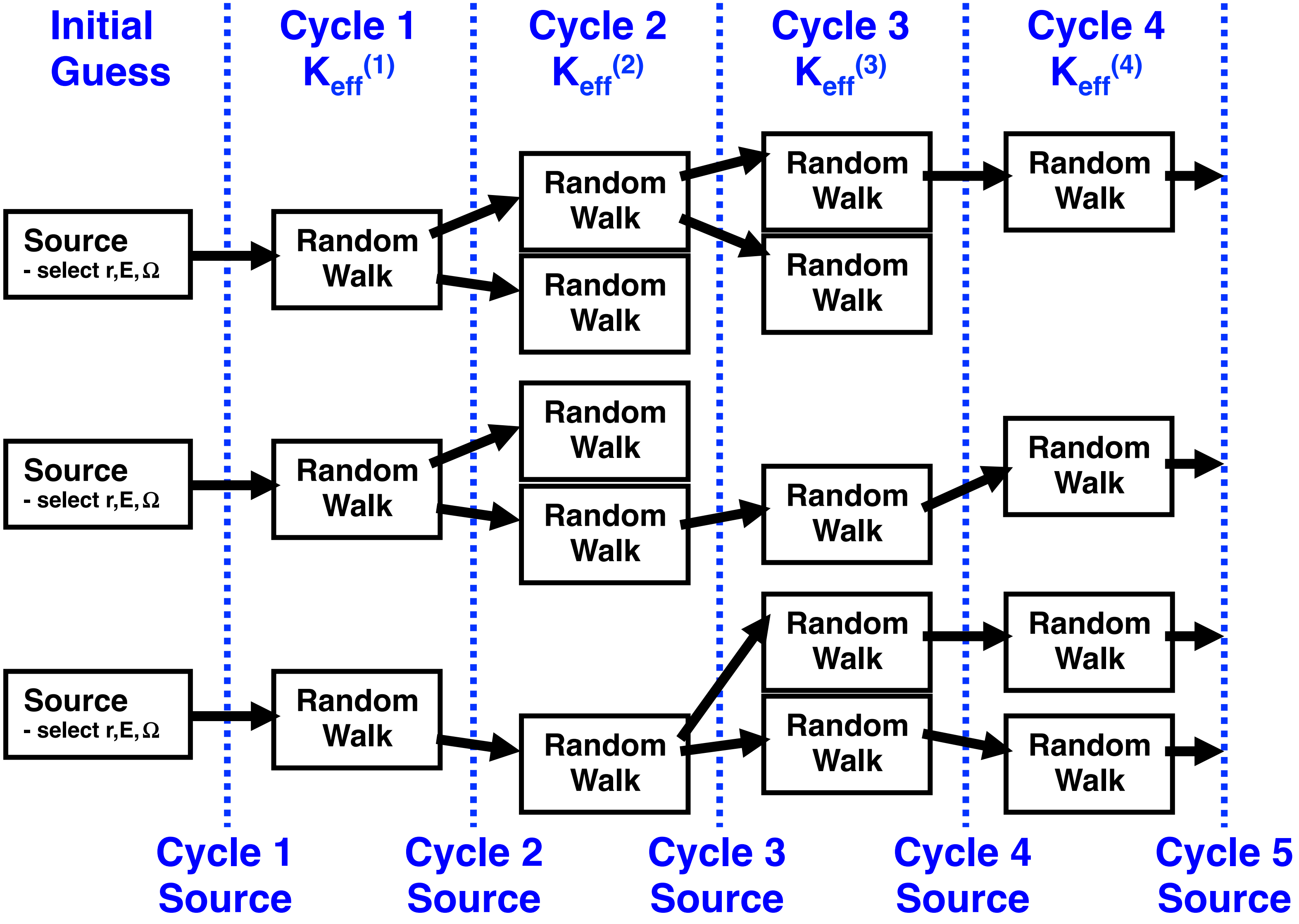
$$[\,L + T\,]\,\Psi_k = [S + 1/k\ M\,]\,\Psi_k$$

- The factor 1/k changes the relative level of the fission source, to balance the equation & permit a steady-state solution

- Criticality

Supercritical:	$K_{eff} > 1$
Critical:	$K_{eff} = 1$
Subcritical:	$K_{eff} < 1$

Monte Carlo Eigenvalue calculation



Iterate (cycle) until converged, then more to accumulate tallies

K_{eff} Eigenvalue Equation

- **A common misinterpretation: K_{eff} >1 means "power is rising"**
  - **Not true !**
  - **The factor 1/K_{eff} in the transport equation is the eigenvalue required to make the equation balance for a steady-state solution (stationary eigenfunction)**
  - **Reactor designers & analysts instead think of reactivity:**

$$\rho = \frac{k_{eff} - 1}{k_{eff}}$$

  - **Think of reactivity as a "potential" for power to rise or fall**
    - If it is not cancelled out by some control, then power would rise.
    - **In practice, positive reactivity is cancelled out by negative reactivity from control rods, soluble boron, fission product poisoning, temperature changes, etc.**
  - **The job of reactor designers is:**
    - Calculate the reactivity for a specific reactor configuration.
    - **If the reactivity is positive, some changes need to be made to introduce negative reactivity. Conversely for negative reactivity.**

Statistics Review

- Probability Density Function & Random Sampling
- Continuous PDF & CDF
- Discrete PDF & CDF
- Mean, Standard Deviation, Standard Deviation of the Mean

Introduction

Probability ?

What are the odds of …..

• Being audited by the IRS this year	100	to	1
• Losing your luggage on a U.S. flight	176	to	1
• Being dealt 4 aces on an opening poker hand	4,164	to	1
• Being struck by lightning in your lifetime	9,100	to	1
• Being hit by a baseball at a major league game	300,000	to	1
• Drowning in your bathtub this year	685,000	to	1
• Winning the Powerball jackpot with 1 ticket	292,201,338	to	1

Yet we all still keep buying Powerball tickets, but don’t worry too much about lightning…

Simple Random Sampling (1)

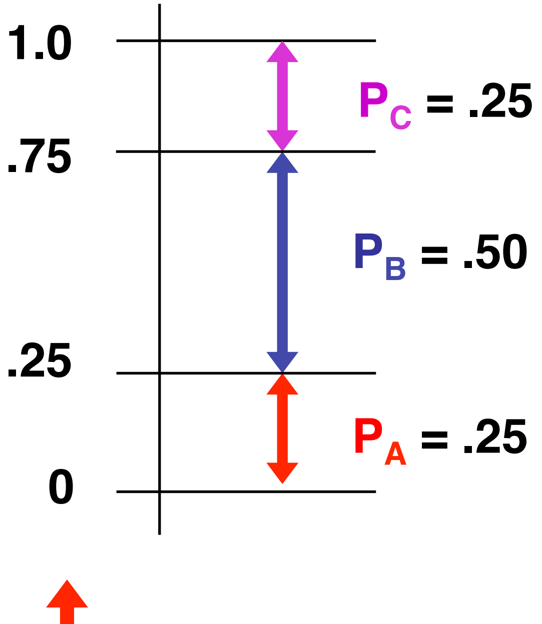
- Suppose we have 3 items, A, B, and C
  - P_A = probability of randomly picking item A = 25% = 0.25
  - P_B = probability of randomly picking item B = 50% = 0.50
  - P_C = probability of randomly picking item C = 25% = 0.25

  - $P_A + P_B + P_C = 1.0$

- Random sampling - pick A or B or C

Generate a random number $\mathcal{R}$
in the range (0,1)

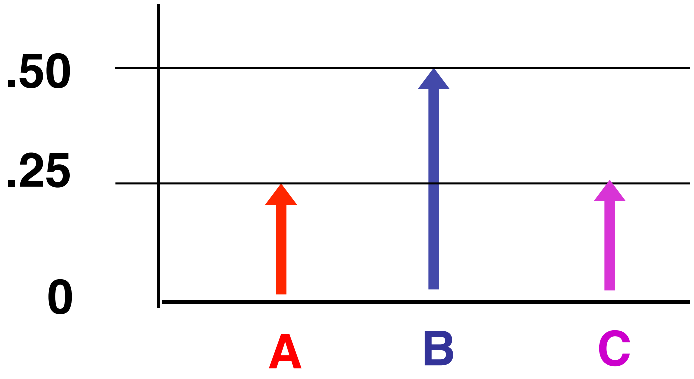
If $\mathcal{R} < .25$ ➜ select A
Else If $.25 < \mathcal{R} < .75$ ➜ select B
Otherwise ➜ select C



Cumulative Probabilities

Simple Random Sampling (2)

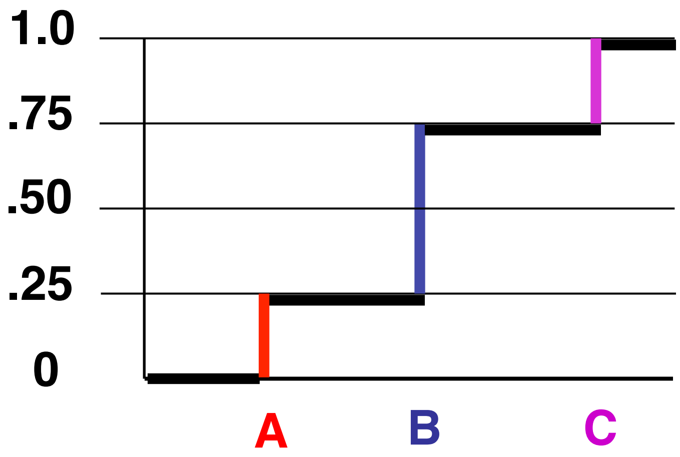
- Random sampling - pick A or B or C
  - P_A = probability of randomly picking item A = 25% = 0.25
  - P_B = probability of randomly picking item B = 50% = 0.50
  - P_C = probability of randomly picking item C = 25% = 0.25
  - $P_A + P_B + P_C = 1.0$



Discrete Probabilities

Generate a random number $\mathcal{R}$ in the range (0,1),

Pick A, B, or C



Cumulative Probabilities

Probability Density Functions

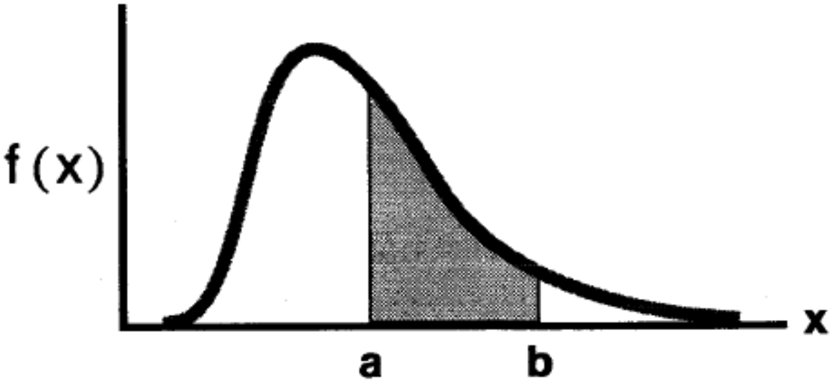
- **Continuous Probability Density**

$f(x)$ = probability density function (PDF)

$f(x) \geq 0$

$$\text{Probability}\{a \leq x \leq b\} = \int_a^b f(x)dx$$

$$\text{Normalization:} \quad \int_{-\infty}^{\infty} f(x)dx = 1$$



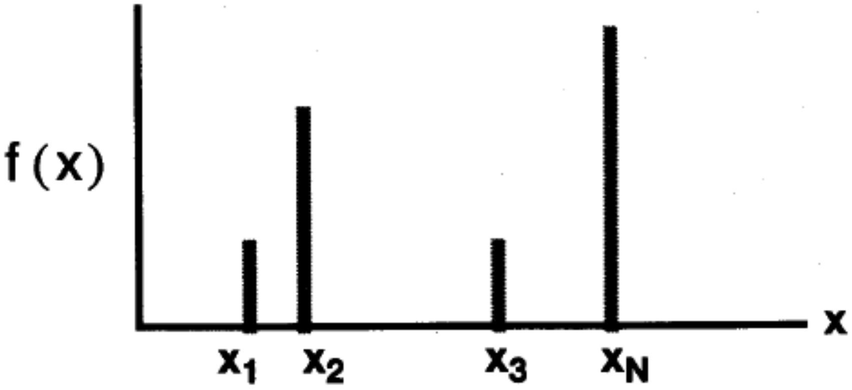
- **Discrete Probability Density**

$\{ f_k \},\ k = 1,\ldots,N, \quad \text{where } f_k = f(x_k)$

$f_k \geq 0$

$$\text{Probability}\{ x = x_k \} = f_k$$

$$\text{Normalization:} \quad \sum_{k=1}^{N} f_k = 1$$

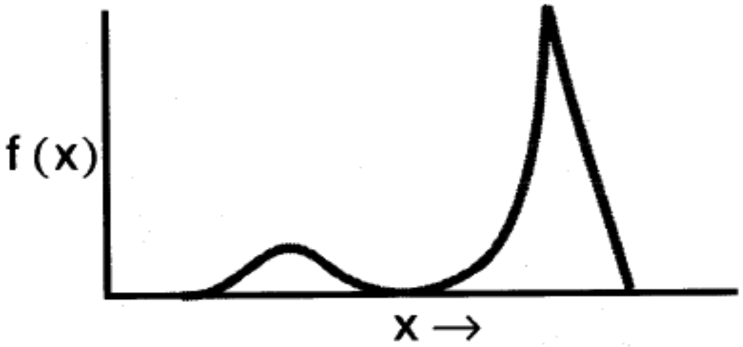


Random Sampling

The key to Monte Carlo methods is the notion of *random sampling*.

- **The problem can be stated this way:**

  Given a probability density, f(x), produce a sequence of $\hat{x}$'s.
  The $\hat{x}$'s should be distributed in the same manner as f(x).



- **Use of random sampling distinguishes Monte Carlo from other methods**

- **When Monte Carlo is used to solve the Boltzmann transport equation:**
  - **Random sampling models the outcome of physical events**
    (e.g., neutron collisions, fission process, sources, …..)
  - **Computational geometry models the arrangement of materials**

Continuous PDF & CDF

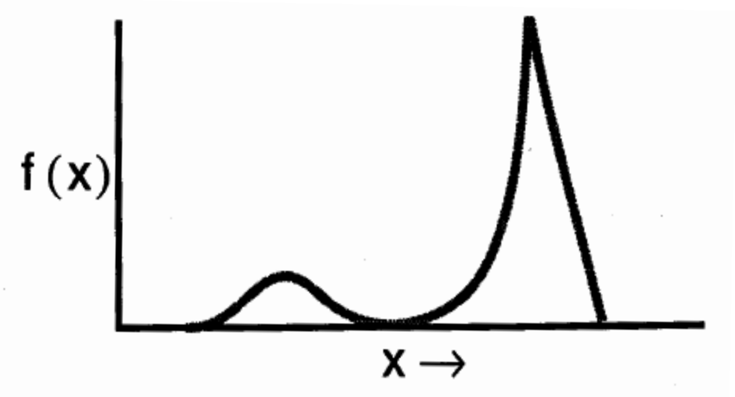
- **Probability Density Function (PDF)**

$f(x)$ = probability density function (PDF)

$f(x) \geq 0$

$$\text{Probability}\{a \leq x \leq b\} = \int_a^b f(x)dx$$

$$\text{Normalization:} \quad \int_{-\infty}^{\infty} f(x)dx = 1$$



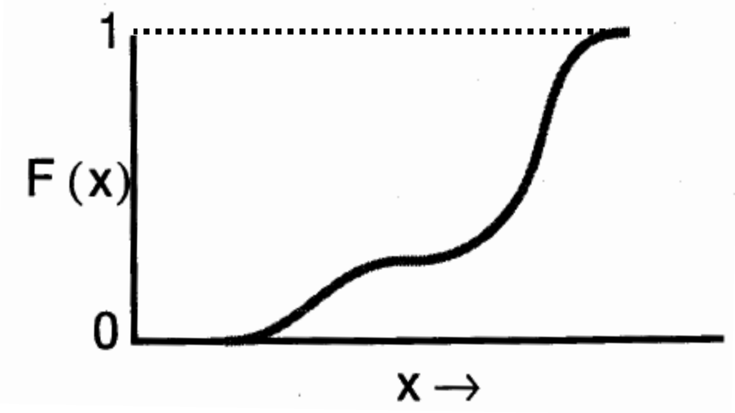
- **Cumulative Distribution Function (CDF)**

$$F(x) = \int_{-\infty}^{x} f(x')dx'$$

$$0 \leq F(x) \leq 1$$

$$\frac{dF(x)}{dx} \geq 0$$

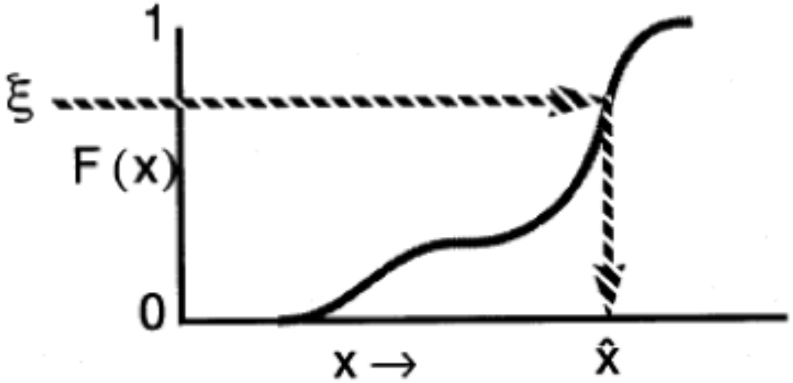
$$F(-\infty) = 0, \qquad F(\infty) = 1$$



Direct Sampling

- **Direct solution of** $\hat{x} = F^{-1}(\xi)$

  Solve for $\hat{x}$: $\xi = \int_{-\infty}^{\hat{x}} f(x)dx$



- **Sampling procedure**
  - **Generate ξ**
  - **Determine $\hat{x}$ such that $F(\hat{x}) = \xi$**
- **Advantages**
  - **Straightforward mathematics & coding**
  - **"High-level" approach**
- **Disadvantages**
  - **Often involves complicated functions**
  - **In some cases, F(x) cannot be inverted (e.g., Klein-Nishina)**

Rejection Sampling

- **Von Neumann:**

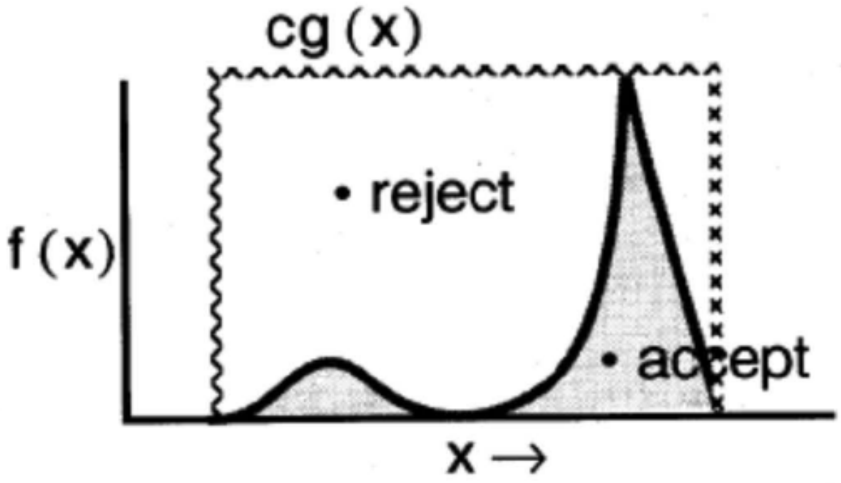
  " .... *it seems objectionable to compute* a *transcendental function of* a *random number.* "

- **Select a bounding function, g(x), such that**
  - $c \cdot g(x) > f(x)$ for all x
  - g(x) is an easy-to-sample PDF

- **Sampling Procedure:**
  - sample x' from g(x): $x' \leftarrow G^{-1}(\xi_1)$
  - test: $\xi_2 \cdot c\, g(x') < f(x')$

    if ***true***, accept x', done

    if ***false***, reject x', try again



- **Advantages**
  - Simple computer operations
- **Disadvantages**
  - "Low-level" approach, sometimes hard to understand

Mean & Standard Deviation

- Given a set of random samples, $x_1, x_2, \ldots, x_{N,}$
  - Mean $$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j$$
  - Population variance & standard deviation $$\sigma^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \left(\frac{1}{N}\sum_{j=1}^{N} x_j\right)^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2 \qquad \sigma = \sqrt{\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2}$$
  - Variance & standard deviation <u>of the mean</u> $$\sigma_{\bar{x}}^2 = \frac{\sigma^2}{N} \qquad \sigma_{\bar{X}} = \frac{1}{\sqrt{N}} \cdot \sqrt{\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2}$$

Monte Carlo codes calculate <u>mean</u> values for tallies, & report the <u>standard deviation of the mean</u>

In the definitions above, some of the “N” terms should really be “N-1”. MCNP & many other codes ignore that, since N is very large.

Random Numbers & Random Sampling

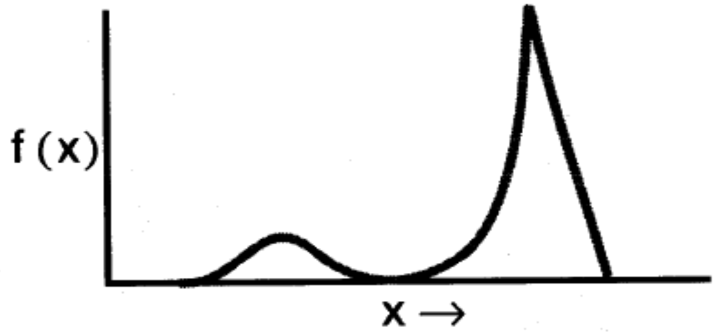
Introduction

The key to Monte Carlo methods is the notion of *random sampling*.

- **The problem can be stated this way:**

  Given a probability density, f(x), produce a sequence of $\hat{X}$'s.

  The $\hat{X}$'s should be distributed in the same manner as f(x).



- **Random sampling distinguishes Monte Carlo from other methods**
- **When Monte Carlo is used to solve the Boltzmann transport equation:**
  - **Random sampling models the outcome of physical events (e.g., neutron collisions, fission process, sources, …..)**
  - **Computational geometry models the arrangement of materials**

Monte Carlo & Random Sampling

Categories of random sampling

- **Random number generator** - uniform PDF on (0,1)
- Sampling from **analytic PDFs** - normal, exponential, Maxwellian, …
- Sampling from **tabulated PDFs** - angular PDFs, spectrum, …

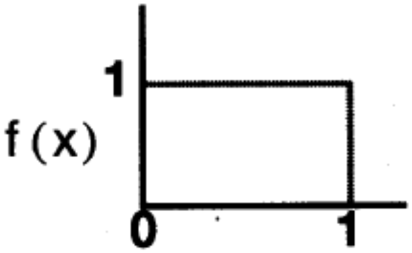
For Monte Carlo codes…

- **Random numbers, ξ, are produced by the RN generator on (0,1)**
- Non-uniform random variates are produced from the ξ' s by:
  - **Direct inversion**
  - **Rejection methods**
  - **Transformations**
  - **Composition (mixtures)**
  - **Sums, products, ratios, …**
  - **Table lookup + interpolation**
  - **Lots (!) of other tricks**
- **Typically < 5 - 10% of total CPU time**

Random Number Generators

"Randomness is a negative property; it is the absence of any pattern."
Richard W. Hamming, 1991

- Numbers are not random; a sequence of numbers can be.
- Truly random sequences are generally not desired on a computer.
- RNG
  - Function which generates a sequence of numbers which appear to have been randomly sampled from a uniform distribution on (0,1)
  - Repeatable (deterministic)
  - Pass statistical tests for randomness
  - Typical usage in codes: r = rang()
  - Also called "pseudo-random number generators"



- All other random sampling is performed using this basic RNG
- Note that the probability of something occurring also varies between 0 & 1 …..

Random Number Generators

Most production-level Monte Carlo codes for particle transport use linear congruential random number generators:

$$S_{i+1} = S_i \bullet g + c \quad \mathrm{mod}\ 2^m$$

S_i = seed, g = multiplier, c = adder, 2^m = modulus

- **Simple, fast, robust, over 50 years of heavy-duty use**
- **Theory is well-understood** (e.g., DE Knuth, Vol. 2, 177 pages)
- **Not the "best" generators, but good enough - RN's are used in unpredictable ways during particle simulation**
- **To achieve reproducibility for vector or parallel calculation, there must be a fast, direct method for skipping ahead (or back) in the random sequence**

Simple RNG - Example #1

S_{k+1} = [g·S_k + C] mod p,   with g=47, C=1, S_0=1, P=100

```
s( 0) = 1
s( 1) = (47x1  + 1) mod 100 =   48 mod 100 = 48
s( 2) = (47x48 + 1) mod 100 = 2257 mod 100 = 57
s( 3) = (47x57 + 1) mod 100 = 2680 mod 100 = 80
s( 4) = (47x80 + 1) mod 100 = 3761 mod 100 = 61
s( 5) = (47x61 + 1) mod 100 = 2868 mod 100 = 68
s( 6) = (47x68 + 1) mod 100 = 3197 mod 100 = 97
s( 7) = (47x97 + 1) mod 100 = 4560 mod 100 = 60
s( 8) = (47x60 + 1) mod 100 = 2821 mod 100 = 21
s( 9) = (47x21 + 1) mod 100 =  988 mod 100 = 88
s(10) = (47x88 + 1) mod 100 = 4137 mod 100 = 37
s(11) = (47x37 + 1) mod 100 = 1740 mod 100 = 40
s(12) = (47x40 + 1) mod 100 = 1881 mod 100 = 81
s(13) = (47x81 + 1) mod 100 = 3808 mod 100 =  8
s(14) = (47x8  + 1) mod 100 =  377 mod 100 = 77
s(15) = (47x77 + 1) mod 100 = 3620 mod 100 = 20
s(16) = (47x20 + 1) mod 100 =  941 mod 100 = 41
s(17) = (47x41 + 1) mod 100 = 1928 mod 100 = 28
s(18) = (47x28 + 1) mod 100 = 1317 mod 100 = 17
s(19) = (47x17 + 1) mod 100 =  800 mod 100 =  0
s(20) = (47x0  + 1) mod 100 =    1 mod 100 =  1
s(21) = (47x1  + 1) mod 100 =   48 mod 100 = 48
s(22) = (47x48 + 1) mod 100 = 2257 mod 100 = 57
```

Simple RNG - Examples #2 & #3

Example #2: $S_{k+1} = [\ g \cdot S_k + C\ ]\ \mathrm{mod}\ p,$

with $g=5$, $c=1$, $S_0=1$, $p=100$

```
s( 0) = 1
s( 1) = (5x1  + 1) mod 100 =   6 mod 100 =  6
s( 2) = (5x6  + 1) mod 100 =  31 mod 100 = 31
s( 3) = (5x31 + 1) mod 100 = 156 mod 100 = 56
s( 4) = (5x56 + 1) mod 100 = 281 mod 100 = 81
s( 5) = (5x81 + 1) mod 100 = 406 mod 100 =  6
s( 6) = (5x6  + 1) mod 100 =  31 mod 100 = 31
etc.
```

Example #3: $S_{k+1} = [\ g \cdot S_k + C\ ]\ \mathrm{mod}\ p,$

with $g=5$, $c=0$, $S_0=1$, $p=100$

```
s( 0) = 1
s( 1) = (5x1 ) mod 100 =   5 mod 100 =  5
s( 2) = (5x5 ) mod 100 =  25 mod 100 = 25
s( 3} = (5x25) mod 100 = 125 mod 100 = 25
s( 4) = (5x25) mod 100 = 125 mod 100 = 25
etc.
```

Typical Linear Congruential RNGs

- Multiplicative congruential method - Lehmer

$S_k = g \cdot S_{k-1} + c \mod 2^m,$ $0 < S_k < 2^m,$ integer

$\xi_k = S_k / 2^m,$ $0 \le \xi_k < 1,$ real

- Typical parameters

	2^m	Period	g	c
RACER (KAPL)	2^{47}	2^{45}	84,000,335,758,957	0
RCP (BAPL)	2^{48}	2^{48}	2^9+1	59,482,192,516,946
MORSE (ORNL)	2^{47}	2^{45}	5^{15}	0
VIM (ANL)	2^{48}	2^{46}	5^{19}	0
RANF (CRAY)	2^{48}	2^{46}	44,485,709,377,909	0
G. Marsaglia	2^{32}	2^{32}	69069	1
MCNP6 (default)	2^{48}	2^{46}	5^{19}	0
MCNP6 (opt)	2^{63}	2^{63}	(6 options)	1 or 0

MCNP5 & MCNP6 RNG

- MCNP5 & MCNP6 Linear congruential generator (LCG)

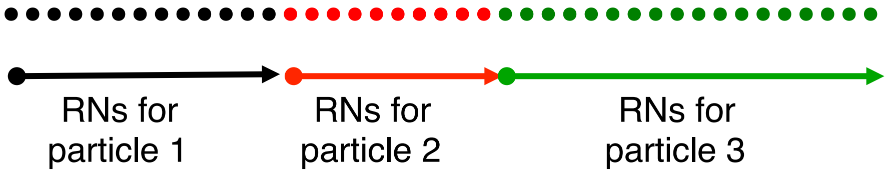
  $$S_{n+1} = g\, S_n + c \mod 2^m$$

  - See Knuth for rules for selecting g,c,m so that period is maximized & correlation minimized
  - 7 different LCGs are available -- chosen based on the spectral test, Knuth's tests, & Marsaglia's DIEHARD tests
  - LCG(g, c, 2^m):
    - **Traditional MCNP,** **period = $2^{46} \approx 7\text{x}10^{14}$**
      - LCG(5^{19}, 0, 2^{48})
    - **L'Ecuyer 63-bit Mixed LCGs,** **period = $2^{63} \approx 9\text{x}10^{18}$**
      - LCG(9219741426499971445, 1, 2^{63})
      - LCG(2806196910506780709, 1, 2^{63})
      - LCG(3249286849523012805, 1, 2^{63})
    - **L'Ecuyer 63-bit Multiplicative LCGs,** **period = $2^{61} \approx 2\text{x}10^{18}$**
      - LCG(3512401965023503517, 0, 2^{63})
      - LCG(2444805353187672469, 0, 2^{63})
      - LCG(1987591058829310733, 0, 2^{63})

[L’Ecuyer, **Math. Comp.**, 68, **249-260 (1999)]**

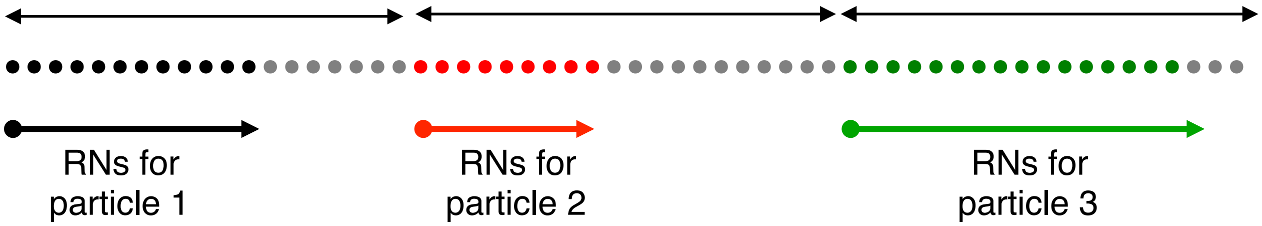
Using RNGs in Particle Transport MC Codes

- Naïve use, in many older codes & student codes



  – Problem: Can't start Particle-2 until Particle-1 is finished, etc.
  Can't do parallel processing of different particles

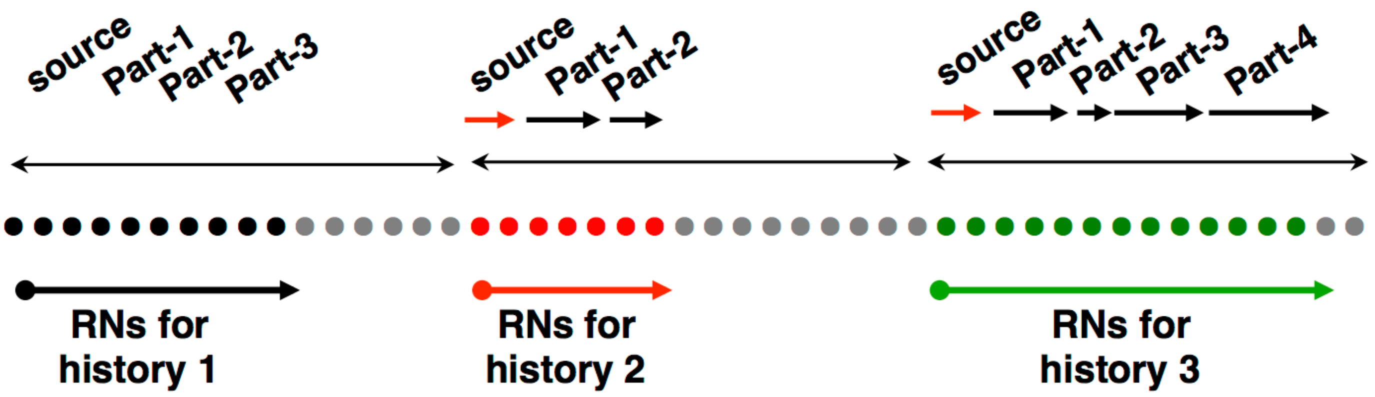
- MCNP, VIM, RACER, MC21, & many other production codes
  – Partition RN sequence into equal-length subsequences, one for each particle



  – Can process all particles in parallel
  – Length of each subsequence is called the stride
  – Must have a fast way to skip-ahead in the RN sequence

Using RNGs in Particle Transport MC Codes

- **Histories vs particles**
  - With splitting &/or secondary particle creation, the number of particles in a given history is not known in advance
  - Need to partition RN sequence by history, not by particle



  - With this scheme, can process histories in parallel, but not particles in same history
  - Must have a predictable scheme for banking/unbanking particles in a given history (e.g., LIFO)

Random Sampling

"Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin."

John Von Neuman, 1951

Introduction

Probability ?

What are the odds of …..

• Being audited by the IRS this year	100	to	1
• Losing your luggage on a U.S. flight	176	to	1
• Being dealt 4 aces on an opening poker hand	4,164	to	1
• Being struck by lightning in your lifetime	9,100	to	1
• Being hit by a baseball at a major league game	300,000	to	1
• Drowning in your bathtub this year	685,000	to	1
• Winning the Powerball jackpot with 1 ticket	292,201,338	to	1

Yet we all still keep buying Powerball tickets, but don’t worry too much about lightning…

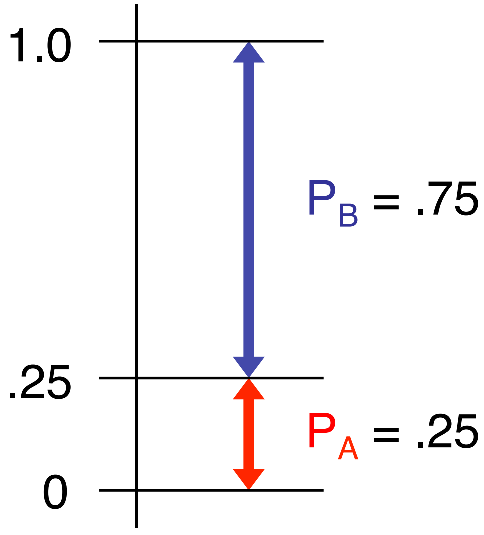
Simple Random Sampling (1)

- **Suppose we have 2 items, A and B**
  - **P_A = probability of randomly picking item A = 25% = 0.25**
  - **P_B = probability of randomly picking item B = 75% = 0.75**
  - **$P_A + P_B = 1.0$**

- **Random sampling - pick A or B**

Generate a random number $\mathcal{R}$ in the range (0,1)

If $\mathcal{R} < .25$ ➜ select A
Otherwise ➜ select B



Cumulative Probabilities

Simple Random Sampling (2)

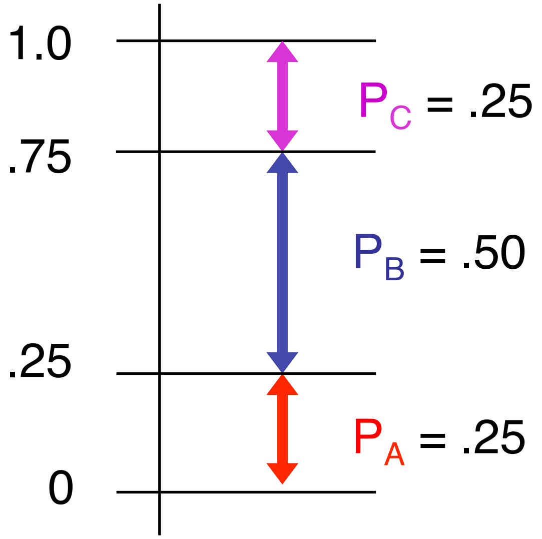
- Suppose we have 3 items, A, B, and C
  - P_A = probability of randomly picking item A = 25% = 0.25
  - P_B = probability of randomly picking item B = 50% = 0.50
  - P_C = probability of randomly picking item C = 25% = 0.25

  - $P_A + P_B + P_C = 1.0$

- Random sampling - pick A or B or C

Generate a random number $\mathcal{R}$ in the range (0,1)

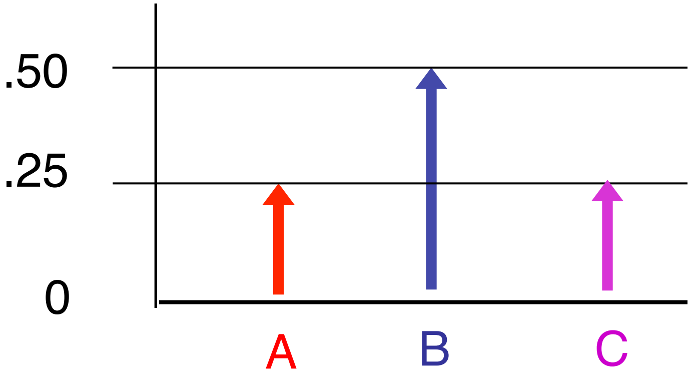
If	$\mathcal{R} < .25$	- select A
Else If	$.25 < \mathcal{R} < .75$	- select B
Otherwise		- select C



Cumulative Probabilities

Simple Random Sampling (3)

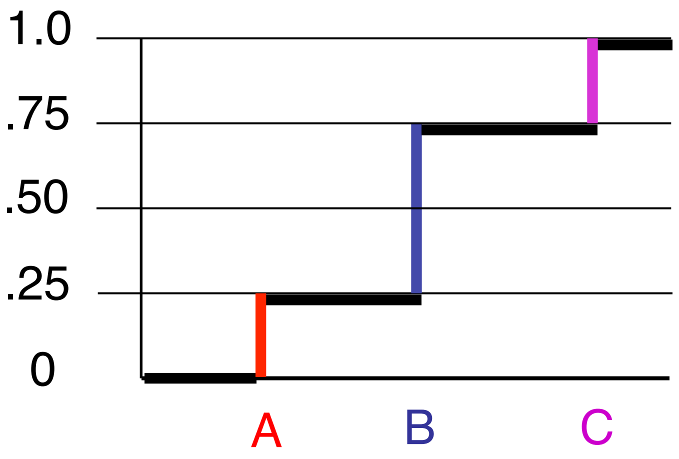
- **Random sampling - pick A or B or C**
  - **P_A = probability of randomly picking item A = 25% = 0.25**
  - **P_B = probability of randomly picking item B = 50% = 0.50**
  - **P_C = probability of randomly picking item C = 25% = 0.25**
  - **$P_A + P_B + P_C = 1.0$**



Discrete Probabilities

Generate a random number $\mathcal{R}$ in the range (0,1),

Pick A, B, or C



Cumulative Probabilities

Probability Density Functions

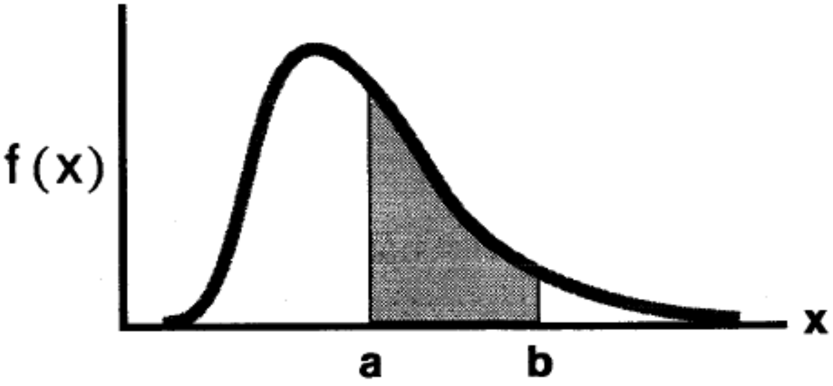
- **Continuous Probability Density**

f(x) = probability density function (PDF)

$f(x) \geq 0$

$$\text{Probability}\{a \leq x \leq b\} = \int_a^b f(x)dx$$

$$\text{Normalization:} \quad \int_{-\infty}^{\infty} f(x)dx = 1$$



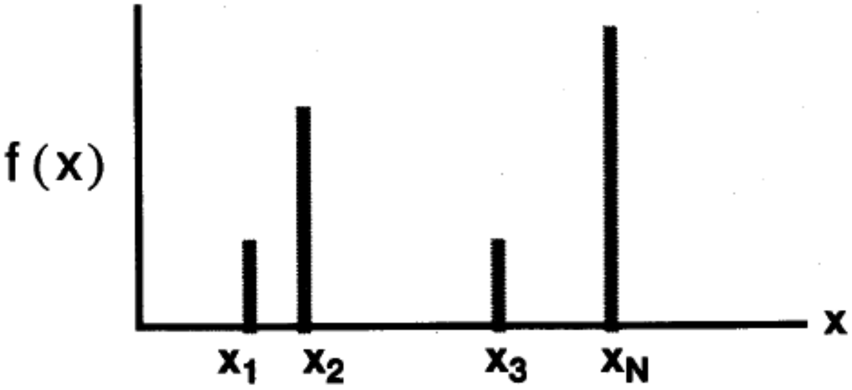
- **Discrete Probability Density**

$$\{ f_k \}, \ k = 1,\ldots,N, \quad \text{where } f_k = f(x_k)$$

$f_k \geq 0$

$$\text{Probability}\{ x = x_k \} = f_k$$

$$\text{Normalization:} \quad \sum_{k=1}^{N} f_k = 1$$



Continuous PDF & CDF

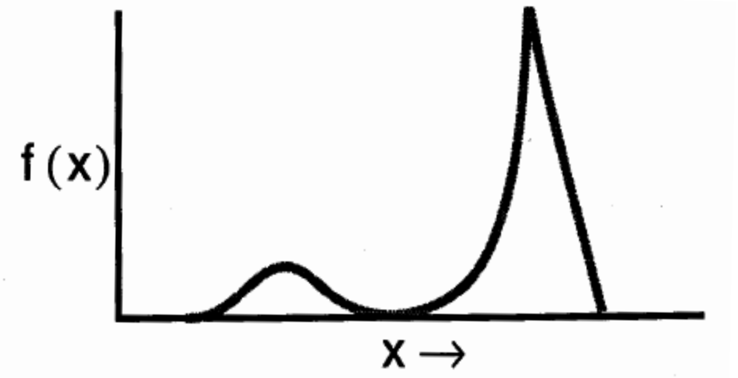
- **Probability Density Function (PDF)**

$f(x)$ = probability density function (PDF)

$f(x) \geq 0$

$$\text{Probability}\{a \leq x \leq b\} = \int_a^b f(x)dx$$

$$\text{Normalization:} \quad \int_{-\infty}^{\infty} f(x)dx = 1$$



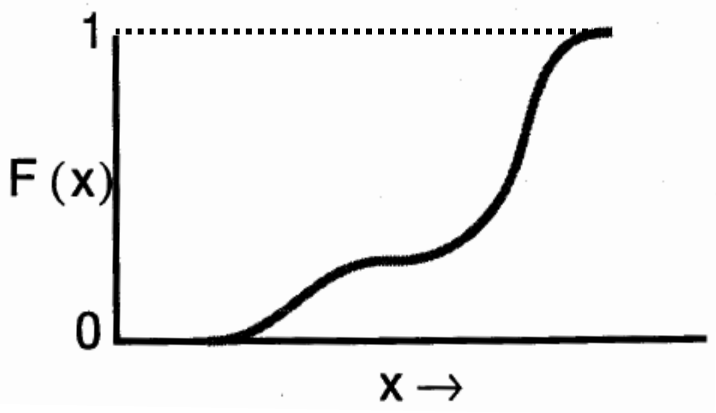
- **Cumulative Distribution Function (CDF)**

$$F(x) = \int_{-\infty}^{x} f(x')dx'$$

$0 \leq F(x) \leq 1$

$$\frac{dF(x)}{dx} \geq 0$$

$F(-\infty) = 0, \quad F(\infty) = 1$



Note: convention is to use f(x) for PDF, F(x) for CDF

Discrete PDF & CDF

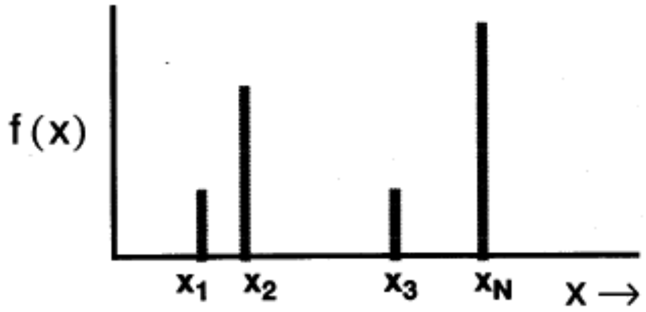
Discrete PDF's

- **Probability Density Function (PDF)**

$\{ f_k \}$, where $f_k = f(x_k)$, $k=1,\ldots,N$

$$f_k \geq 0$$

$$\sum_{j=1}^{N} f_j = 1$$



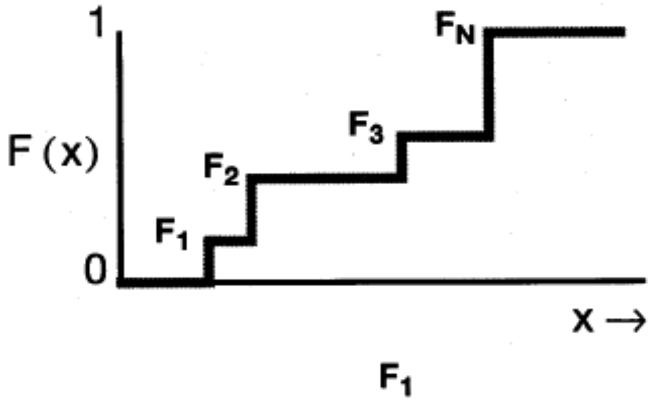
- **Cumulative Distribution Function (CDF)**

$\{ F_k \}$, where $F_k = \sum_{j=1} f_j$, $k=1, \ldots, N\text{-}1$

and

$$F_0 = 0,$$

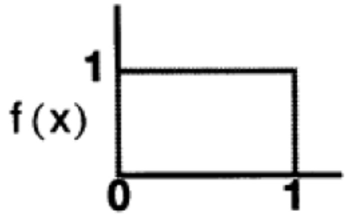
$$F_N = 1$$

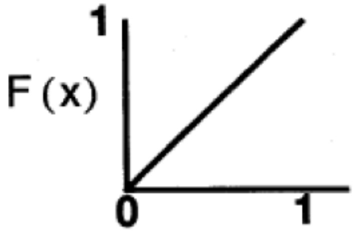


Note: convention is to use f_J for PDF, F_J for CDF

Fundamental RNG

- **Random Number Generator**
  - **Not strictly "random", but good enough**
    - Pass statistical tests for randomness
    - Reproducible sequence
  - **Uniform PDF on (0,1)**
  - **Must be easy to compute**





- **Linear Congruential Method**
  - **Algorithm**

$$
\begin{aligned}
S_0 &= \text{ initial seed, odd integer, } < M \\
S_k &= G \cdot S_{k-1} + c \quad \text{mod } M, \quad k = 1,2, \ldots.. \\
\xi_k &= S_k / M
\end{aligned}
$$

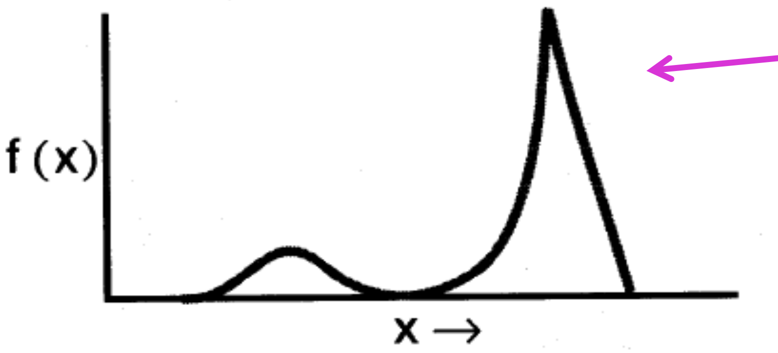
- **Usage**
  - **In algorithms, usually denote RN uniform on (0,1) by ξ ("xye")**
  - **In codes, invoke basic RN generator by: r = rang()**
  - **Each new usage of ξ or rang() generates a new RN**

Random Sampling

The key to Monte Carlo methods is the notion of *random sampling*.

- **The problem can be stated this way:**

  Given a probability density, f(x), produce a sequence of $\hat{x}$'s.
  The $\hat{x}$'s should be distributed in the same manner as f(x).



Given f(x),
Randomly choose x

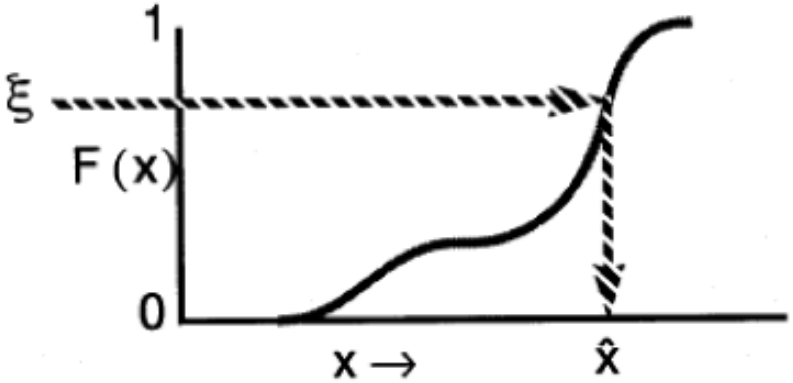
- **The use of random sampling distinguishes Monte Carlo from other methods**

- **When Monte Carlo is used to solve the integral Boltzmann transport equation:**
  - **Random sampling models the outcome of physical events (e.g., neutron collisions, fission process, sources, …..)**
  - **Computational geometry models the arrangement of materials**

★★★★★ Direct Sampling ★★★★★

- Direct solution of $x = F^{-1}(\xi)$

Solve for x: $$\xi = \int_{-\infty}^{x} f(y)\,dy$$



- **Sampling procedure**
  - Generate ξ
  - Determine x such that F(x) = ξ

- **Advantages**
  - Straightforward mathematics & coding
  - "High-level" approach

- **Disadvantages**
  - Often involves complicated functions
  - In some cases, F(x) cannot be inverted (e.g., Klein-Nishina)

Discrete PDFs

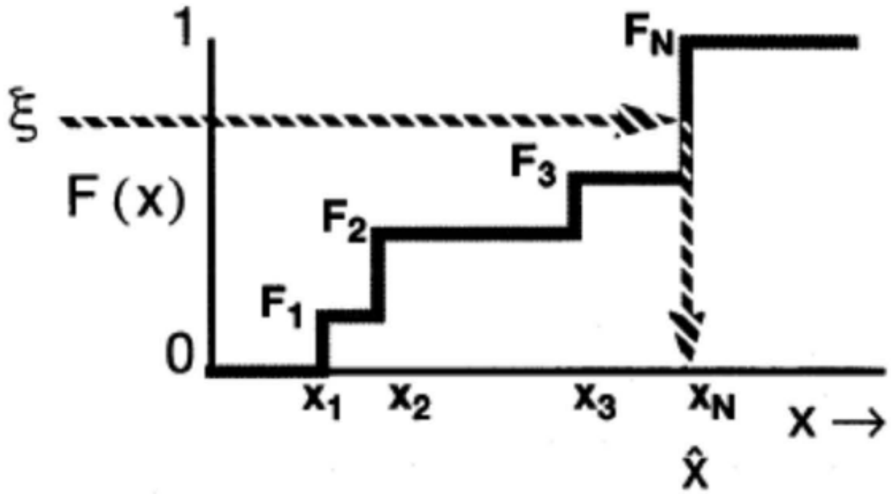
- **Sampling from Discrete PDF's - Conventional Procedure**

Direct Solution of $\mathbf{x'} \leftarrow \mathbf{F^{-1}(\xi)}$

(1) Generate $\boldsymbol{\xi}$

(2) Determine k such that $F_{k-1} \le \xi < F$

(3) Return $\mathbf{x'} = x_k$



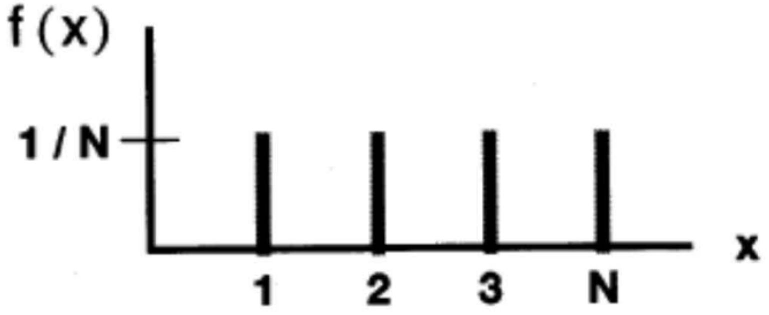
- **Step (2) requires a <u>table search</u>**
  - **Linear table searches require *O(N)* time - use when N small**
  - **Binary table searches require *O(lnN)* time - use when N large**

- **For some discrete PDFs, F_k' s are <u>not</u> precomputed.**
  - **Use linear search, with F_k's computed on-the-fly as needed**

Discrete Uniform PDF

- **Example - Sampling from Discrete Uniform PDF**

- **Discrete Uniform PDF**
  - $f_k = 1 / N, \quad k = 1, \ldots, N$
  - $F_k = k / N, \quad F_0=0, \quad F_N= 1$

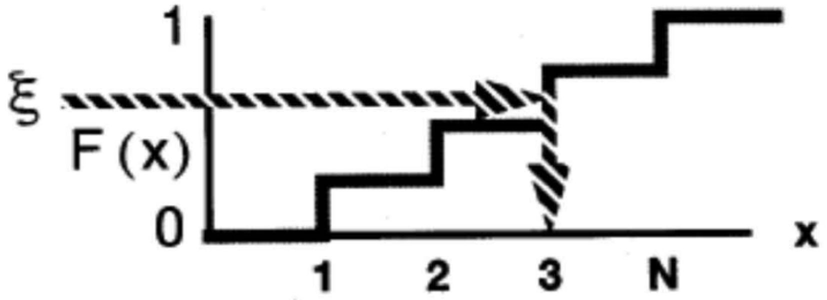


- **Sampling procedure:**
  - Could use table search method, ...
  - Easier, for this special case:

    $k \leftarrow 1 + \lfloor N \xi \rfloor$,

    where $\lfloor y \rfloor$ is the "floor" function,
    largest integer < y

  - Fortran: `k = 1 +    int( N*rang() )`
    C: `k = 1 + floor( N*rang() )`
  - Note: must be sure that $1 \leq k \leq N$



Discrete PDFs - Examples

- Example – Pick 1 Powerball number, uniform integer in [1,60]

k = int(1 + 60*rang())

- Example - loaded die, faces show 2,2,3,4,5,5 – simulate 1 roll

```
pdf(1:6) =  [ 0./6., 2./6., 1./6., 1./6., 2./6., 0./6. ]
cdf(1:6) =  [ 0./6., 2./6., 3./6., 4./6., 6./6., 6./6. ]

r = rang()
do j = 1, 6
  if(  r < cdf(j)  ) then
    k = j
    exit
  endif
enddo
{result is k}
```

This coding is a simple linear search to determine an integer k in the range [1,6]

Search for the first occurrence of $\xi \le \text{cdf}(j)$

Random Sampling -- Discrete PDFs

- **Multigroup Scattering**

  – **Scatter from group g to group g', where 1 ≤ g' ≤ G**

$$f_{g'} = \frac{\sigma_{g \to g'}}{\sum_{k=1}^{G} \sigma_{g \to k}}$$

- **Selection of scattering nuclide for a collision**

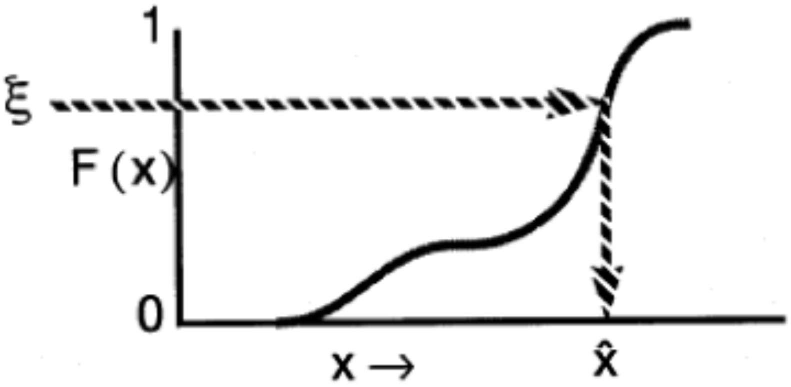
  – **K = number of nuclides in composition**

$$f_k = \frac{N^{(k)} \sigma_s^{(k)}}{\sum_{j=1}^{K} N^{(j)} \sigma_s^{(j)}}$$

★★★★★ Direct Sampling ★★★★★

- Direct solution of $x = F^{-1}(\xi)$

Solve for x: $$\xi = \int_{-\infty}^{x} f(y)\,dy$$



- **Sampling procedure**
  - Generate ξ
  - Determine x such that F(x) = ξ

- **Advantages**
  - Straightforward mathematics & coding
  - "High-level" approach

- **Disadvantages**
  - Often involves complicated functions
  - In some cases, F(x) cannot be inverted (e.g., Klein-Nishina)

Continuous PDFs - Exponential

Examples - Sampling from an Exponential PDF

PDF: $$f(x) = \Sigma \cdot e^{-\Sigma x}, \qquad x > 0$$

CDF: $$F(x) = \int_0^x f(y)\,dy = \int_0^x \Sigma \cdot e^{-\Sigma y}\,dy = -e^{-\Sigma y}\Big|_0^x = 1 - e^{-\Sigma x}$$

Direct sampling:

Solve for x: F(x) = ξ

Solving $\xi = 1 - e^{-\Sigma x}$ gives: $x \leftarrow \; -\ln(1-\xi)/\Sigma$

or

$$x \leftarrow \; -\ln\xi/\Sigma$$

Although (1- ξ) ≠ ξ,
both ξ and (1- ξ) are uniformly distributed on (0,1),
so that we can use either in the random sampling procedure.

i.e., the numbers are different, but the <u>distributions are the same</u>

Continuous PDFs – Power Law on [0,1]

Example - Sampling from power law PDF in range [0,1],

$$\textit{Note}: \quad (n+1) \text{ is necessary, so that} \int_0^\infty f(x')dx' = 1$$

PDF: $f(x) = (n+1)\, x^n, \quad n>0, \quad 0 \le x \le 1$

$= 0 \qquad x < 0, \text{ or } \quad x > 1$

CDF:

$$F(x) = \int_0^x f(y)dy = \int_0^x (n+1)\cdot y^n\, dy = (n+1)\cdot \left.\frac{y^{n+1}}{n+1}\right|_0^x = x^{n+1}, \qquad 0 \le x \le 1$$

Sampling scheme: $F(x) = \xi$, solve for x

$x^{n+1} = \xi$

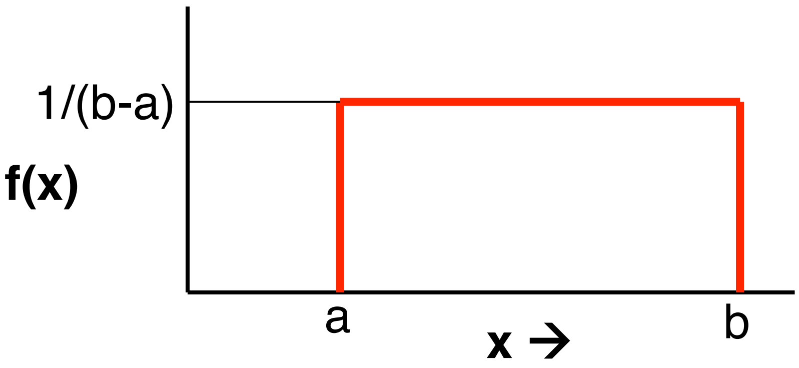
$x \leftarrow \xi^{1/(n+1)}$

For power laws on [0,1]:

n=1:	$f(x) = 2x$,	$F(x) = x^2$,	$x \leftarrow \sqrt{\xi}$
n=2:	$f(x) = 3x^2$,	$F(x) = x^3$,	$x \leftarrow \sqrt[3]{\xi}$
n=3:	$f(x) = 4x^3$,	$F(x) = x^4$,	$x \leftarrow \sqrt[4]{\xi}$

Continuous PDFs - Uniform

Example - Sampling from uniform PDF in range (a,b), Histogram with 1 bin



PDF: $f(x) = 1/(b-a), \quad a \le x \le b$

$= 0 \quad x<a, \text{ or } x>b$

CDF: $F(x) = (x-a)/(b-a), \quad a \le x \le b$

Sampling scheme: $F(x) = \xi$, solve for x

$(x-a)/(b-a) = \xi$

$$x \leftarrow a + (b-a)\,\xi$$

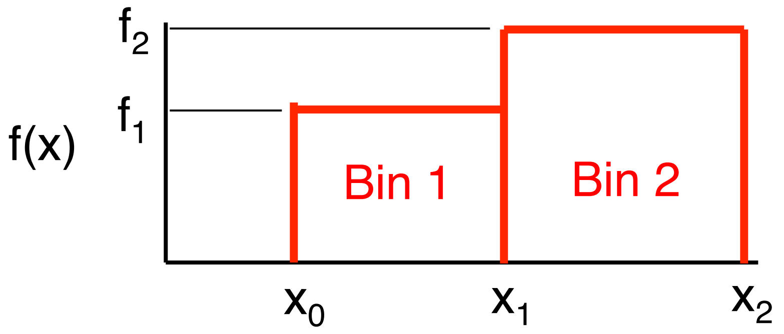
Note: Often implemented as:

$$f = \xi$$

$$x \leftarrow (1-f)\,a + f\,b$$

Continuous PDFs - Histogram

Example - Sampling from histogram with 2 bins



$A_1 = (x_1 - x_0) \cdot f_1$

$A_2 = (x_2 - x_1) \cdot f_2$

$p_1 = \text{Prob}\{\ x_0 < x < x_1\ \} = A_1 / (A_1 + A_2)$

$p_2 = \text{Prob}\{\ x_1 < x < x_2\ \} = A_2 / (A_1 + A_2)$

$p_1 + p_2 = 1$

Two-step sampling procedure:

1. **Select a bin, b:**

   If $\xi_1 <$ p_1, select b = bin 1

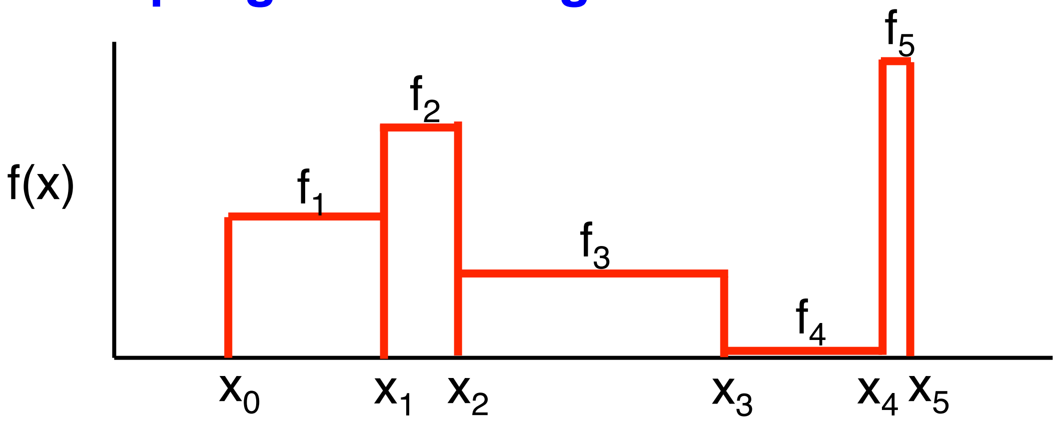
   otherwise, select b = bin 2

2. **Sample x uniformly within bin:**

   $$x \leftarrow x_{b-1} + \xi_2 \cdot (x_b - x_{b-1})$$

Continuous PDFs - Histogram

Example - Sampling from Histogram PDF

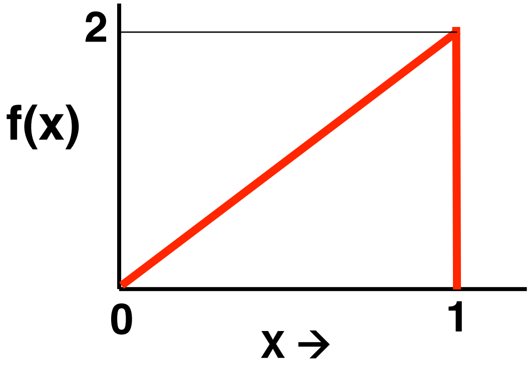


Two-step sampling: **(1) Sample from discrete PDF to select a bin**
(2) Sample from uniform PDF within bin

- **Discrete PDF:** $p_k = f_k \cdot (x_k - x_{k-1})$, $k = 1, \ldots, N$, $\Sigma p_k = 1$
  - **Generate ξ_1**
  - **Use table search to select k**
- **Uniform sampling within bin k**
  - **Generate ξ_2**
  - **Then,** $x \leftarrow x_{k-1} + (x_k - x_{k-1}) \cdot \xi_2$

Continuous PDFs – Linear (1)

Example - Sampling from an increasing linear PDF in range [0,1]



PDF: $f(x) = 2\,x, \quad 0 \le x \le 1$

CDF: $F(x) = x^2, \quad 0 \le x \le 1$

Sampling scheme: $F(x) = \xi,$ solve for x

$x^2 = \xi$

$x \leftarrow \mathrm{sqrt}(\xi)$

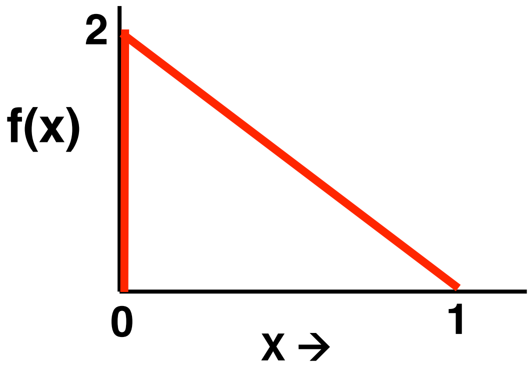
While not obvious, 2 alternative schemes for sampling x are:

$x \leftarrow \max(\xi_1, \xi_2)$

$x \leftarrow 1 - \mathrm{abs}(\xi_1 - \xi_2)$

Continuous PDFs – Linear (2)

Example - Sampling from a decreasing linear PDF in range [0,1]



PDF: $f(x) = 2 - 2x, \qquad 0 \le x \le 1$

CDF: $F(x) = 2x - x^2, \qquad 0 \le x \le 1$

Sampling scheme: $F(x) = \xi$, solve for x

$2x-x^2 = \xi$

$x^2 - 2x + 1 = 1 - \xi$

$(x-1)^2 = 1 - \xi$

$x - 1 = \pm \text{sqrt}(1-\xi)$

Choose the minus sign for correct range in x:

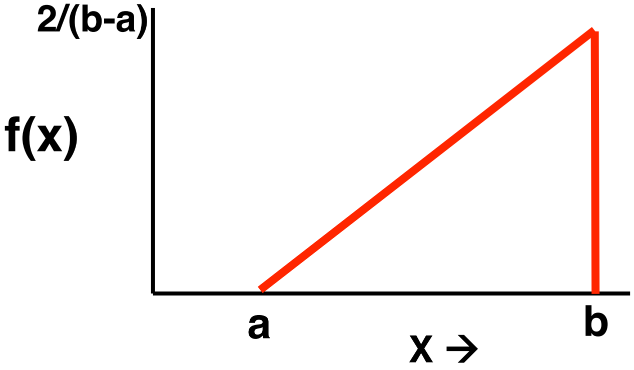
$$x \leftarrow 1 - \text{sqrt}(1-\xi)$$

Or, since ξ and 1-ξ have the same distribution:

$$x \leftarrow 1 - \text{sqrt}(\xi)$$

Continuous PDFs – Linear (3)

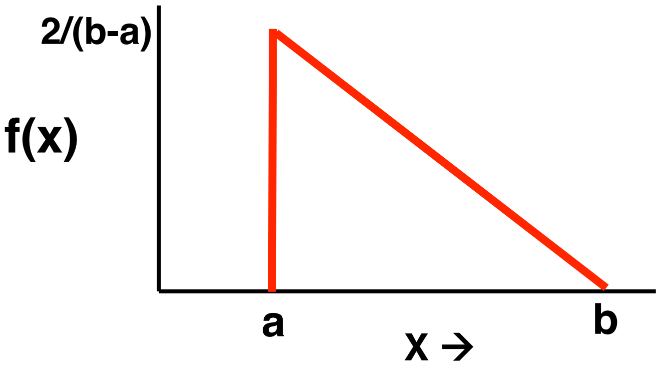
Increasing linear PDF



Random sampling can be done with a simple shifting & scaling of the unit PDF:

$$x \leftarrow a + (b\text{-}a)\,\mathrm{sqrt}(\ \xi\ )$$

Decreasing linear PDF

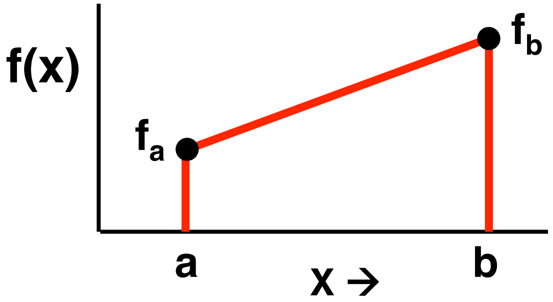


Random sampling can be done with a simple shifting & scaling of the unit PDF:

$$x \leftarrow a + (b\text{-}a)\,(1 - \mathrm{sqrt}(\xi))$$

Continuous PDFs – Linear (4)

Example - Sampling from linear PDF in range [a,b], 1 bin



PDF: $f(x) = f_a + m\,(x\text{-}a)$, $m = (f_b\text{-}f_a)/(b\text{-}a)$, $a \le x \le b$

CDF: $F(x) = (m/2)\,x^2 + (f_a\text{-}ma)\,x + (ma^2/2 - f_a a)$

$= A\,x^2 + B\,x + C$

Sampling scheme: $F(x) = \xi$, solve for x

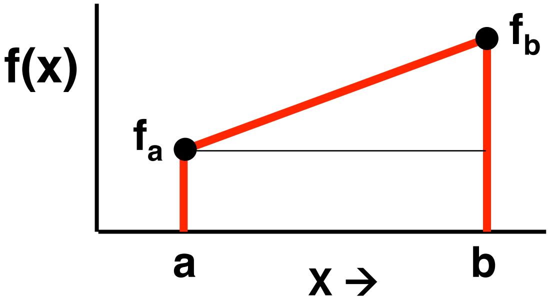
$x = \{ -B \pm \mathrm{sqrt}(B^2 - 4AC) \} / 2A$

➔ Awfully complicated, and sensitive to numerical roundoff

➔ There must be a simpler scheme (there is …)

Continuous PDFs – Linear (5)

Example - Sampling from linear PDF in range [a,b], 1 bin



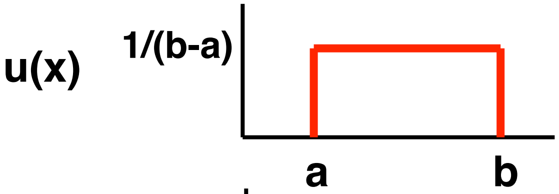
Composition method #1

Decompose the original PDF into the sum of 2 PDFs, uniform + linear:

$$f(x) = p_u\, u(x) + p_l\, l(x)$$

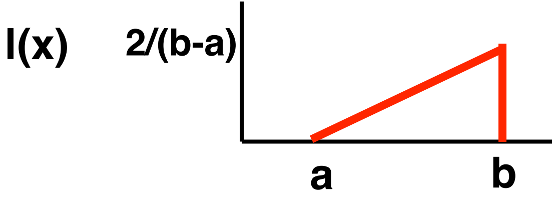
u(x) = uniform on $a \le x \le b$,

$p_u = \{ \min(f_a, f_b)\,(b-a) \} \;/\; \{ .5(f_a+f_b)\,(b-a) \}$



l(x) = linear on $a \le x \le b$,

$p_l = \{ .5\, \mathrm{abs}(f_b-f_a)\,(b-a) \} \;/\; \{ .5(f_a+f_b)\,(b-a) \}$

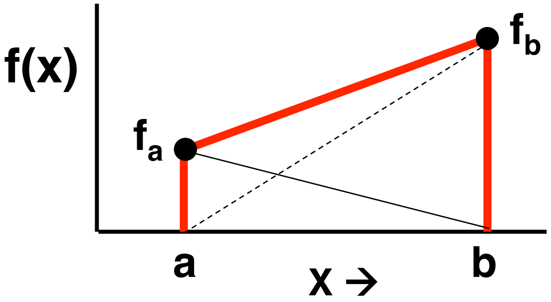


Sampling scheme:

```
if( $\xi_1 < p_u$ )
    $x \leftarrow a + (b-a)\,\xi_2$
else
    if( $f_b > f_a$ )    $x \leftarrow a + (b-a)\,\mathrm{sqrt}(\xi_2)$
    else                 $x \leftarrow a + (b-a)\,(1 - \mathrm{sqrt}(\xi_2))$
```

Continuous PDFs – Linear (6)

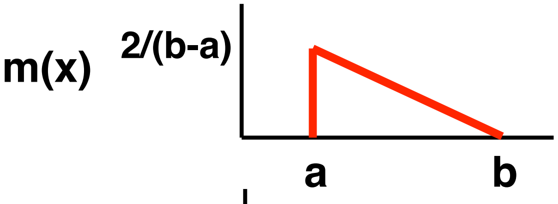
Example - Sampling from linear PDF in range [a,b], 1 bin



Composition method #2

Decompose the original PDF into the sum of 2 PDFs, increasing + decreasing linear:

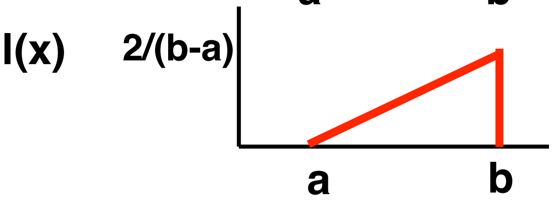
$$f(x) = p_m\, m(x) + p_l\, l(x)$$



$m(x)$ = linear decreasing on $a \le x \le b$,

$p_m = \{ .5\, f_a\, (b-a) \} \;/\; \{ .5(f_a+f_b)\, (b-a) \}$

$= f_a \,/\, (f_a+f_b)$



$l(x)$ = linear increasing on $a \le x \le b$,

$p_l = \{ .5\, f_b\, (b-a) \} \;/\; \{ .5(f_a+f_b)\, (b-a) \}$

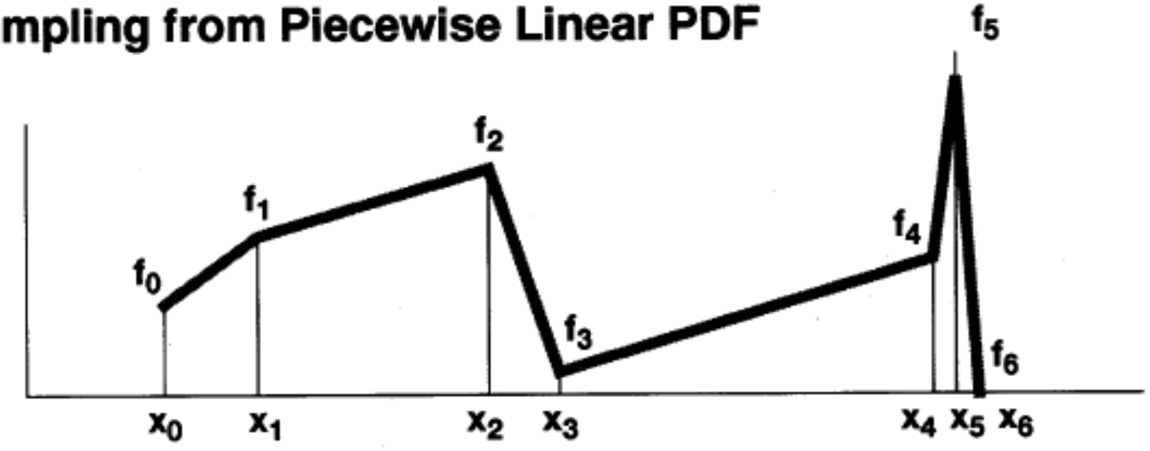
$= f_b \,/\, (f_a+f_b)$

Sampling scheme:

```
if( $\xi_1 < p_l$ )
    $x \leftarrow a + (b-a)\,\mathrm{sqrt}(\xi_2)$
else
    $x \leftarrow a + (b-a)\,(1 - \mathrm{sqrt}(\xi_2))$
```

Continuous PDFs – Linear (7)

Examples — Sampling from Piecewise Linear PDF



Two-step sampling: **(1) Sample from discrete PDF to select a bin**
(2) Sample from linear PDF within bin

- Discrete PDF: $p_k = \frac{(f_k + f_{k-1})}{2} \cdot (x_k - x_{k-1})$, $k = 1, \ldots, N$

— generate ξ
— use table search or alias method to select **K**

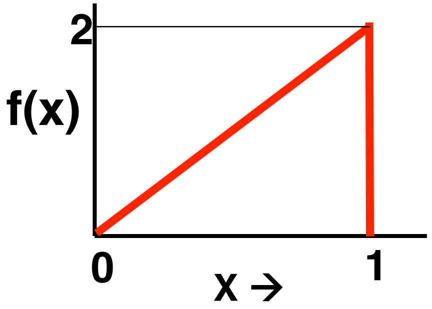
- Linear sampling within bin **K**:

— generate ξ
— then, if $\xi_1 < \frac{f_{k-1}}{f_k + f_{k-1}}$, $\hat{x} \leftarrow x_k - (x_k - x_{k-1})\sqrt{\xi_2}$

otherwise $\hat{x} \leftarrow x_{k-1} + (x_k - x_{k-1})\sqrt{\xi_2}$

Continuous PDFs – Linear (8)

We have seen that a simple, increasing linear PDF in the range [0,1] can be sampled directly by inverting the CDF to obtain:



PDF: $f(x) = 2x, \quad 0 \leq x \leq 1$

CDF: $F(x) = x^2, \quad 0 \leq x \leq 1$

Sampling scheme:

$F(x) = \xi, \quad$ solve for x

$x \leftarrow \text{sqrt}(\ \xi\ )$

While not obvious, some other schemes for sampling x are:

```
x = ξ₁
r = ξ₂
if( r > x ) x = r
```

$x \leftarrow \max(\ \xi_1, \xi_2\ )$

$x \leftarrow 1 - \text{abs}(\ \xi_1 - \xi_2\ )$

Why consider these other schemes?

Sqrt() function used to be very expensive. The other schemes involve only simple non-arithmetic operations & were much faster.

Today, sqrt() operations & computers are very fast – sqrt() is as fast as generating a 2nd RN. We usually go with the more obvious direct method.

BUT, the older schemes are still commonly used in production MC codes. Learn to recognize them.

Rejection Sampling

- **Von Neumann:**

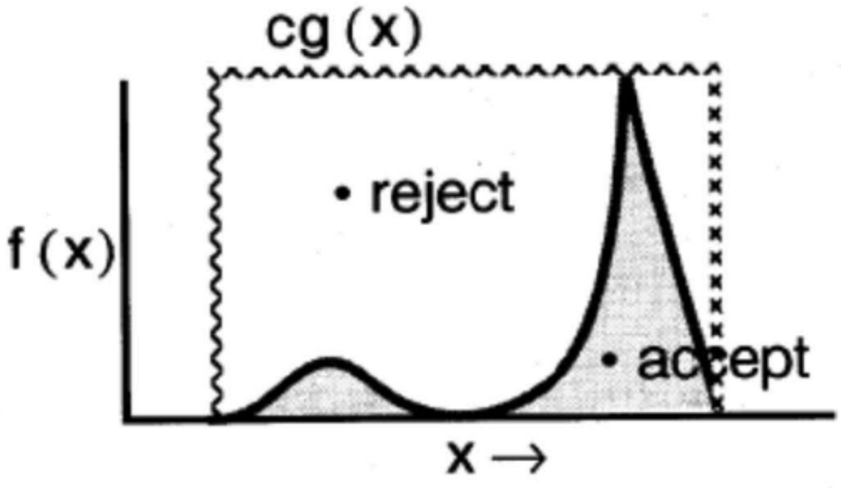
  " .... *it seems objectionable to compute a transcendental function of a random number.* "

- **Select a bounding function, g(x), such that**
  - $c \geq g(x) > f(x)$ for all x
  - g(x) is an easy-to-sample PDF

- **Sampling Procedure:**
  - sample x' from g(x): $x' \leftarrow G^{-1}(\xi_1)$
  - test: $\xi_2 \leq c\,g(x') < f(x')$

    if ***true***, accept x', done

    if ***false***, reject x', try again



- **Advantages**
  - **Simple computer operations**
- **Disadvantages**
  - **“Low-level” approach, sometimes hard to understand**

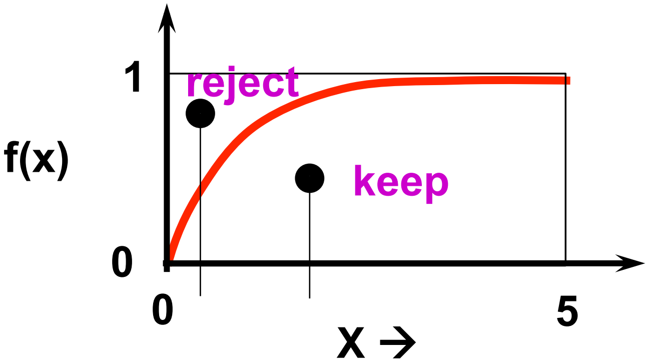
Rejection Sampling - Examples

- Sample from a PDF

  $f(x) = c \cdot \text{erf}(x), \quad 0 \le x \le 5.$

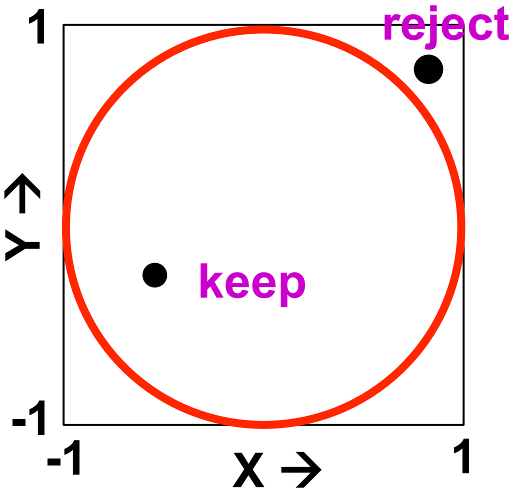
  note: $\text{erf}(\infty) = 1.$

```
Do
   xtry = 5.*rang()
   ftry = 1.*rang()
   if( ftry <= erf(xtry) ) exit
Enddo
x = xtry
```



- Select (x,y) points uniformly in a disk

```
Do
   x = 2.*rang() - 1.
   y = 2.*rang() – 1.
   if(  x**2 + y**2  <  1.0 )   exit
Enddo
```



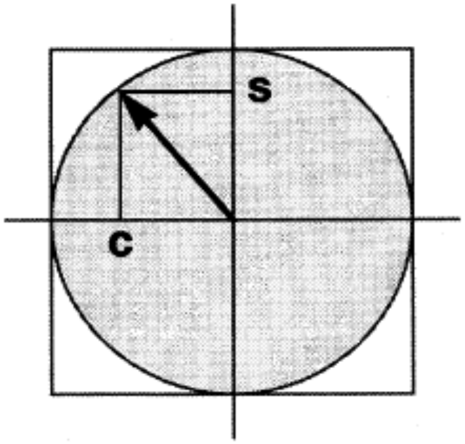
Direct vs. Rejection - 2D Direction Cosines

Example — 2D Isotropic

$$f(\vec{\rho}) = \frac{1}{2\pi}, \qquad \vec{\rho} = (u, v)$$

Rejection ***(old vim)***

```
     SUBROUTINE AZIRN_VIM( S, C )
    IMPLICIT DOUBLE PRECISION  (A-H, O-Z)
100 R1=2.*RANF() - 1.
     R1SQ=R1*R1
     R2=RANF()
     R2SQ=R2*R2
     RSQ=R1SQ+R2SQ
     IF(1.-RSQ)100,105,105
105 S=2.*R1*R2/RSQ
     C=(R2SQ-R1SQ)/RSQ
     RETURN
     END
```



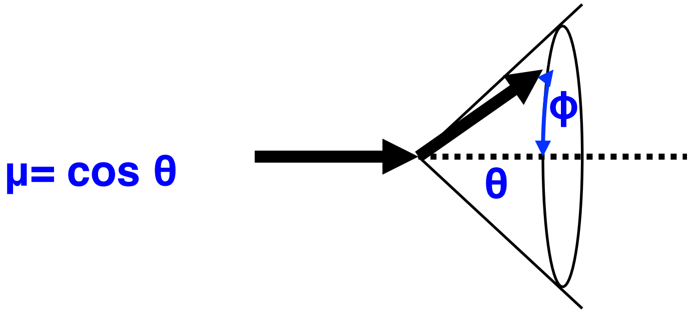
Direct ***(racer, new vim)***

```
     subroutine azirn_new( s, c )
     implicit double precision  (a-h,o-z)
     parameter ( twopi = 2.*3.14159265 )
     phi = twopi*ranf()
     c = cos(phi)
     s = sin(phi)
     return
     end
```

Isotropic Scatter – Sampling the Scattering Angle

- **Consider isotropic scattering**
  - **Any direction is equally likely**
  - **Interpret as:**

    "pick a random point on a unit sphere,
    then get direction-cosines"



- **Rejection method for scatter angle sampling**
  - **Pick x,y,z randomly in unit cube**
  - **If x,y,z outside unit sphere, reject and try again**
  - **If x,y,z inside unit sphere, scale so that $x^2+y^2+z^2 = 1$**
  - **Get direction-cosines of angles, u,v,w**

- **Direct method for scatter angle sampling**

$$f(\hat{\Omega}) = \frac{1}{4\pi}, \qquad \frac{d\hat{\Omega}}{4\pi} = \frac{\sin\theta\cdot d\theta}{2}\cdot\frac{d\phi}{2\pi}$$

$$f(\theta,\phi) = \frac{\sin\theta\cdot d\theta}{2}\cdot\frac{d\phi}{2\pi}, \qquad 0\le\theta\le\pi,\quad 0\le\phi\le 2\pi$$

$$f(\theta) = \int_0^{2\pi} f(\theta,\phi)\,d\phi = \frac{\sin\theta}{2}$$

$$\mu = \cos\theta, \quad d\mu = -\sin\theta\cdot d\theta, \qquad -1\le\mu\le+1$$

$$f(\mu) = f(\theta)\left|\frac{d\theta}{d\mu}\right| = \frac{\sin\theta}{2}\cdot\frac{1}{\sin\theta} = \frac{1}{2}$$

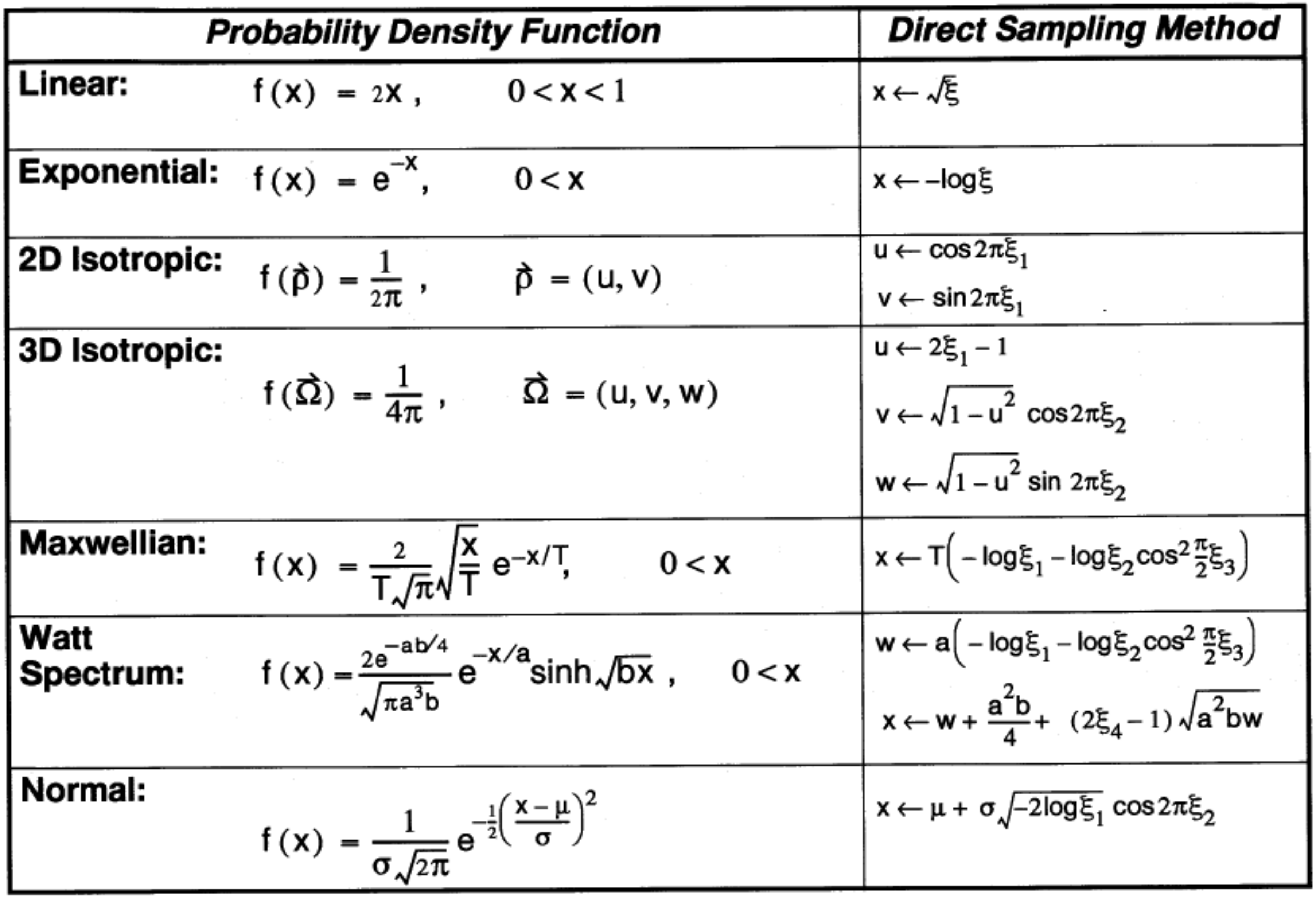
➜ **μ is distributed uniformly in [-1,1]**

➜ **φ is distributed uniformly in [0,2π]**

$$\mu \leftarrow 2\xi_1 - 1$$

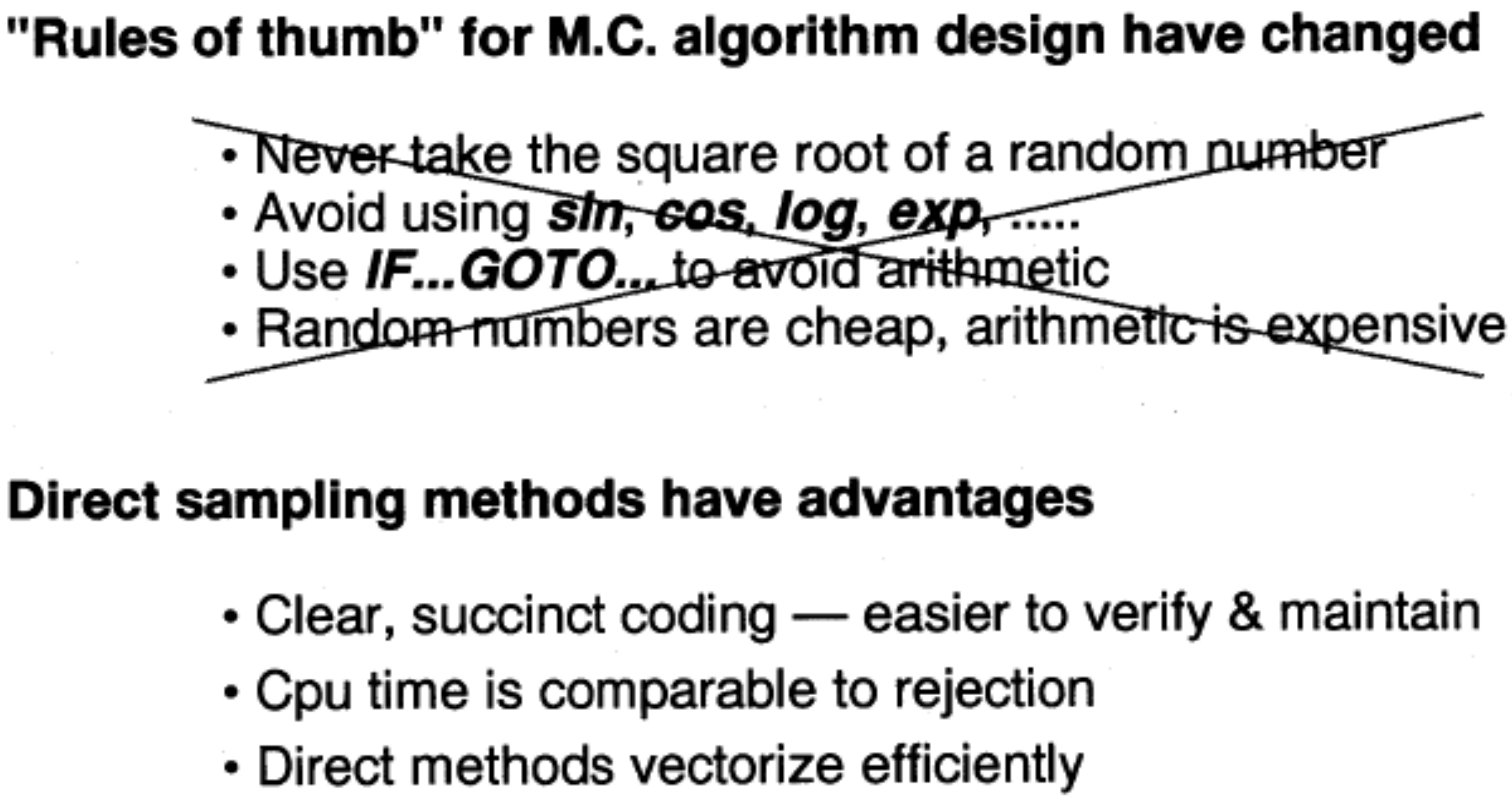
$$\phi \leftarrow \xi_2\ 2\,\pi$$

Direct Sampling – Common PDFs



Probability Density Function			*Direct Sampling Method*
Linear:	$f(x) = 2x$,	$0 < x < 1$	$x \leftarrow \sqrt{\xi}$
Exponential:	$f(x) = e^{-x}$,	$0 < x$	$x \leftarrow -\log\xi$
2D Isotropic:	$f(\vec{\rho}) = \frac{1}{2\pi}$,	$\vec{\rho} = (u, v)$	$u \leftarrow \cos 2\pi\xi_1$ $v \leftarrow \sin 2\pi\xi_1$
3D Isotropic:	$f(\vec{\Omega}) = \frac{1}{4\pi}$,	$\vec{\Omega} = (u, v, w)$	$u \leftarrow 2\xi_1 - 1$ $v \leftarrow \sqrt{1-u^2}\cos 2\pi\xi_2$ $w \leftarrow \sqrt{1-u^2}\sin 2\pi\xi_2$
Maxwellian:	$f(x) = \frac{2}{T\sqrt{\pi}}\sqrt{\frac{x}{T}}\, e^{-x/T}$,	$0 < x$	$x \leftarrow T\left(-\log\xi_1 - \log\xi_2 \cos^2 \frac{\pi}{2}\xi_3\right)$
Watt Spectrum:	$f(x) = \frac{2e^{-ab/4}}{\sqrt{\pi a^3 b}} e^{-x/a} \sinh\sqrt{bx}$,	$0 < x$	$w \leftarrow a\left(-\log\xi_1 - \log\xi_2 \cos^2 \frac{\pi}{2}\xi_3\right)$ $x \leftarrow w + \frac{a^2 b}{4} + (2\xi_4 - 1)\sqrt{a^2 bw}$
Normal:	$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$		$x \leftarrow \mu + \sigma\sqrt{-2\log\xi_1}\cos 2\pi\xi_2$

Software Considerations



"Rules of thumb" for M.C. algorithm design have changed

- ~~Never take the square root of a random number~~
- ~~Avoid using ***sin*, *cos*, *log*, *exp***, ...~~
- ~~Use ***IF...GOTO...*** to avoid arithmetic~~
- ~~Random numbers are cheap, arithmetic is expensive~~

Direct sampling methods have advantages

- Clear, succinct coding — easier to verify & maintain
- Cpu time is comparable to rejection
- Direct methods vectorize efficiently

Mean & Standard Deviation

- Given a set of random samples, $x_1, x_2, \ldots, x_N,$
  - Mean $$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j$$
  - Population variance & standard deviation $$\sigma^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \left(\frac{1}{N}\sum_{j=1}^{N} x_j\right)^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2 \qquad \sigma = \sqrt{\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2}$$
  - Variance & standard deviation of the mean $$\sigma_{\bar{x}}^2 = \frac{\sigma^2}{N} \qquad \sigma_{\bar{X}} = \frac{1}{\sqrt{N}} \cdot \sqrt{\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2}$$

Monte Carlo codes calculate mean values for tallies, & report the standard deviation of the mean

In the definitions above, some of the "N" terms should really be "N-1". MCNP & many other codes ignore that, since N is very large.

Random Sampling -- References

Every Monte Carlo code developer who works with random sampling should own & read these references:

– D. E. Knuth, The Art of Computer Programming, Vol. 2: Semi-numerical Algorithms, 3rd Edition, Addison-Wesley, Reading, MA (1998).

– L. Devroye, Non-Uniform Random Variate Generation, Springer-Verlag, NY (1986). ★

– J. von Neumann, "Various Techniques Used in Conjunction with Random Digits," *J. Res. Nat. Bur. Stand. Appl. Math Series* 3, 36-38 (1951). ★

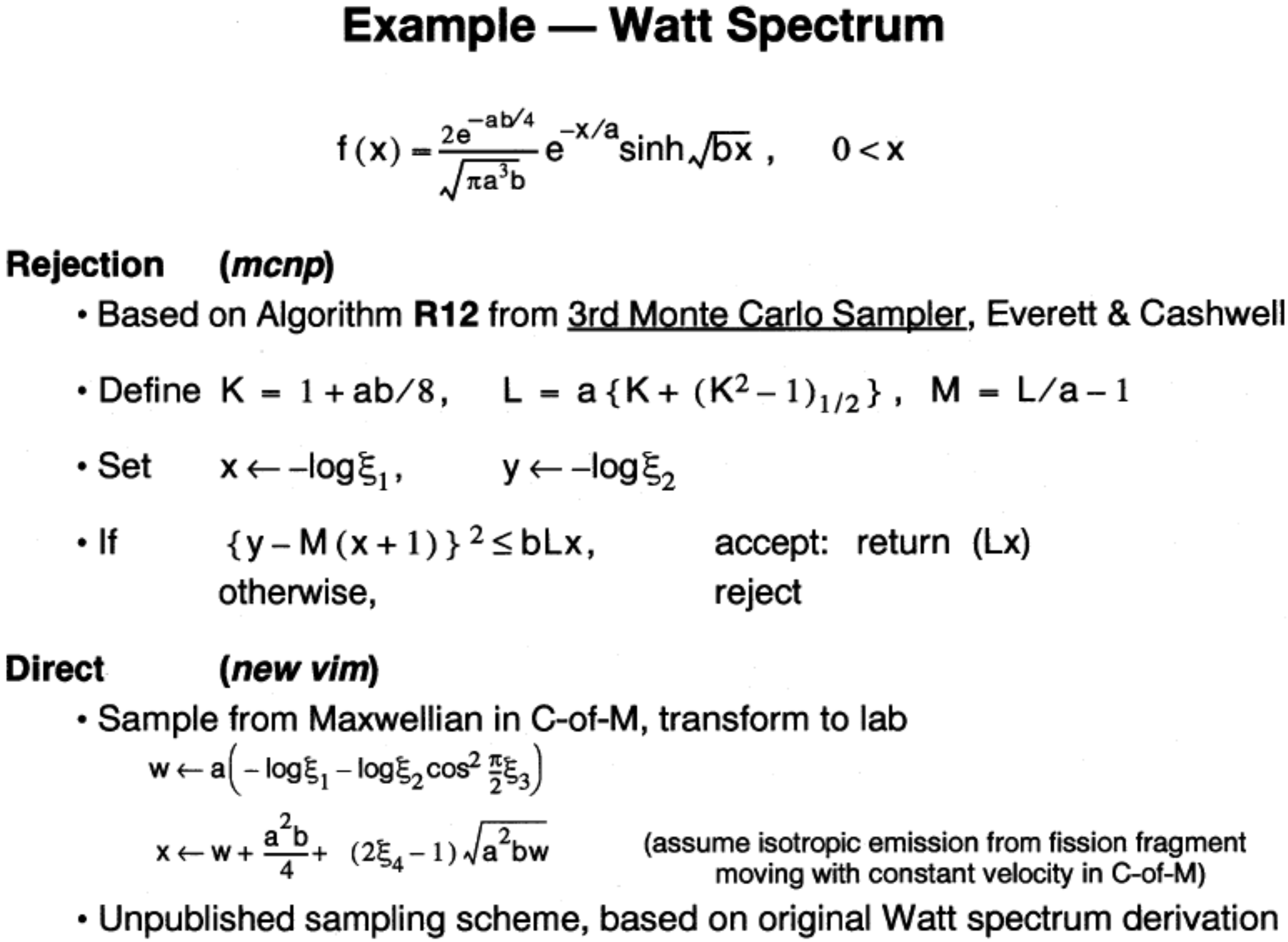
– C. J. Everett and E. D. Cashwell, "A Third Monte Carlo Sampler," LA9721-MS, Los Alamos National Laboratory, Los Alamos, NM (1983). ★

– H. Kahn, "Applications of Monte Carlo," AECU-3259, Rand Corporation, Santa Monica, CA (1954). ★

★= Included in References on class CD

Extra Topics

Direct vs. Rejection - Watt



Example — Watt Spectrum

$$f(x) = \frac{2e^{-ab/4}}{\sqrt{\pi a^3 b}} e^{-x/a} \sinh\sqrt{bx}\ , \qquad 0 < x$$

Rejection ***(mcnp)***

- Based on Algorithm **R12** from 3rd Monte Carlo Sampler, Everett & Cashwell
- Define $K = 1 + ab/8, \quad L = a\{K + (K^2 - 1)_{1/2}\}, \quad M = L/a - 1$
- Set $x \leftarrow -\log\xi_1, \qquad y \leftarrow -\log\xi_2$
- If $\{y - M(x+1)\}^2 \le bLx,$ accept: return (Lx)
  otherwise, reject

Direct ***(new vim)***

- Sample from Maxwellian in C-of-M, transform to lab

$$w \leftarrow a\left(-\log\xi_1 - \log\xi_2 \cos^2 \tfrac{\pi}{2}\xi_3\right)$$

$$x \leftarrow w + \frac{a^2 b}{4} + (2\xi_4 - 1)\sqrt{a^2 bw}$$

(assume isotropic emission from fission fragment moving with constant velocity in C-of-M)

- Unpublished sampling scheme, based on original Watt spectrum derivation

Stratified Sampling

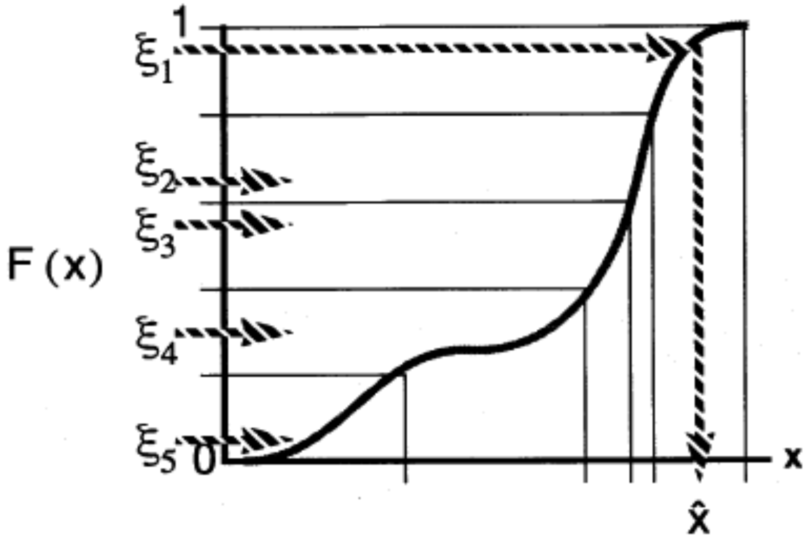
If a specific number of samples, M, is needed from a single distribution:

- Naive approach — repeat the sampling procedure M times

- **Stratified sampling** approach

  — partition the sample space into M disjoint regions of **equal probability**

  — produce 1 sample from each region



- Stratified sampling considerations

  — F(x) must be known & easy to partition

  — The number of partitions, M, must be known in advance

  — Must be relatively easy to sample **within** each given partition

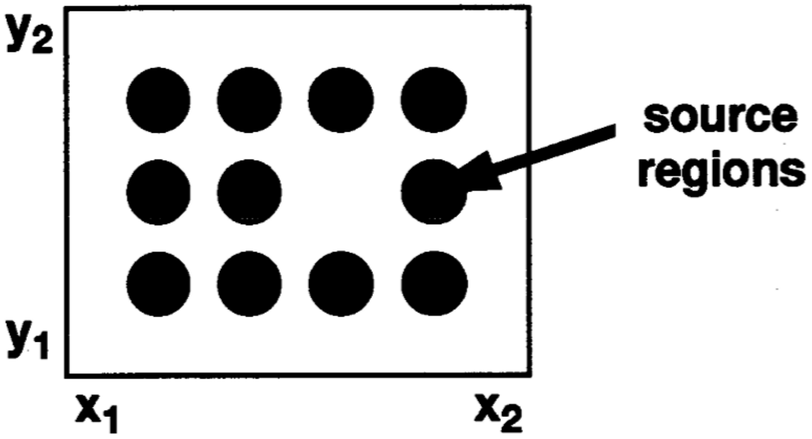
  — Stratification improves the "coverage"

  — Stratified sampling reduces variance, at little or no computing cost

Rejection Method

- Rejection sampling methods are useful when it is difficult or impossible to invert F(x), or when F(x) is no known

- Example - Selection of initial source sites in a reactor, rejection method based on spatial coordinates



– Select a trial site:

$$x' \leftarrow x_1 + (x_2 - x_1)\cdot\xi_1$$

$$y' \leftarrow y_1 + (y_2 - y_1)\cdot\xi_2$$

– If (x',y') is inside a fuel pin (shaded region), then accept (x',y').

– Otherwise, reject (x',y') and repeat

– Efficiency of rejection sampling ~ (volume source region) / (total volume)

Weighted Sampling

It is sometimes useful to sample from an alternate PDF

$$f(x)\,dx = \left[\frac{f(x)}{g(x)}\right] g(x)\,dx = h(x)\,g(x)\,dx$$

& then "correct" the result via either weight factors or a 2nd sampling stage

Weighted Sampling

- To sample $\hat{x}$ from f(x),
  - — first, sample $\hat{x}$ from g(x)
  - — then, multiply the "weight" assigned to $\hat{x}$ by $\dfrac{\text{right answer}}{\text{wrong answer}} = \dfrac{f(\hat{x})}{g(\hat{x})}$

- Note that g(x) must be >0 whenever f(x)>0.
- Also, g(x) must be normalized so that $\int g(x)\,dx = 1$

- **Example — survival biasing of collisions**

  If a collision occurs, $P_{survive} = \dfrac{\Sigma_S}{\Sigma_T}$ is the probability of surviving.

  Instead of sampling the outcome, always choose survival & multiply the "weight" by $P_{survive}$

Splitting & Russian Roulette

Combined Russian Rouletting & Splitting

- Russian Roulette — kill off some particles, but conserve total weight
- Splitting — create extra identical particles, but conserve total weight

- Definitions

  wgt = Particle weight

  For the region containing the particle:

  $\mathbf{w_{high}}$ = upper bound on weight, if wgt larger — split

  $\mathbf{w_{low}}$ = lower bound on weight, if wgt lower — roulette

  $\mathbf{w_{ave}}$ = weight to assign survivors, $\mathbf{w_{low}} < \mathbf{w_{ave}} < \mathbf{w_{high}}$

  Then,

  $\mathbf{wgt} / \mathbf{w_{ave}}$ = probability of surviving split/roulette

- Combined game for split/roulette:

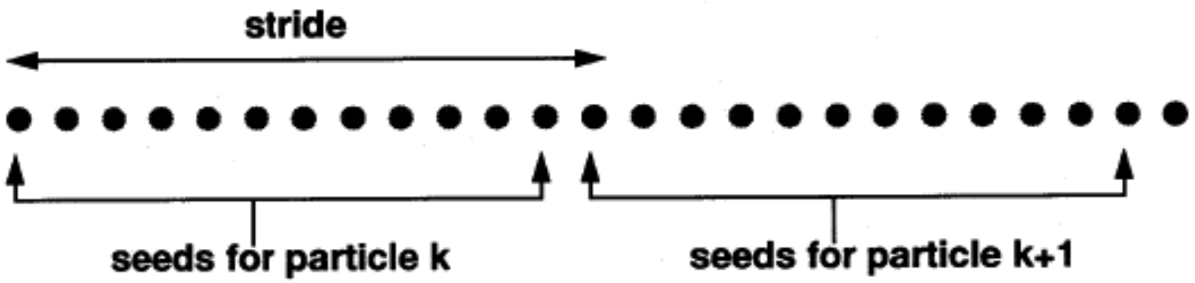
  if $\mathbf{wgt} < \mathbf{w_{low}}$ or $\mathbf{w_{high}} < \mathbf{wgt}$,

  create **n** particles of weight $\mathbf{w_{ave}}$, where $\mathbf{n} \leftarrow \left\lfloor \frac{\mathbf{wgt}}{\mathbf{w_{ave}}} + \xi \right\rfloor$

Random Number Generators - Reproducibility

Reproducibility of a Particle History

- use separate, distinct random sequence for each particle
- starting seeds for separate particles are separated by "stride"



- stride should be large enough to prevent overlap (for most histories)

— 1000 is common for reactor analysis problems

- splitting & variance reduction not needed for in-core physics
- reduces total random number usage

— 4,297 is the "old" default for MCNP & VIM

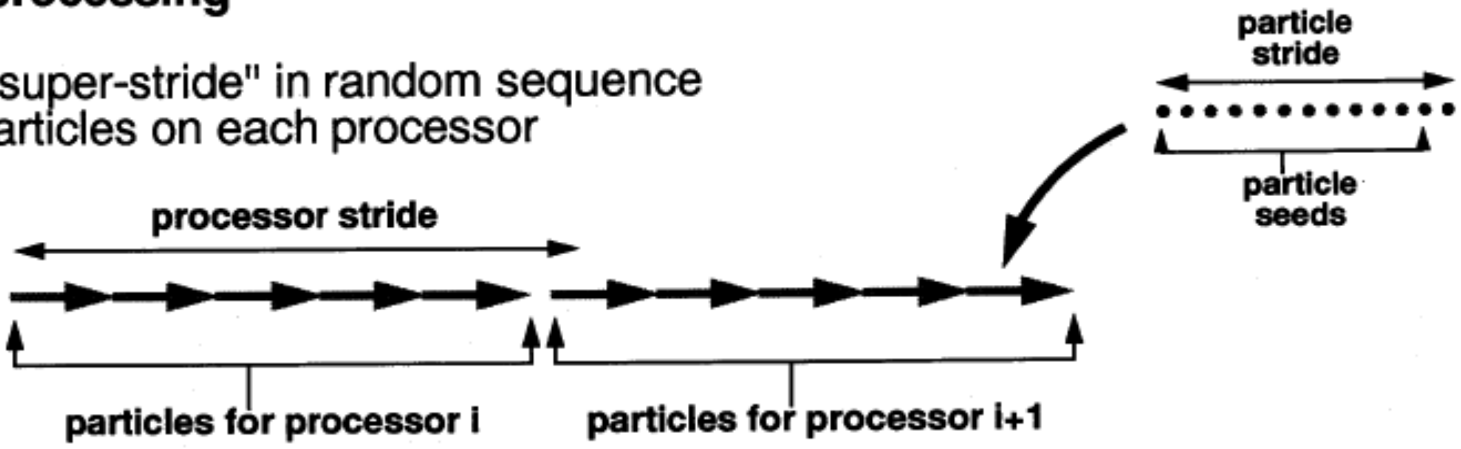
— 152,917 is the default for MCNP & VIM

- prepared for lots of splitting & variance reduction
- potential for lots of secondary particles

Random Number Generators - Reproducibility

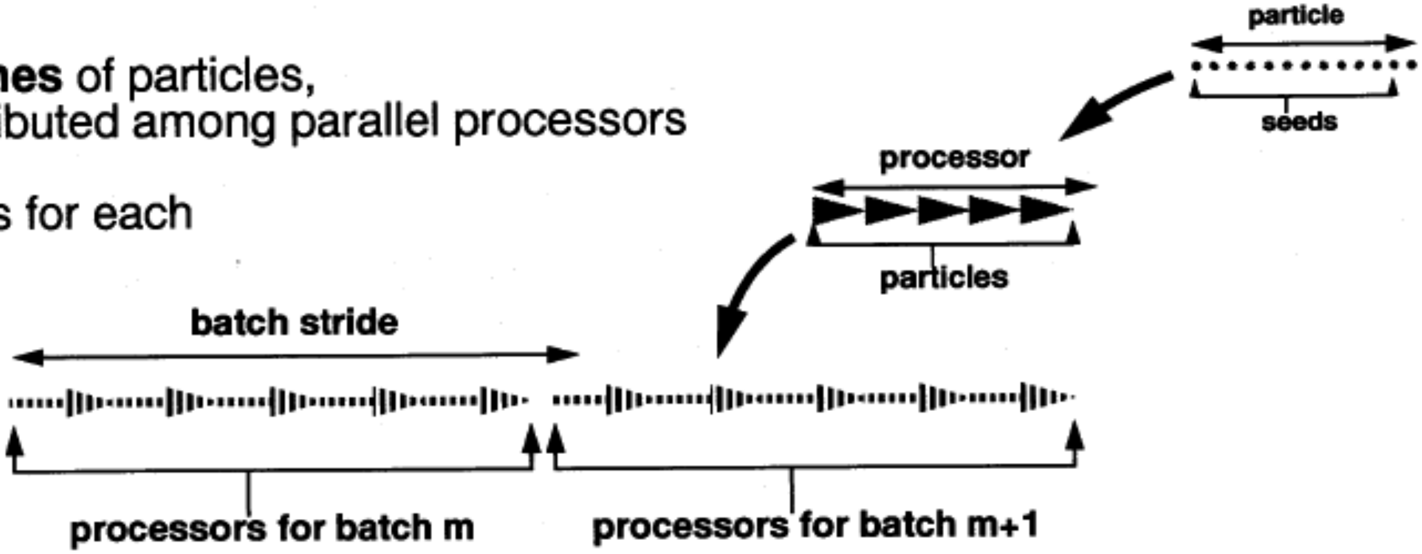
Parallel processing

- take "super-stride" in random sequence for particles on each processor



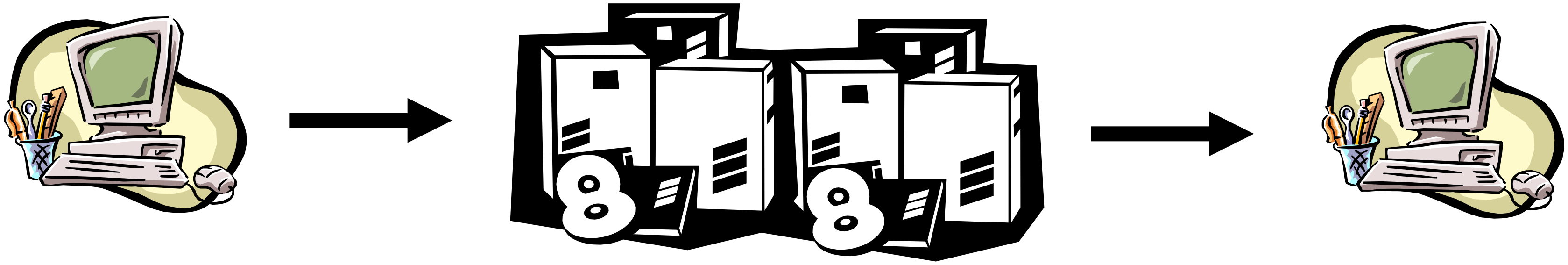
Eigenvalue Problems

- **batches** of particles, distributed among parallel processors
- seeds for each



Computational Geometry

Engineering Model vs. Computational Model



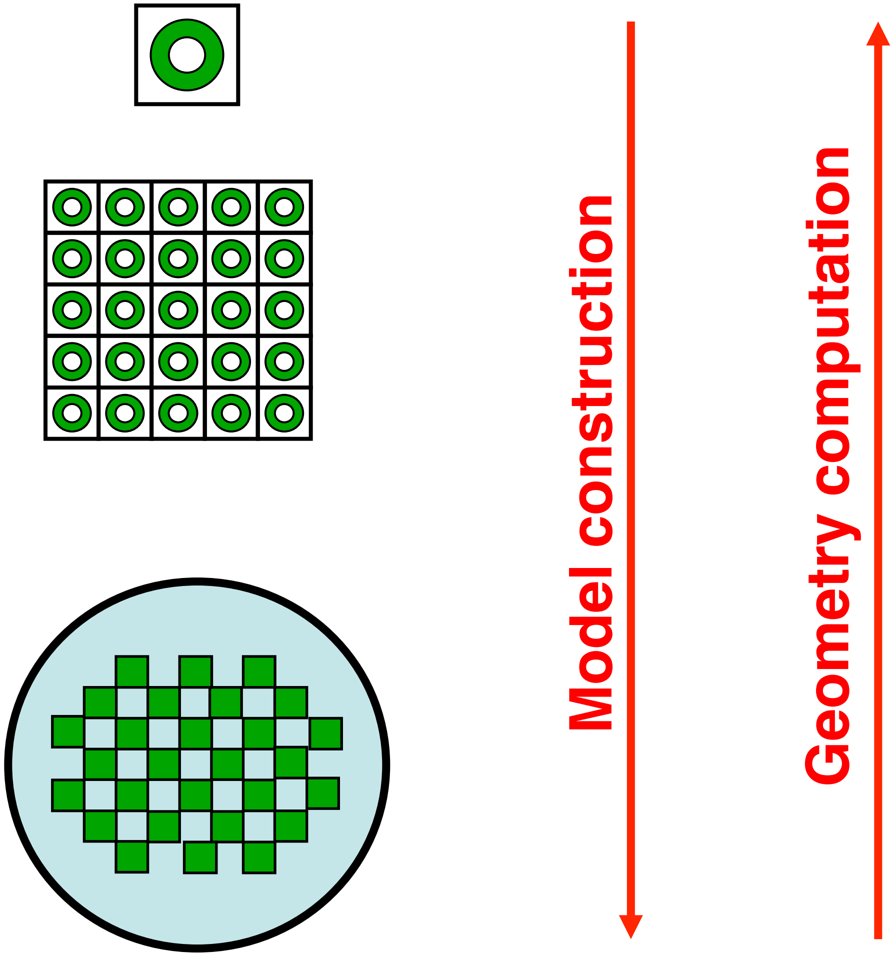
Model Generation | Large-scale Computation | Post-processing

Engineering Model | Computational Model | Engineering Model

- **Model Generation**
  - Focus on engineering productivity
  - Describes “reality” to computer
  - Interactive, batch, or CAD
- **Large-scale Computation**
  - Focus on efficiency & capabilities
  - Data structures should be compact & regular
  - Computational model often hidden from user
- **Post-Processing**
  - Interpretation of results
  - Visualization

Modeling vs. Computation

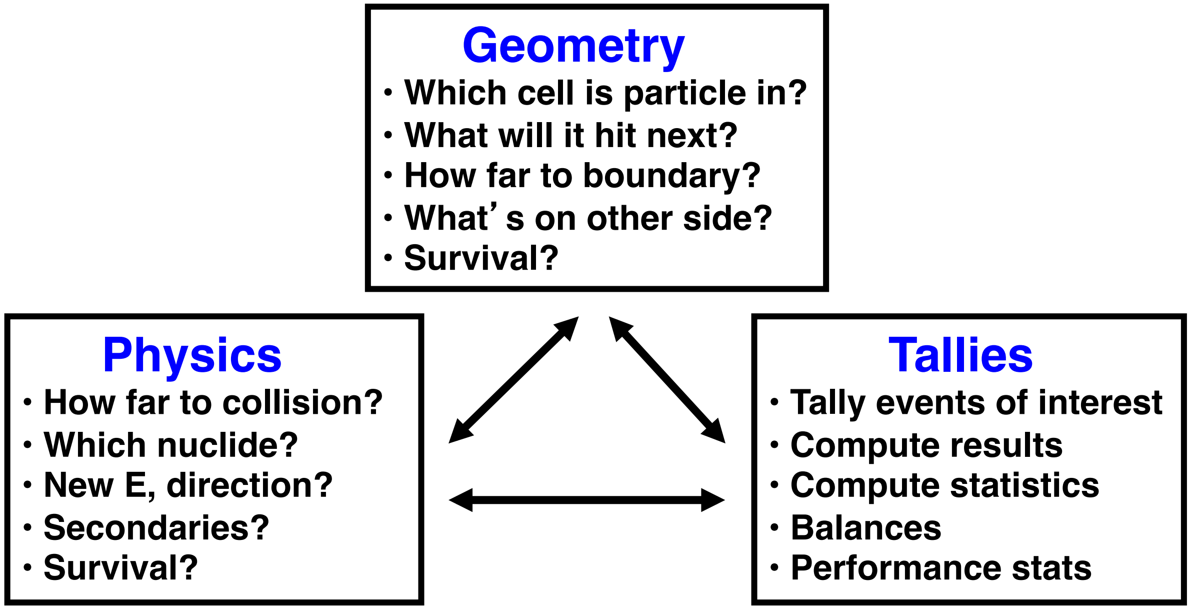
- Element geometry
- Elements --> assemblies
- Assemblies --> core
- Core + peripherals
  --> 3D model



Model construction

Geometry computation

Monte Carlo Geometry



Geometry

- Which cell is particle in?
- What will it hit next?
- How far to boundary?
- What's on other side?
- Survival?

Physics

- How far to collision?
- Which nuclide?
- New E, direction?
- Secondaries?
- Survival?

Tallies

- Tally events of interest
- Compute results
- Compute statistics
- Balances
- Performance stats

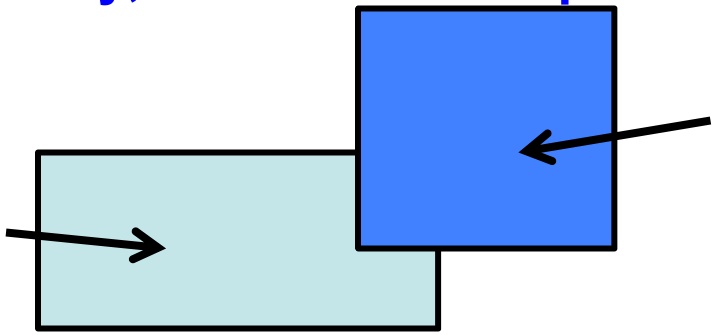
mcnp, rcp, vim, racer, sam, tart, morse, keno, tripoli, mcbend, monk, o5r, recap, andy, …

Development of particular geometric capabilities is driven by applications:

- **Shielding & experiment analysis**
  - Irregular geometry
  - Moderate number of regions & compositions
- **Reactor core analysis**
  - Regular geometry
  - Very many regions & compositions

Comments on 3D Computational Geometry (1)

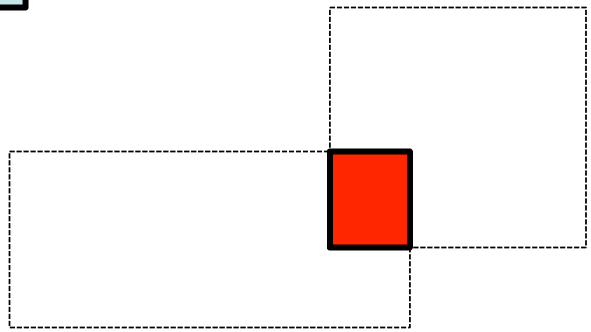
- At the most fundamental level, 3D computational geometry is an exercise in Set Theory, the same concepts we all learned as kids



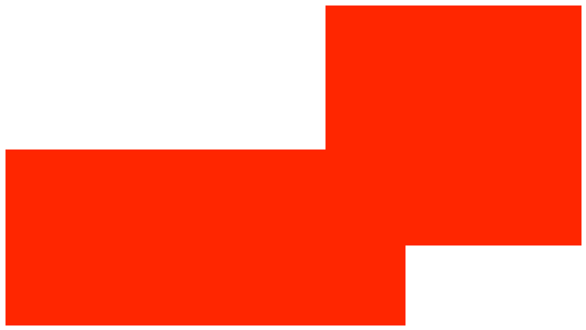
Set of all x,y,z points inside box A

Set of all x,y,z points inside box B

Intersection of sets A & B

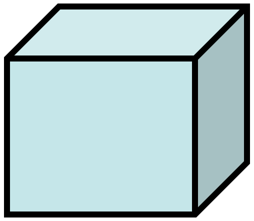


Union of sets A & B



Comments on 3D Computational Geometry (2)

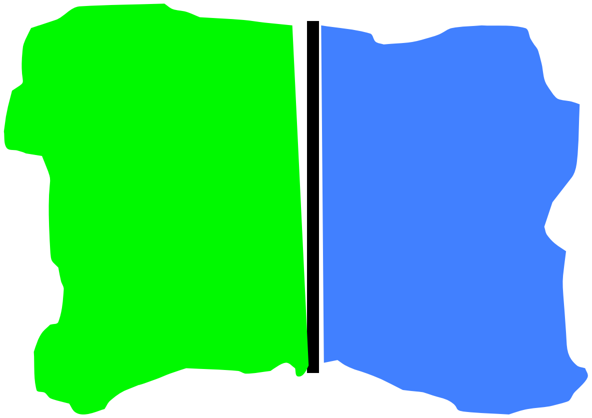
- Some codes use primitive bodies (box, sphere, etc.) in defining the sets of points to consider



Set of all x,y,z points inside box

- Other codes use half-spaces – all the points on one side of a surface

Set of all x,y,z points on minus side of surface



Set of all x,y,z points on plus side of surface

- A little thought should convince you that either scheme can be used in set theory for defining objects in space

Computational Algorithm - Geometric View

```
Repeat for all $k_{eff}$ cycles
.     Repeat for all histories in cycle
.     .     Repeat while particles are left in history
.     .     .     While particle wgt > 0
.     .     .     .     Repeat until collision
.     .     .     .     .     Repeat for each universe level
.     .     .     .     .     .     Repeat for surfaces of 3D region
.     .     .     .     .     .     .        Distance calculation
.     .     .     .     .     .     . . .
.     .     .     .     .     . . .
.     .     .     .     .     Boundary crossing
.     .     .     .     .     Neighbor search
.     .     .     .     .     Roulette/split
.     .     .     .     . . .
.     .     .     .     Collision analysis
.     .     .     .     Roulette/split
.     .     .     . . .
.     .     . . .
.     .     Update tallies
.     . . .
.     Update tallies, source, & $k_{eff}$
. . .
```

1 reactor calculation requires ~10^{12} distance calculations

Computational Geometry

- Every point in space that a particle could possibly reach must be defined in the geometry model – no gaps or overlaps of regions

- Cells (3D volumes) are defined by their bounding surfaces
  - Boundary representation
  - Combinatorial geometry, with either surfaces or primitive bodies
  - CSG - constructive solid geometry, tree structure with boolean operators
  - Mesh geometry
  - For some codes, disjoint volumes must have different cell numbers
  - For MCNP & others, disjoint volumes may have the same cell number

- Properties are assigned to each cell
  - Material, density, temperature, importance, etc.

- Tallies are defined for particular cells or surfaces, reaction types, & estimator types

Basic Geometry Operations

- **Locate**

  Given a point in space, determine what cell it is in

- **Distance to surface**

  **Given a point & direction in a particular cell,
  determine the distance to the next surface of that cell**

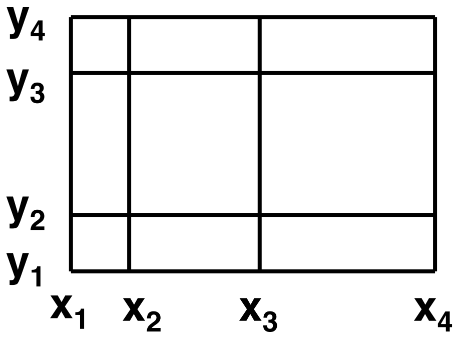
- **Neighbor search**

  **For a particle which has hit a bounding surface of a cell,
  determine the cell to be entered next**

- **Boundary conditions**

  **For a particle which has hit a cell bounding surface
  declared to be periodic or reflecting,
  determine the new position & direction and cell to be entered next**

Simple Case - Mesh Geometry



- **Particle**
  Position = (x,y,z), Direction = (u,v,w)

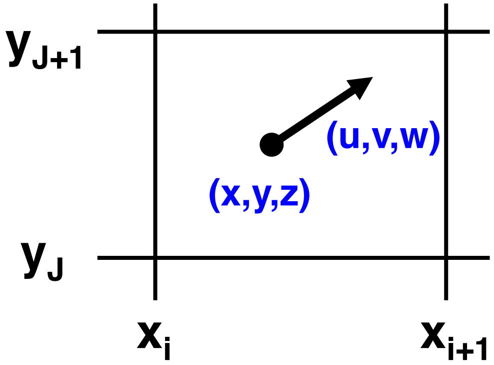
- **Cell number**
  (i,j,k), indices in mesh

- **Locate**
  i: binary search to find x-interval containing x
  j: binary search to find y-interval containing y
  k: binary search to find z-interval containing z

- **Distance**
  - **Use signs of (u,v,w) to select surfaces, then compute 3 distances:**

    if u>0, $d_x = (x_{i+1}-x)/u$, otherwise $d_x = (x_i-x)/u$
    … similar for d_y & d_z

  - **Distance: $d = \min(d_x, d_y, d_z)$**



- **Neighbor search**
- **Boundary conditions**

MCNP Geometry

- MCNP uses a "combinatorial geometry" based on surfaces
  - Define surfaces, specify sense (which side of surface)
  - Define cells using surfaces & operators (intersection, union, complement)
  - Can also group cells together into a universe, and embed that universe inside another cell
  - Can also group cells together into a universe, repeat that universe in a lattice arrangement, and embed that universe inside another cell
  - Assign materials to cells
  - Assign other properties to cells (e.g., density, temperature, importance)
  - Define tallies using cell or surface numbers

Surfaces

- **In MCNP, surface types include:**

1st order:	planes
2nd order:	spheres, cylinders, cones, ellipsoid, hyperboloid, paraboloid, general quadric
4th order:	elliptical & circular torus (axes parallel to x, y, or z)

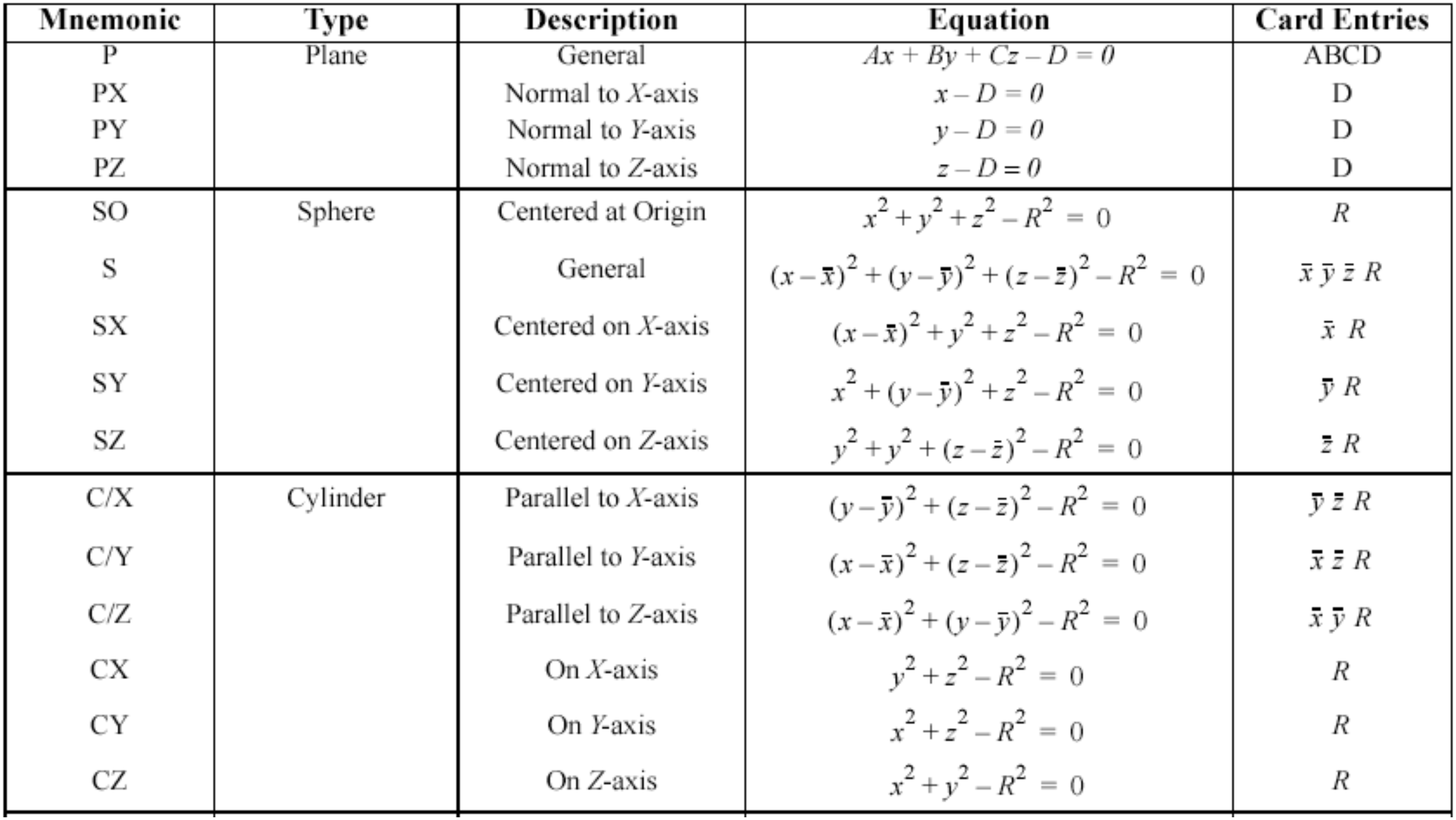
- **Quadratic polynomial for surface:**

$$F(x,y,z) = ax^2 + by^2 + cz^2 + dxy + eyz + fzx + gx + hy + jz + k$$

- Surface is defined by: $F(x,y,z) = 0$
- Surface is either infinite or closed
- Normalization convention: factor of leading 2nd order term is positive

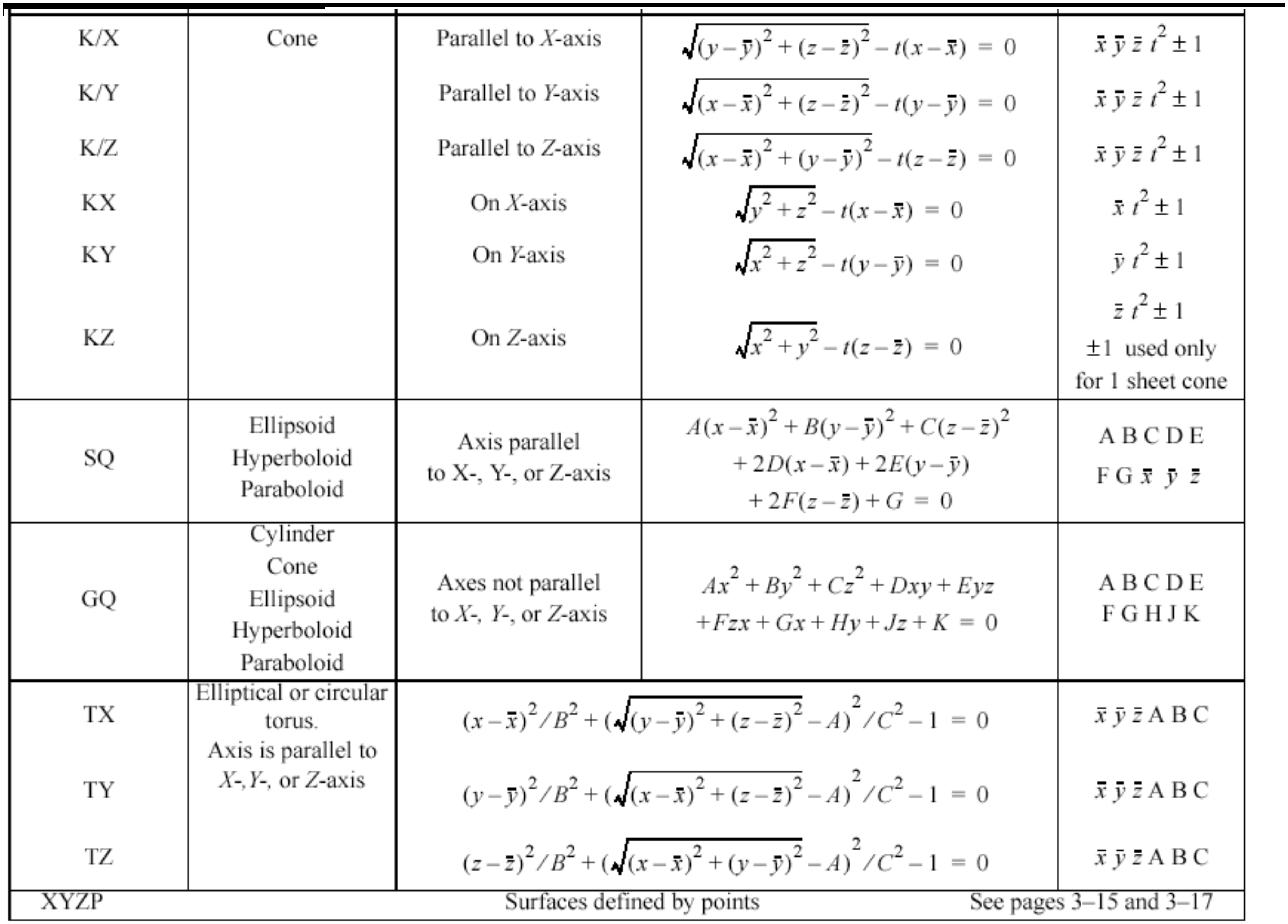
MCNP Surfaces

Table 3.1: MCNP Surface Cards



Mnemonic	Type	Description	Equation	Card Entries
P	Plane	General	$Ax + By + Cz - D = 0$	ABCD
PX		Normal to *X*-axis	$x - D = 0$	D
PY		Normal to *Y*-axis	$y - D = 0$	D
PZ		Normal to *Z*-axis	$z - D = 0$	D
SO	Sphere	Centered at Origin	$x^2 + y^2 + z^2 - R^2 = 0$	R
S		General	$(x - \bar{x})^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ R$
SX		Centered on *X*-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	$\bar{x}\ R$
SY		Centered on *Y*-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	$\bar{y}\ R$
SZ		Centered on *Z*-axis	$y^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{z}\ R$
C/X	Cylinder	Parallel to *X*-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{y}\ \bar{z}\ R$
C/Y		Parallel to *Y*-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{z}\ R$
C/Z		Parallel to *Z*-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ R$
CX		On *X*-axis	$y^2 + z^2 - R^2 = 0$	R
CY		On *Y*-axis	$x^2 + z^2 - R^2 = 0$	R
CZ		On *Z*-axis	$x^2 + y^2 - R^2 = 0$	R

MCNP Surfaces



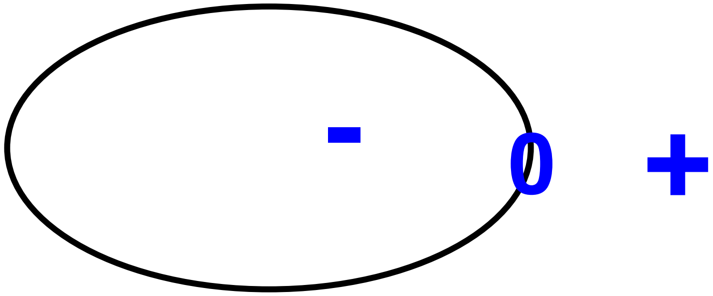
K/X	Cone	Parallel to X-axis	$\sqrt{(y-\bar{y})^2+(z-\bar{z})^2}-t(x-\bar{x}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2 \pm 1$
K/Y		Parallel to Y-axis	$\sqrt{(x-\bar{x})^2+(z-\bar{z})^2}-t(y-\bar{y}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2 \pm 1$
K/Z		Parallel to Z-axis	$\sqrt{(x-\bar{x})^2+(y-\bar{y})^2}-t(z-\bar{z}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2 \pm 1$
KX		On X-axis	$\sqrt{y^2+z^2}-t(x-\bar{x}) = 0$	$\bar{x}\ t^2 \pm 1$
KY		On Y-axis	$\sqrt{x^2+z^2}-t(y-\bar{y}) = 0$	$\bar{y}\ t^2 \pm 1$
KZ		On Z-axis	$\sqrt{x^2+y^2}-t(z-\bar{z}) = 0$	$\bar{z}\ t^2 \pm 1$ ± 1 used only for 1 sheet cone
SQ	Ellipsoid Hyperboloid Paraboloid	Axis parallel to X-, Y-, or Z-axis	$A(x-\bar{x})^2+B(y-\bar{y})^2+C(z-\bar{z})^2$ $+2D(x-\bar{x})+2E(y-\bar{y})$ $+2F(z-\bar{z})+G = 0$	A B C D E F G $\bar{x}$ $\bar{y}$ $\bar{z}$
GQ	Cylinder Cone Ellipsoid Hyperboloid Paraboloid	Axes not parallel to X-, Y-, or Z-axis	$Ax^2+By^2+Cz^2+Dxy+Eyz$ $+Fzx+Gx+Hy+Jz+K = 0$	A B C D E F G H J K
TX	Elliptical or circular torus. Axis is parallel to X-,Y-, or Z-axis		$(x-\bar{x})^2/B^2+(\sqrt{(y-\bar{y})^2+(z-\bar{z})^2}-A)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
TY			$(y-\bar{y})^2/B^2+(\sqrt{(x-\bar{x})^2+(z-\bar{z})^2}-A)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
TZ			$(z-\bar{z})^2/B^2+(\sqrt{(x-\bar{x})^2+(y-\bar{y})^2}-A)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
XYZP		Surfaces defined by points		See pages 3–15 and 3–17

Sense

- For a given point in space, (x,y,z), and surface equation, F(x’ ,y’ ,z’)=0, the sense of the point with respect to the surface is defined as:

Inside the surface,	sense < 0,	if	F(x,y,z) < 0
Outside the surface,	sense > 0,	if	F(x,y,z) > 0
On the surface,	sense = 0,	if	F(x,y,z) = 0

[Must be careful to consider computer roundoff!]

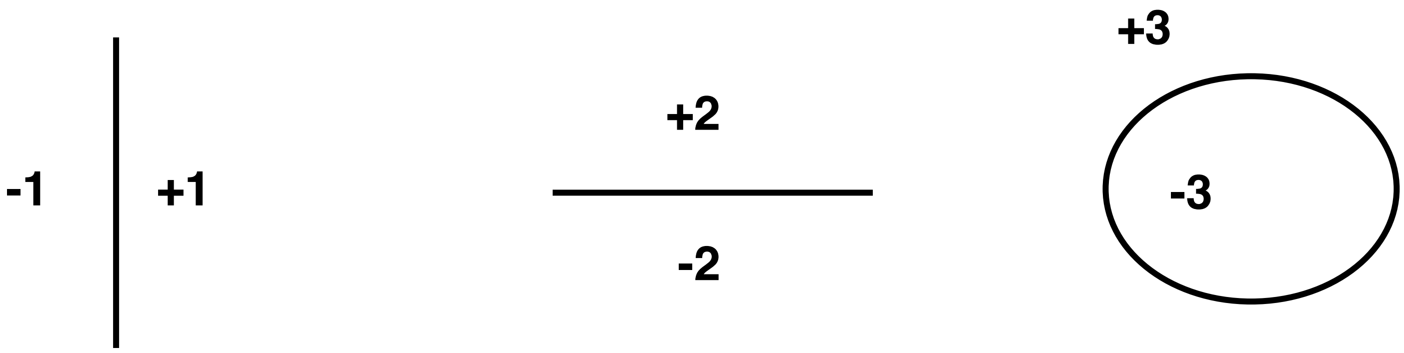


Note: Outward surface normal points in direction of + sense

Sides

- A surface divides space into positive & negative sides

  – MCNP convention: +1 = positive side of surface 1
  -1 = negative side of surface 1



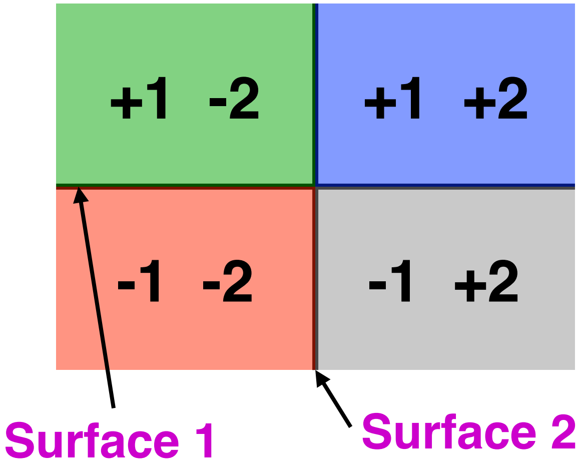
  – If not sure which side is + or -, pick a point & substitute into surface function, F(x,y,z) -- see if result is + or -

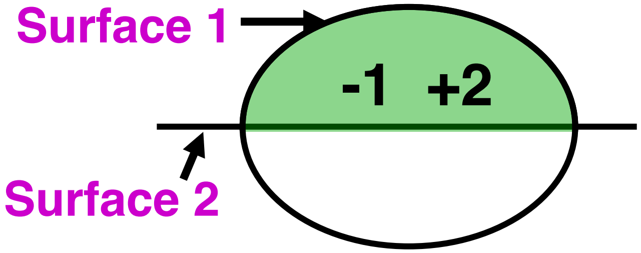
Intersection & Union of Sides

MCNP convention:

Blank signifies intersection

+1 -2 = intersection of
+side of surface 1 and
-side of surface 2

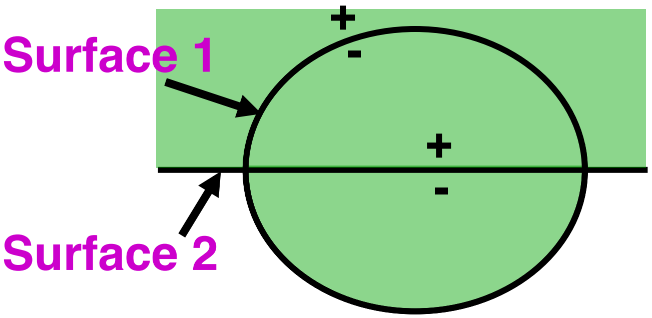




MCNP convention:

Colon signifies union

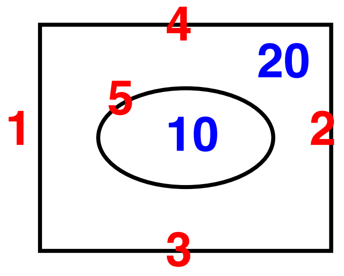
-1 : 2 == union of
-side of surface 1 with
+side of surface 2



Cells

- A cell is defined to be the
  - Intersection of half-spaces defined by a list of signed surface numbers

    Example: cell 10 -5
    cell 20 +1 -2 +3 -4 +5



  - Union of half-spaces defined by signed surface numbers

    Example: cell 43 +1 : -2

  - The complement of another cell (i.e., volume NOT in other cell)

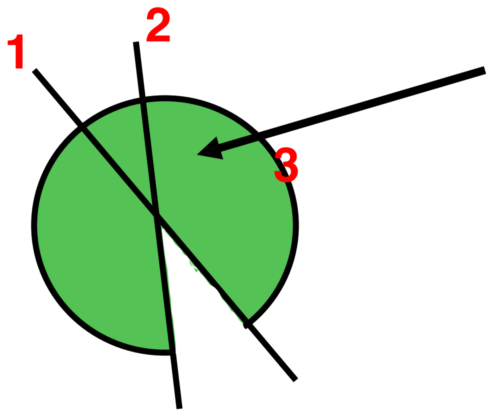
    Example: cell 30 #50

  - A combination of the above

    Example: cell 57 (+1 -2) : 3 #50

Cells

- Cells do not have to be convex, & can be reentrant



(-3 +1) : (-3 -2 -1)

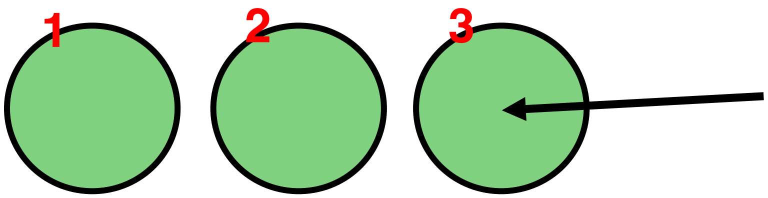
or

(-3 +1) : (-3 -2)

or

-3 (+1 : -2)

- Cells may involve discontiguous regions



Cell 10 -1 : -2 : -3

Cell 20 #10
or 1 2 3

Locate Operations

Given point (x,y,z), determine which cell it is contained in:

```
For(  cell = 1 … n_cells  ) {
        Foreach   surf  in  cell  {
                Evaluate    $S_{surf} = \text{sign}\{ F_{surf}(x,y,z) \}$
                Does   $S_{surf}$   match the sense from the cell definition?
        }
        If all surface-senses for (x,y,z) matched the cell definition,
            then exit & return cell as the result
}
```

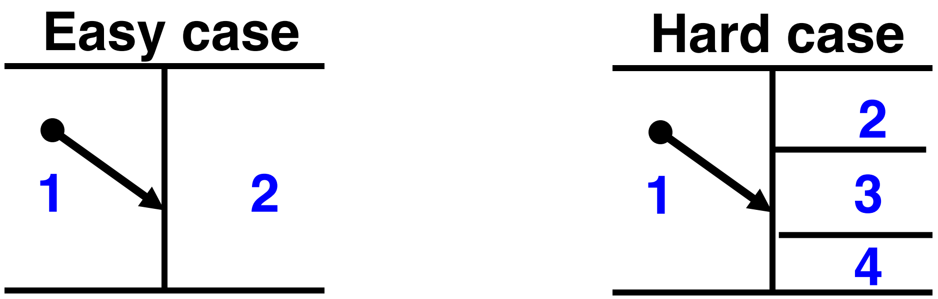
Distance Calculation

**Given point (x,y,z) in cell I,
determine the distance to the cell boundary**

```
d <-- infinity

Foreach surf in cell I {

        If surf is part of the external boundary of cell I {

                Evaluate $d_{surf}$ = smallest positive root of
                            $F_{surf}( x+du, y+dv, z+dw ) = 0$

                $d = \min( d, d_{surf} )$
        }
}
return the value of d
```

Neighbor Search

- When a cell boundary is reached, what's on the other side?



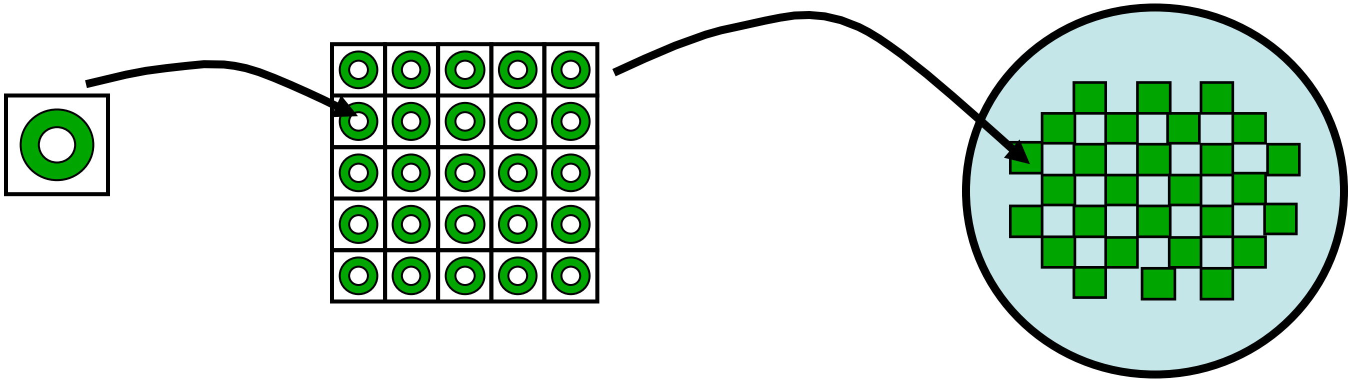
- Most codes build "neighbor lists" during tracking
  - For each bounding surface of cell, remember list of neighbors
  - Initially, neighbor lists are empty
  - Check all cells having surface in common, until one is found satisfying all sense conditions for the particle position
  - Save it
  - Later, check neighbor lists first, only do search if necessary

- Neighbor search is expensive at first, cheap later

- Tracking speeds up as calculation progresses

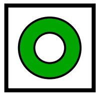
Embedded Geometry - Universes

- In most real-world applications, there is a need for modeling detailed geometry with many repeating units

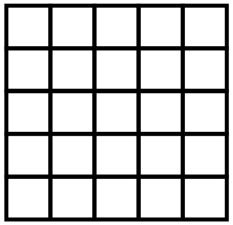


- All production Monte Carlo codes provide capabilities for multiple levels of nested geometry
  - Called "universes" in MCNP
  - A collection of cells may be grouped into a "universe"
  - Universe may be embedded in another cell,
    with the universe 'clipped' by the cell boundaries

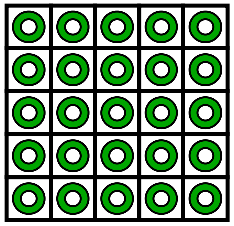
Universes & Lattices



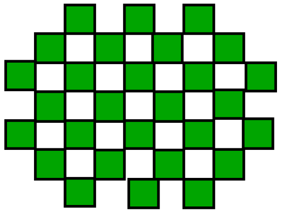
Universe 1 - cells for detailed fuel pin



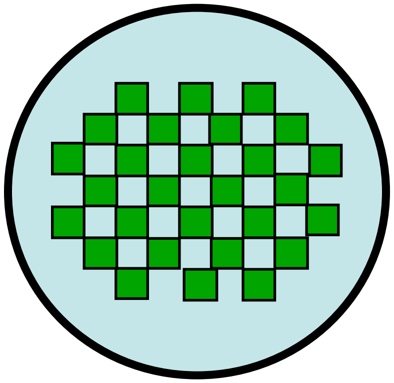
Universe 2 - lattice of cells for fuel assembly



Universe 2, with cells filled by Universe 1



Universe 3 - lattice of cells for reactor



"Real world" - final geometry

Body Geometry

- Some Monte Carlo codes use primitive bodies rather than surfaces for defining cells (e.g., MORSE, KENO, ITS, VIM)

SPH - sphere
BOX - box
RPP - box
RCC - cylinder
WED - wedge

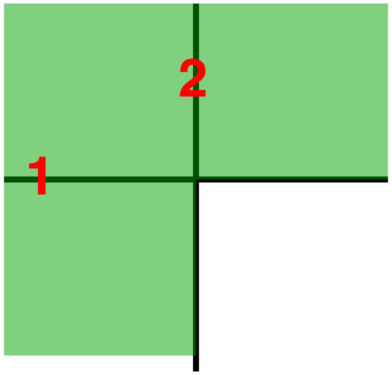
ELL - ellipsoid
REC - right elliptic cylinder
RHP - hexagonal prism
HEX - hexagonal prism
ARB - arbitrary polyhedron
TRC - truncated cone

- Usually called "combinatorial geometry"
  - Invented by MAGI in ~1956, used in SAM-CE & other codes
  - Space inside the body has a negative sense, outside a positive sense
  - Boolean operators AND, OR, NOT may be used to combine bodies (like MCNP's intersection, union, & complement operators)
  - MCNP allows body geometry input (calls them "macrobodies"), but internally converts them to lists of surfaces

Special Topics - Simple Cells

- **Simple cells are those which can be constructed using only intersections, with no union operators**
- **Some Monte Carlo codes require that all cells be simple cells. Union operators are not allowed.**
- **Tracking through simple cells is fast, at the expense of more complex geometry input & setup**
  - **For simple cells, the logic to find the distance to boundary is simple - check the distance to each of the cell surfaces & keep only the smallest positive distance**

Special Topics - Simple Cells



Consider the example at the left.

Using the union operator, the cell is described by: +1 : -2

Without the union operator, separate cells must be defined & then assigned the same material properties:

	+1,	-1 -2	
or	-2,	+1 +2	
or	+1 -2,	+1 +2,	-1 -2

Special Topics -Distance Calculations

- **3D Surface**
  - **$F(x,y,z) = 0$**
    - Linear: ∇F = constant
    - Quadratic: $\nabla F = f(x,y,z)$, $\nabla^2 F$ = constant
- **Distance calculation**
  - **S = directed distance from (x_0,y_0,z_0) along (u,v,w) to $F(x,y,z)=0$**
    = smallest positive root of $F(x_0+su, y_0+sv, z_0+sw) = 0$
  - **General form: $As^2 + 2Bs + C = 0$, $D = B^2 - AC$**
    - 27 combinations of A, B, C >0, =0, <0
    - Only 12 yield valid solutions:

$s = -C/(2B)$	if	(A=0, C<0, B>0)	or	(A=0, C>0, B<0)
$s = (-B-\sqrt{D})/A$	if	(A>0, C>0, B<0, D>0)	or	(A<0, C>0, B>0, D>0)
	or	(A<0, C>0, B<0, D>0)	or	(A<0, C>0, B=0, D>0)
$s = (-B+\sqrt{D})/A$	if	(A>0, C<0, B>0, D>0)	or	(A>0, C<0, B<0, D>0)
	or	(A>0, C<0, B=0, D>0)	or	(A<0, C<0, B>0, D>0)
	or	(A>0, C=0, B<0, D>0)	or	(A<0, C=0, B>0, D>0)
$s = \infty$		otherwise		

Special Topics -Distance Calculations

- **Noting that $C = F(x_0,y_0,z_0)$ = sense at (x_0,y_0,z_0), the valid solutions can be simplified using the known surface sense §:**

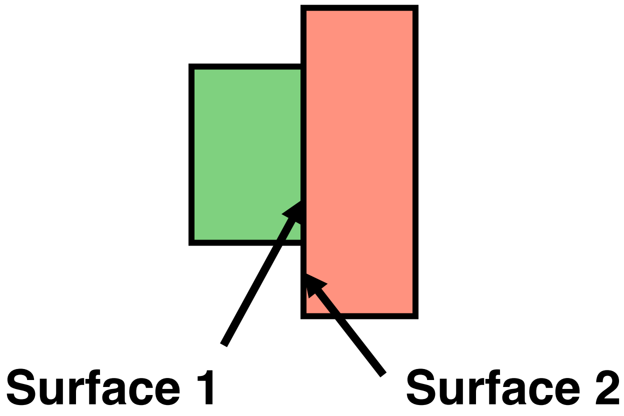
$$
\begin{array}{lll}
s' = -C/(2B) & \text{if} & (A=0,\ D>0) \\
s' = (-B-\sqrt{D})/A & \text{if} & (A\neq 0,\ D>0,\ \S>0) \\
s' = (-B+\sqrt{D})/A & \text{if} & (A\neq 0,\ D>0,\ \S<0) \\
s' = \infty & \text{otherwise} &
\end{array}
$$

And

$$
\begin{array}{ll}
s = s' & \text{if } s'>0 \\
 = \infty & \text{otherwise}
\end{array}
$$

Special Topics - Common Surfaces

- If 2 surfaces coincide, neighbor searches become more complicated & tracking can slow down significantly



- Most MC codes check for coincident surfaces & eliminate one of them (replacing it by the other)

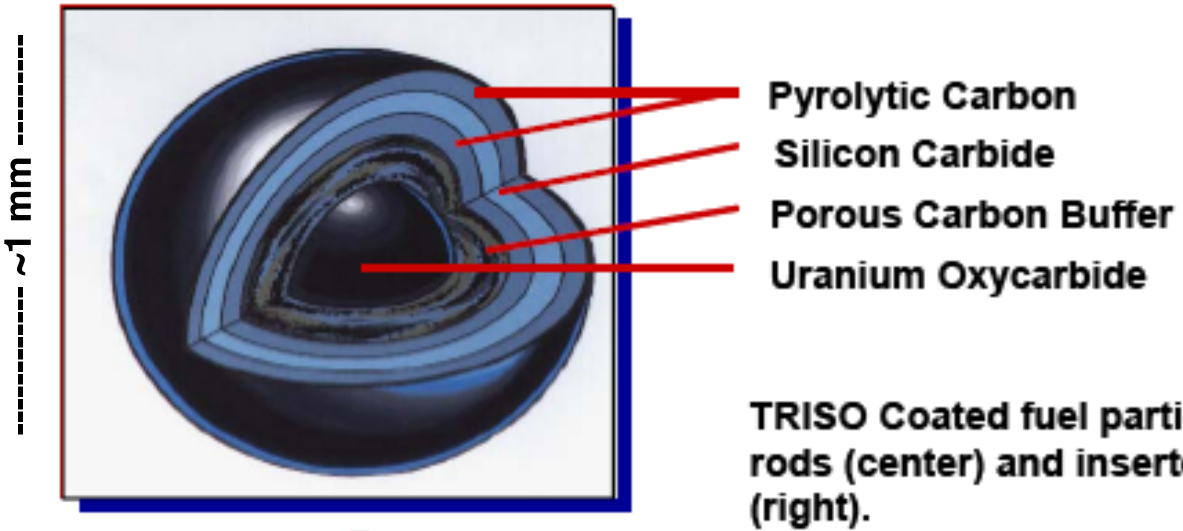
- The tolerance for coincident surfaces usually defaults to a small separation distance (e.g., 1.e-4 cm). For problems with unusual geometry (very small or very large), this may have to be changed in the code or code input.

Stochastic Geometry & HTGR Modeling (optional)

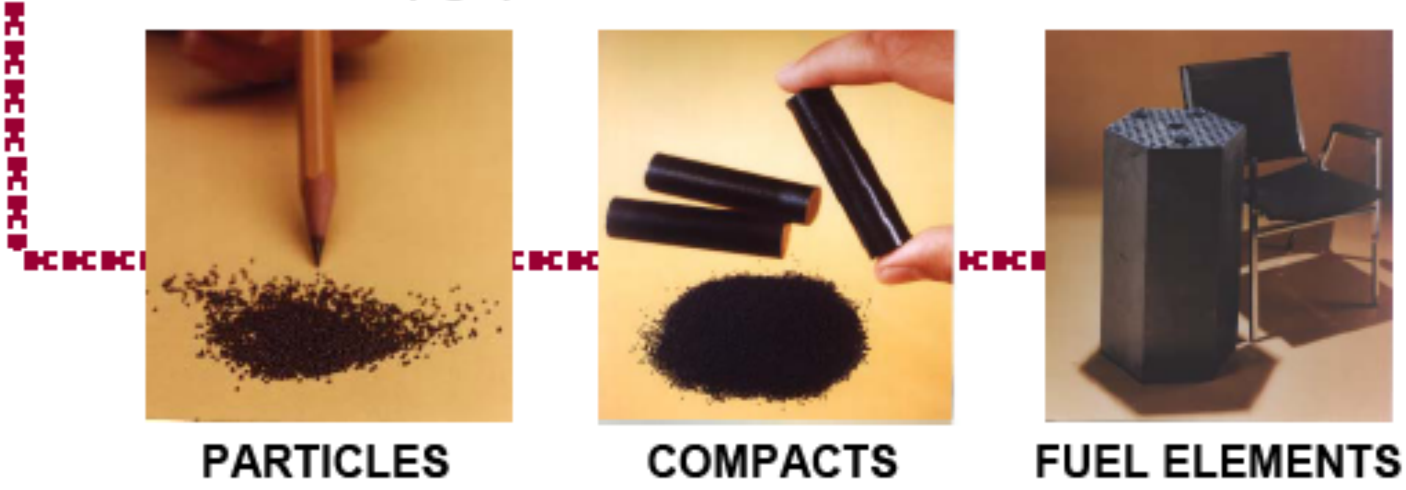
Introduction

- Much interest lately in analyzing HTGRs
  - **Fuel kernels with several layers of coatings**
  - **Very high temperatures**
  - **Contain fission products**
  - **Safety aspects …**
- Double heterogeneity problem
  - **Fuel kernels randomly located within fuel elements**
  - **Fuel elements may be "compacts" or "pebbles" (maybe random)**
  - **Challenging computational problem**
- Monte Carlo codes can faithfully model HTGRs
  - **Full 3D geometry**
  - **Multiple levels of geometry, including embedded lattices**
  - **Random geometry ?????**

Example - Very High Temperature Gas Cooled Reactor



TRISO Coated fuel particles (left) are formed into fuel rods (center) and inserted into graphite fuel elements (right).



P. E. MacDonald, et al., "NGNP Preliminary Point Design – Results of the Initial Neutronics and Thermal-Hydraulic Assessments During FY-03", INEEL/EXT-03-00870 Rev. 1, Idaho National Engineering and Environmental Laboratory (2003).

Example - GT-MHR Modeling

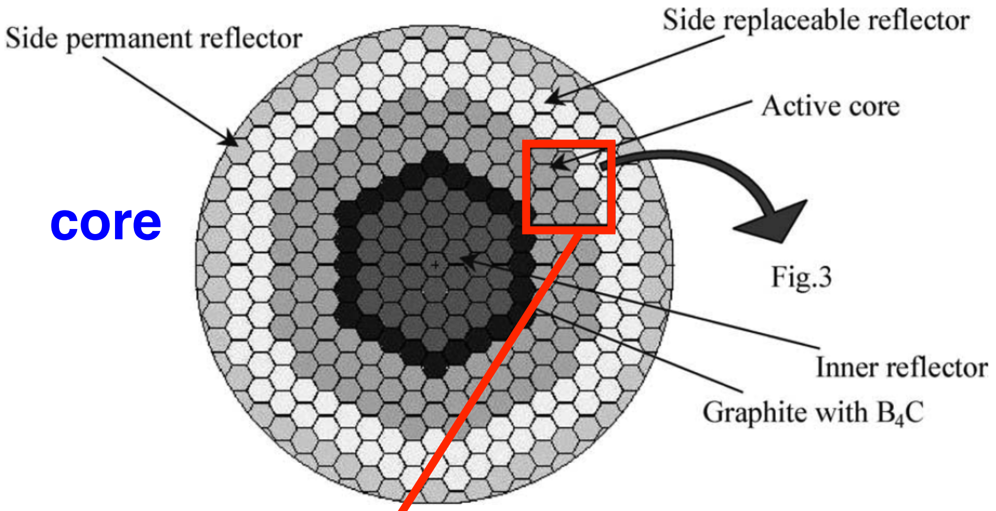


Fig. 2. A cross-section of the GT-MHR homogeneous core with hexagonal structure (HTR1).

Plukiene, R. and Ridikas, D., Modeling of HTGRs with Monte Carlo: from a homogeneous to an exact heterogeneous core with microparticles. Annals of Nuclear Energy 30, 1573-1585 (2003).

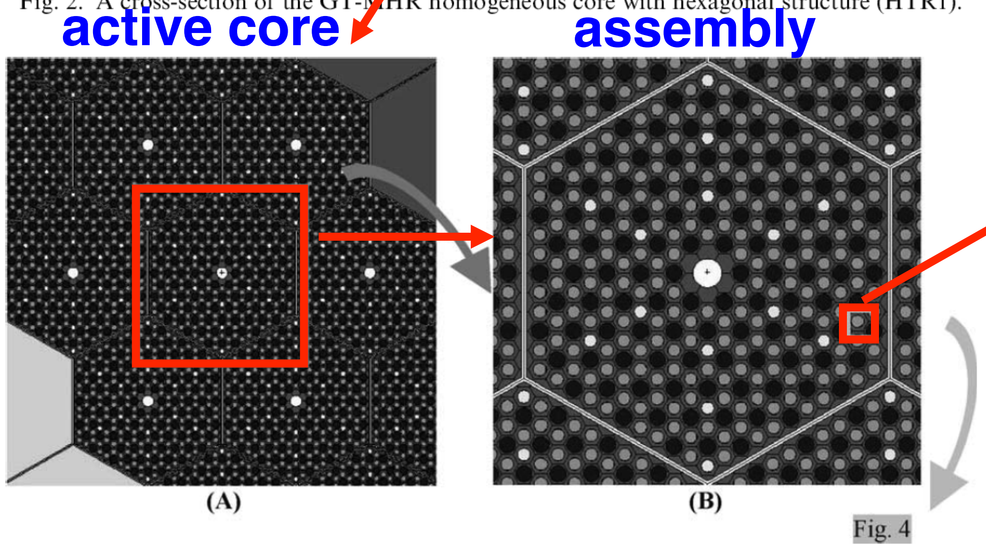


Fig. 3. Fragments of single-heterogeneous GT-MHR (HTR2): (A) an active core structure: three rings of hexagonal fuel columns; (B) magnified view of a separate fuel assembly. Fuel compacts are presented in small grey circles, burnable poison compacts in light grey. Bigger diameter holes stand for He channels, while the rest material represents the graphite matrix.

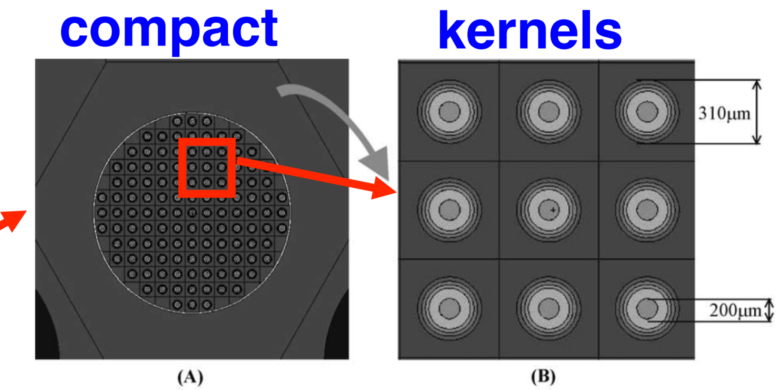


Fig. 4. Fragments of double-heterogeneous GT-MHR (HTR3): (A) fuel element (compact) cross section with coated fuel particles; (B) magnified view of coated fuel particles: spherical kernels of PuO_{2-x} are surrounded by protective coatings made of PyC_{buffer}, PyC I, SiC and PyC II layers correspondingly. The same structure is valid for particles containing burnable poison—natural Er_2O_3.

Example - Pebble Bed Experiments at Proteus Facility

Core

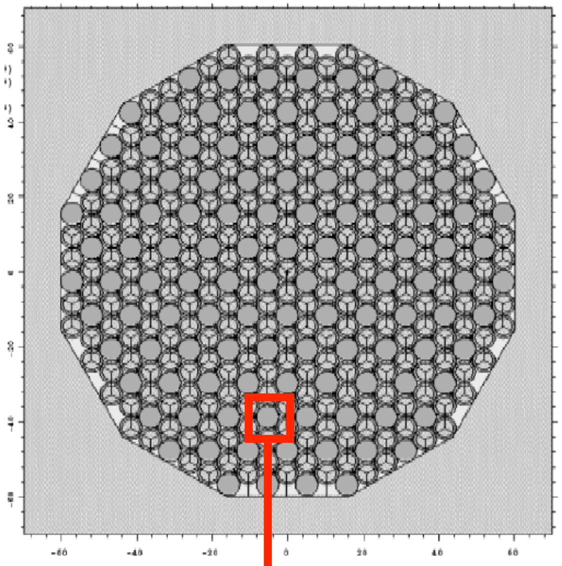


Fig. 3. Cross section of the odd layers of the hcp configurations, case 4 with polyethylene rods. The fi
with the visualization tools of the MCNP program.

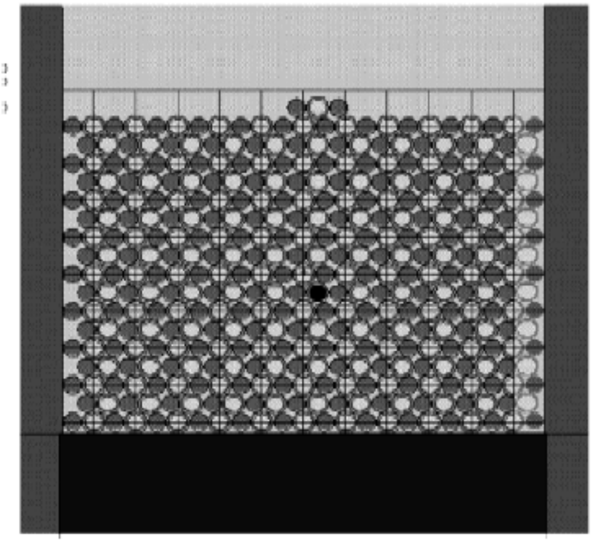


Fig. 5. Case 4, vertical cross section. The black pebble (fuel type) appears magnified in Figs. 6, 7, and 8 to show the heterogeneous details of the fuel pebble.

Difilippo, F.C., Monte Carlo Calculations of Pebble Bed Benchmark Configurations of the PROTEUS Facility. Nucl. Sci. Eng. 143, 240-253 (2003).

Pebbles

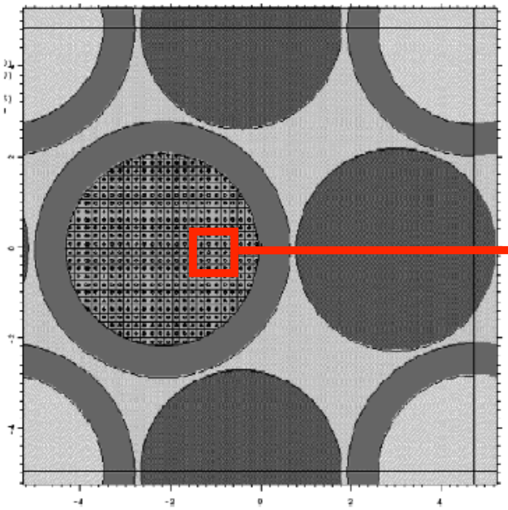


Fig. 6. Magnified fuel pebble of Fig. 5.

Fuel kernel lattice

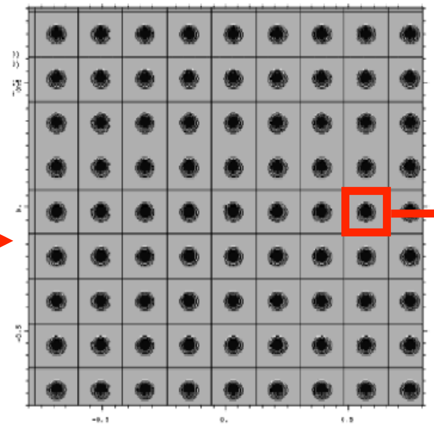


Fig. 7. Details of the cubic lattice of fuel kernels inside the pebble of Fig. 5.

Fuel kernel

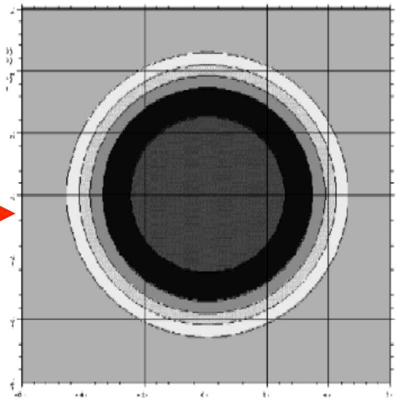


Fig. 8. Fuel kernel with the four coatings at each location of the cubic lattice and inside the fuel region of the pebble shown in Fig. 6.

MCNP Models for HTGRs

- Existing MCNP geometry can handle:
  - **3D description of core**
  - **Fuel compacts or lattice of pebbles**
    - Typically, **hexagonal lattice** with close-packing of spherical pebbles
    - Proteus experiments: ~ 5,000 fuel pebbles
~ 2,500 moderator pebbles
  - **Lattice of fuel kernels within compact or pebble**
    - Typically, **cubic lattice** with kernel at center of lattice element
    - Proteus experiments: ~ 10,000 fuel kernels per pebble
~ 50 M fuel kernels, total
  - **Could introduce random variations in locations of a few thousand cells in MCNP input, but not a few million.**
  - **See papers by: Difilippo, Plukiene et al, Ji-Conlin-Martin-Lee, etc.**

MCNP5 Stochastic Geometry

- **When a neutron enters a new lattice element, a transformation is made to the neutron's position & direction to the local coordinates of the universe embedded in that lattice element. [standard MCNP]**

- Users can flag selected universes as "stochastic" **[new]**
  - **A neutron entering a lattice element containing a stochastic universe undergoes the normal transformations.**
  - **Then, additional random translations are made:**

$$x \leftarrow x + (2\xi_1 - 1) \cdot \delta_x$$

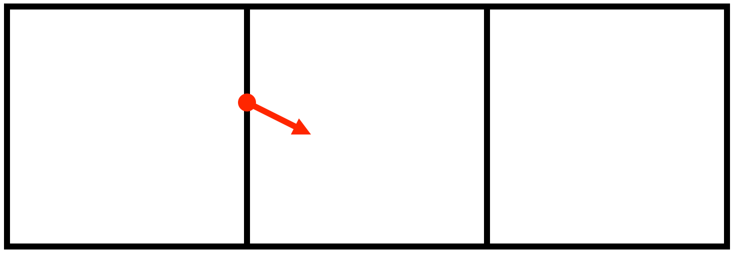
$$y \leftarrow y + (2\xi_2 - 1) \cdot \delta_y$$

$$z \leftarrow z + (2\xi_3 - 1) \cdot \delta_z$$

  - **Then, tracking proceeds normally, with the universe coordinates fixed until the neutron exits that lattice element**

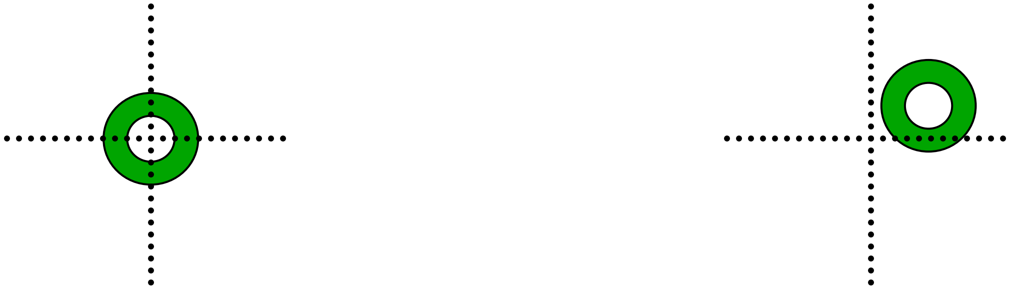
MCNP5 Stochastic Geometry

- **Neutron on lattice edge, about to enter embedded universe**

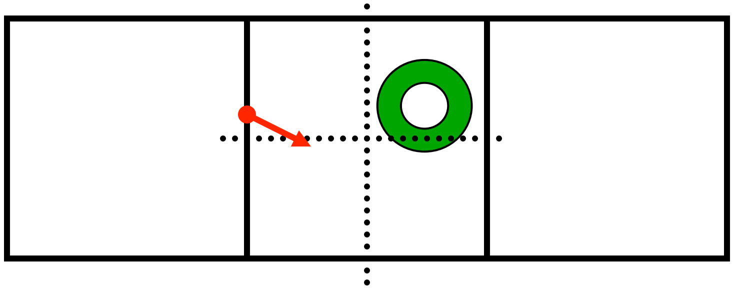


- **Embedded universe,**

before **random translation** after **random translation**



- **Track normally, until neutron exits the lattice element**

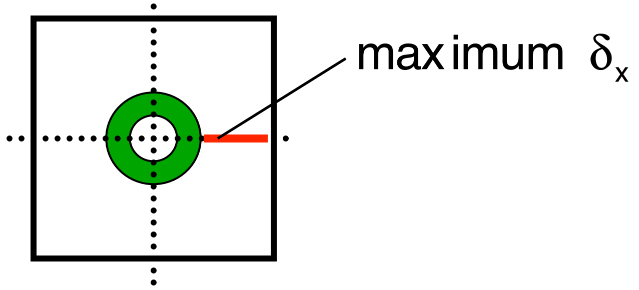


MCNP5 Stochastic Geometry

- On-the-fly random translations of embedded universes in lattice
  - Does not require any extra memory storage
  - Very little extra computing cost - only 3 random numbers for each entry into a stochastic universe

- For K-effective calculations (KCODE problems)
  - If fission occurred within fuel kernel, should have source site in next cycle be at same position within fuel kernel
  - Need to save $\delta_x, \delta_y, \delta_z$ along with neutron coordinates in fission bank
  - On source for next cycle, apply $\delta_x, \delta_y, \delta_z$ after neutron pulled from bank

- **To preserve mass exactly**, rather than on the average stochastically, must choose $\delta_x, \delta_y, \delta_z$ so that fuel kernels are not displaced out of a lattice element



Numerical Results -- HTGR Fuel Kernels

- Infinite array of TRISO fuel kernels in graphite matrix
  - Fuel kernel geometry & composition taken from the NGNP Point Design (MacDonald et al. 2003)

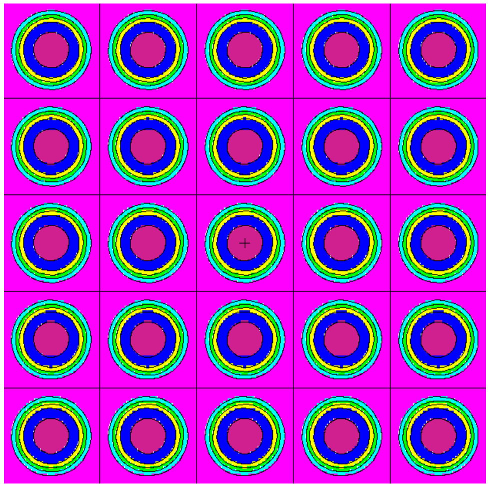
TRISO Fuel Kernel Geometry and Composition

Region #	Name	Outer radius (μ)	Composition	Density (g/cc)
1	Uranium oxycarbide	175	UCO ($UC^{.5}O^{1.5}$)	10.5
2	Porous carbon buffer	275	C	1.0
3	Inner pyrolytic carbon	315	C	1.9
4	Silicon carbide	350	SiC	3.2
5	Outer pyrolytic carbon	390	C	1.9

- Calculations run 4 ways:
  1. Fixed lattice with centered kernels
  2. Fixed lattice with random kernels [MCNP stochastic geometry]
  3. Multiple lattice realizations
  4. Box of randomly place kernels

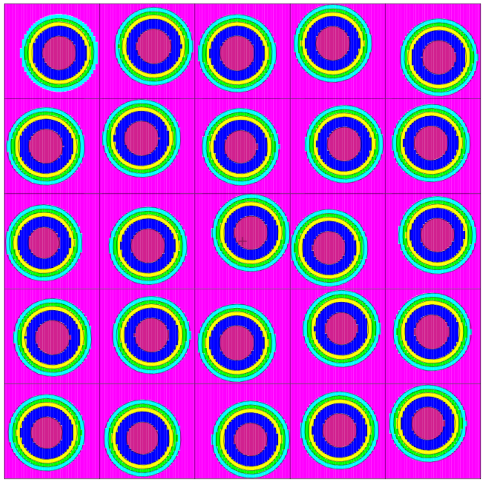
Calculations - Case #1

- Fixed lattice with centered kernels
  - 5x5x5 cubical lattice
  - Lattice edge chosen to preserve the specified packing fraction.
  - Fuel kernels centered within the cubical cells
  - Reflecting boundaries on the outer surfaces
  - Essentially same as Difilipo, Plukiene et al, Ji-Conlin-Martin-Lee
  - No random geometry, standard MCNP5 calculations



Calculations - Case #2

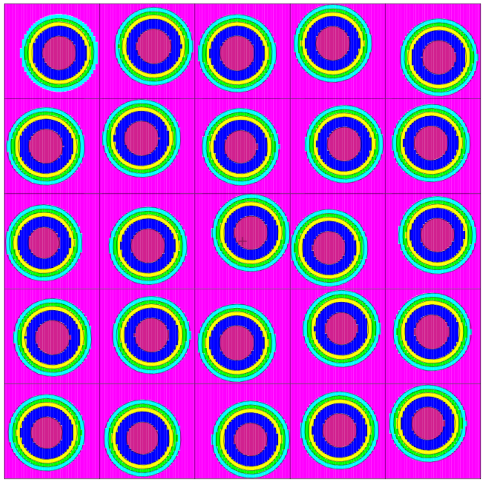
- Fixed lattice with random kernels [MCNP stochastic geometry]
  - 5x5x5 cubical lattice
  - Lattice edge chosen to preserve the specified packing fraction.
  - Fuel kernels randomly placed on-the-fly within the cubical cells
  - Reflecting boundaries on the outer surfaces
  - Uses new MCNP5 stochastic geometry



Fuel kernel displaced randomly within lattice element each time that neutron enters

Calculations - Case #3

- **Multiple lattice realizations**
  - 5x5x5 cubical lattice
  - Lattice edge chosen to preserve the specified packing fraction.
  - Fuel kernels randomly placed in job input within the cubical cells
  - Reflecting boundaries on the outer surfaces
  - Uses standard MCNP5
  - 25 separate calculations, each with different location of kernels in the input files

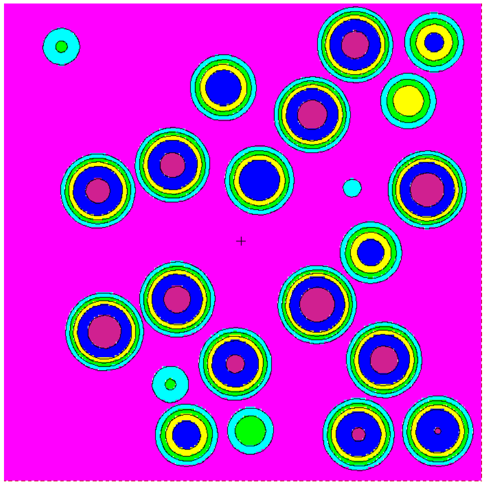


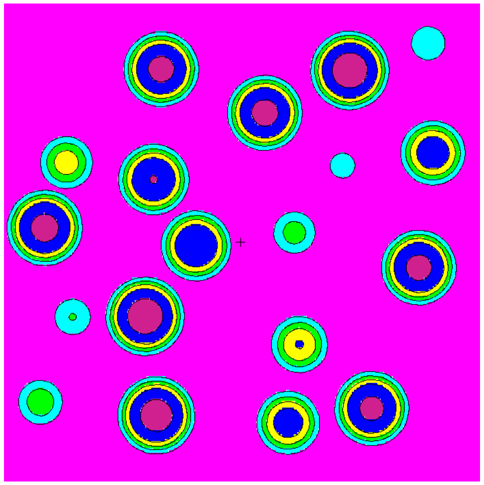
1 realization, fixed lattice with kernel locations chosen randomly in problem input & held constant during each MCNP calculation

Calculations - Case #4

- **Box of randomly placed fuel kernels**
  - Single box with 125 fuel kernels
  - Box size chosen to preserve the specified packing fraction.
  - Fuel kernels randomly placed in job input within the box (using RSA algorithm, Random Sequential Addition)
  - Reflecting boundaries on the outer surfaces
  - Uses standard MCNP5
  - 25 separate calculations, each with different location of kernels in the input files

2 different realizations of "truly random" cases:





Numerical Results

MCNP5 Results for Infinite Lattices of Fuel Kernels

#	Method	K-effective
1	Fixed 5x5x5 lattice with centered spheres	1.1531 ± 0.0004
2	Fixed 5x5x5 lattice with randomly located spheres ("on the fly")	1.1515 ± 0.0004
3	Multiple (25) realizations of 5x5x5 lattice with randomly located spheres	1.1513 ± 0.0004
4	Multiple (25) realizations of randomly packed (RSA) fuel "box"	1.1510 ± 0.0003

Conclusions

- The new stochastic geometry treatment for MCNP5 provides an accurate and effective means of modeling the particle heterogeneity in TRISOL particle fuel
  - Same results as (brute-force) multiple realizations of random geometry input with standard MCNP
  - Negligible difference from "truly random" multiple realizations

- The results indicate that:
  - The neutronic effect of using a fixed lattice is negligible
  - The effect of choosing either a centered spheres or randomly located spheres is also small, at least for the specific fuel geometry that was analyzed during this study

- Future work
  - Examination of finite geometries, including cylindrical fuel compacts, hexagonal fuel blocks, and full core configurations.
  - We will also consider lattices other than simple cubic lattices, such as BCC, FCC, and HCP lattices.

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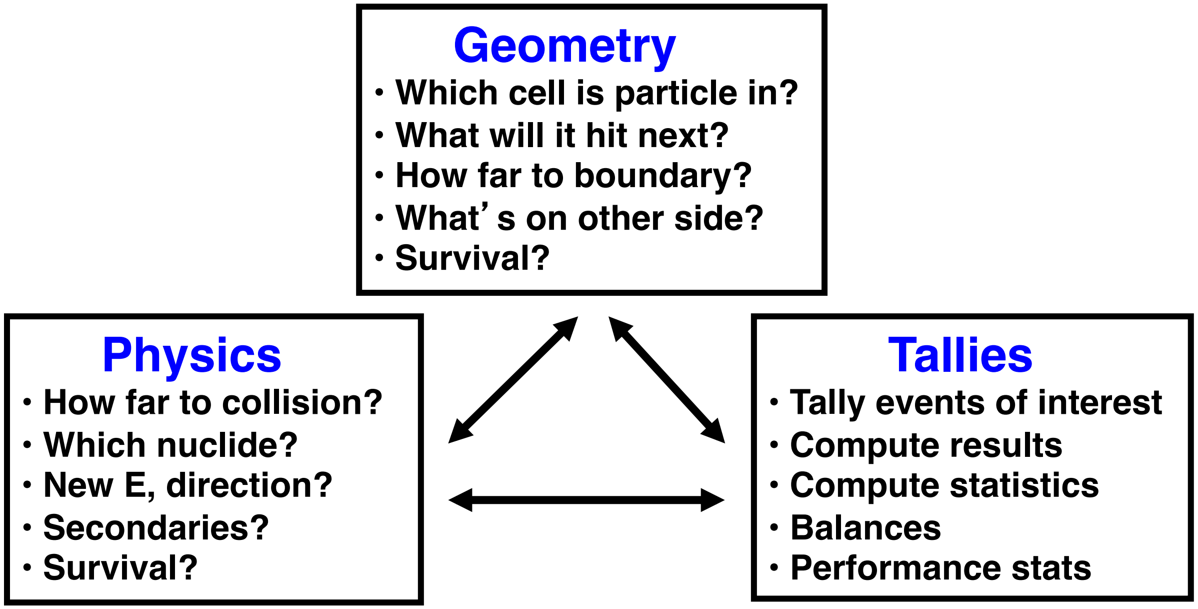
Collision Physics

Monte Carlo Calculations



Geometry

- Which cell is particle in?
- What will it hit next?
- How far to boundary?
- What's on other side?
- Survival?

Physics

- How far to collision?
- Which nuclide?
- New E, direction?
- Secondaries?
- Survival?

Tallies

- Tally events of interest
- Compute results
- Compute statistics
- Balances
- Performance stats

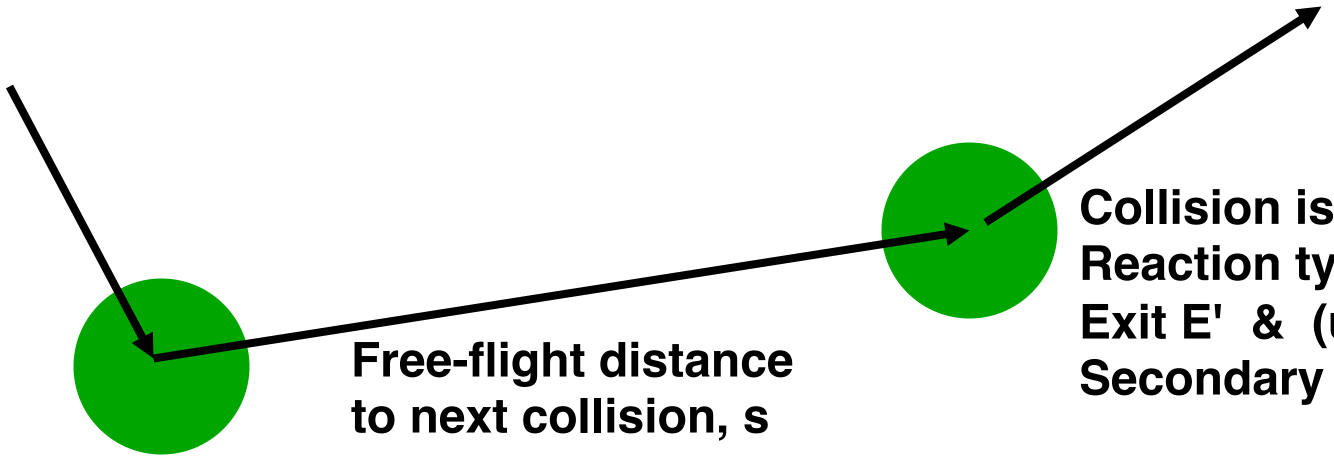
mcnp, rcp, vim, racer, sam-ce, tart, morse, keno, tripoli, mcbend, monk, o5r, recap, andy,…

- **Geometry routines determine the cell & material in that cell**
- **Collision routines model the physical interactions with the material**
  - **Random sampling from PDFs determined by cross-section data**
    - Continuous: flight distance, exit E & direction, …..
    - Discrete: select nuclide, select interaction type, secondaries, …

Monte Carlo Calculations

- After a particle emerges from source or collision, or if the particle is on a cell bounding surface:
  - Randomly sample the free-flight distance to the next interaction
  - If the distance-to-interaction is less than the distance to cell boundary, then move the particle to the interaction point
  - Collision physics at the interaction point:
    - Determine which isotope the interaction is with
    - Determine which reaction type for that isotope
    - Determine the exit energy & direction of the particle
    - Determine if secondary particles were produced
    - Biasing + weight adjustments
    - Tallies of quantities of interest

Collision Physics



Free-flight distance
to next collision, s

Collision isotope,
Reaction type,
Exit E' & (u',v',w'),
Secondary particles

Sampling the Flight Distance

- Given a particle at (x_0,y_0,z_0) with direction (u,v,w) in cell I containing material M, sample the free-flight distance to the next interaction

  – Σ_T = total macroscopic cross-section in material M
  = sum{ $N^k \sigma_T^k$ }, where k = isotopes in material M
  = probability of any interaction per unit distance, units cm^{-1}

  – PDF for flight distance s, where $0 \le s \le \infty$,

  f(s) = {prob interaction p.u.d} · {prob travelling dist s w/o interact}
  $f(s) = \Sigma_T \exp(-\Sigma_T s)$

  – Sampling procedure

  $F(s) = 1 - \exp(-\Sigma_T s)$ ➜ $s = - \ln(\xi) / \Sigma_T$

Selecting the Collision Isotope

- $\Sigma_T = \sum_j N^{(j)} \sigma_T^{(j)}$ where j = isotopes in material M

- **Probability that collision is with isotope k**

$$p_k = \frac{N^{(k)} \sigma_T^{(k)}}{\Sigma_T}$$

- **{ p_k } = set of discrete probabilities for selecting collision isotope**

- **{ P_k } = discrete CDF, P_k = sum{ p_i, i=1,k }, P_0=0**

- **Discrete sampling for collision isotope k**

  table search to determine k such that $P_{k-1} \leq \xi < P_k$

Selecting the Reaction Type

- For collision isotope k,

  $\sigma_T = \sigma_{elastic} + \sigma_{inelastic} + \sigma_{capture} + \sigma_{fission} + \ldots..$

- $p_j = \sigma_j / \sigma_T$ = probability of reaction type j for isotope k

- $\{ p_j \}$ = set of discrete probabilities for selecting reaction type j

- $\{ P_j \}$ = discrete CDF, $P_j = \text{sum}\{ p_i, i=1,j \}$, $P_0=0$

- Discrete sampling for reaction type j

  table search to determine j such that $P_{j-1} \leq \xi < P_j$

Selecting the Reaction Type - Modified

- In many applications, survival biasing is an effective variance reduction technique
  - Survival biasing is also called implicit absorption, nonabsorption weighting, or (loosely) implicit capture
  - $\Sigma_T = \Sigma_{absorption} + \Sigma_{scatter}$ (absorption = disappearance)
  - Probability that particle survives collision = P_{surv} = $\Sigma_{scatter}/\Sigma_T$
  - Probability that particle is absorbed (killed) = $1 - P_{surv}$
- Disallow absorption of particle, & then adjust particle weight to ensure a fair game
  - Tally absorption of $wgt \cdot (1-P_{surv})$
  - Multiply particle weight by P_{surv}
  - When selecting collision isotope: use Σ_S's, not Σ_T's for isotopes
  - When selecting reaction type: don't include σ_A

Sampling Exit Energy & Direction

- Given a collision isotope k & reaction type j, the random sampling techniques used to determine the exit energy and direction, E' and (u',v',w'), depend on
  - Conservation of energy & momentum
  - Scattering laws - either equations or tabulated data

- Examples
  - Isotropic scattering in lab system [example on next slides]
  - Multigroup scattering [example on next slides]
  - Elastic scattering, target-at-rest [example on next slides]
  - Inelastic scattering, MCNP
  - Other collision physics, MCNP

Isotropic Scatter in Lab System

- Elastic scattering from infinite-mass target nucleus
  - No change in energy:

    $$E' = E$$

  - Sample direction from isotropic scattering PDF, $f(u',v',w') = 1 / 4\pi$

    $\varphi = 2\pi\ \xi_1$ ← uniform azimuthal

    $u' = 2\xi_2 - 1$ ← isotropic, uniform in u'

    $v' = \mathrm{sqrt}(1-u'^2)\cos(\varphi)$

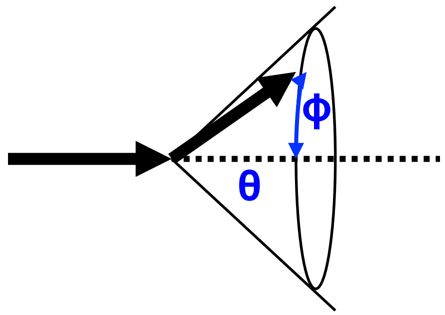
    $w' = \mathrm{sqrt}(1-u'^2)\sin(\varphi)$

Isotropic Scatter – Sampling the Scattering Angle

- **Consider isotropic scattering**
  - **Any direction is equally likely**
  - **Interpret as:**

    "pick a random point on a unit sphere, then get direction-cosines"

$\mu = \cos\theta$



- **Rejection method for scatter angle sampling**
  - **Pick x,y,z randomly in unit cube**
  - **If x,y,z outside unit sphere, reject and try again**
  - **If x,y,z inside unit sphere, scale so that $x^2+y^2+z^2 = 1$**
  - **Get direction-cosines of angles, u,v,w**

- **Direct method for scatter angle sampling**

$$f(\hat{\Omega}) = \frac{1}{4\pi}, \qquad \frac{d\hat{\Omega}}{4\pi} = \frac{\sin\theta \cdot d\theta}{2} \cdot \frac{d\phi}{2\pi}$$

$$f(\theta,\phi) = \frac{\sin\theta \cdot d\theta}{2} \cdot \frac{d\phi}{2\pi}, \qquad 0 \le \theta \le \pi, \quad 0 \le \phi \le 2\pi$$

$$f(\theta) = \int_0^{2\pi} f(\theta,\phi)\,d\phi = \frac{\sin\theta}{2}$$

$$\mu = \cos\theta, \qquad d\mu = -\sin\theta \cdot d\theta, \qquad -1 \le \mu \le +1$$

$$f(\mu) = f(\theta)\left|\frac{d\theta}{d\mu}\right| = \frac{\sin\theta}{2} \cdot \frac{1}{\sin\theta} = \frac{1}{2}$$

➜ **μ is distributed uniformly in [-1,1]**

➜ **ϕ is distributed uniformly in [0,2π]**

$$\mu \leftarrow 2\xi_1 - 1$$

$$\phi \leftarrow \xi_2 \; 2\pi$$

Multigroup Scattering

- **Multigroup approach**
  - **Divide energy range into intervals (groups)**
  - **Use average cross-sections for each group:** $\Sigma_{Tg}, \Sigma_{Sg}, \Sigma_{Ag}, \nu\Sigma_{Fg}$
  - **Use discrete transfer matrix for group-to-group scatter,**

    $\Sigma_{gg'}$ **= cross-section for scatter from group g to group g'**

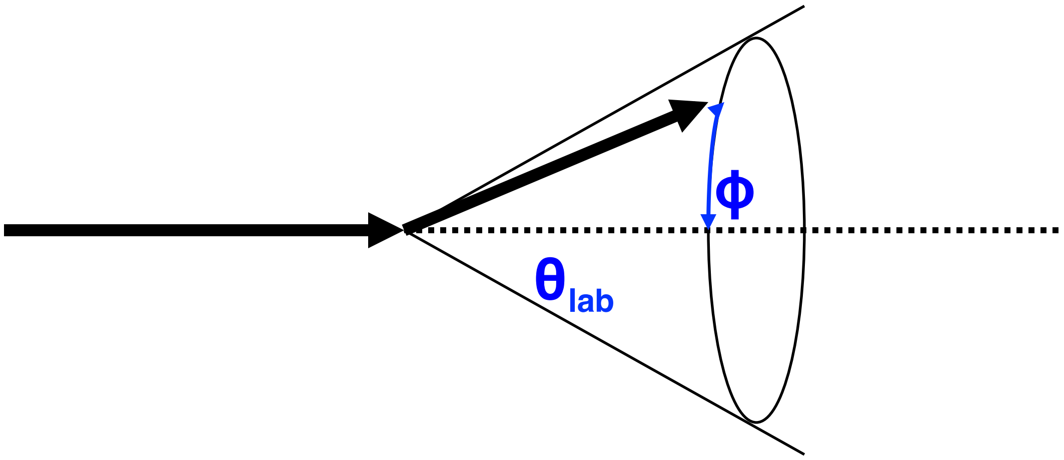
$$\Sigma_{Sg} = \sum_{k=1}^{G} \Sigma_{g\to k}$$

- **Multigroup scattering**
  - **For particle with energy E, determine initial energy group g**
  - **Select exit energy group g' by discrete sampling from** $\Sigma_{gg'}$

$$p_{g'} = \frac{\Sigma_{g\to g'}}{\Sigma_{Sg}}$$

  - **Sample exit energy uniformly within bound of group g'**
  - **Direction**
    - For P_0 scattering - use procedure for isotropic lab scatter
    - For P_1 scattering - sample mu from linear PDF, then select new direction (see next section on elastic scatter)

Elastic Scattering, Target-at-rest



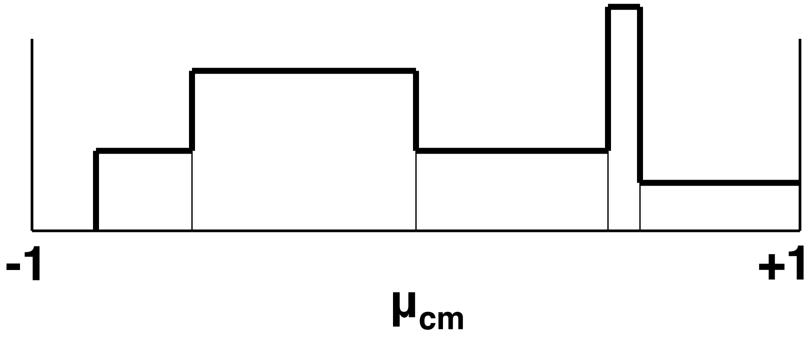
$\mu_{cm} = \cos\,\theta_{cm}$
$\mu_{lab} = \cos\,\theta_{lab}$

θ = scattering angle,
cm or lab

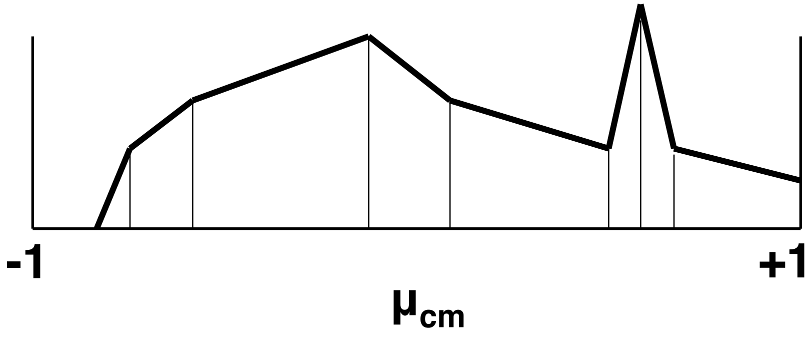
- Sample μ_{cm} from tabulated PDF data, $f(\mu_{cm})$
- Use kinematics to get E'_{lab} & μ_{lab}
- Sample azimuthal angle φ uniformly on $(0,2\pi)$
- Rotate particle direction using μ_{lab} & φ

Sampling the Scattering Direction-cosine, μ_{cm}

- Typical representations for $f(\mu_{cm})$
  - Histogram or Equiprobable Histogram PDF



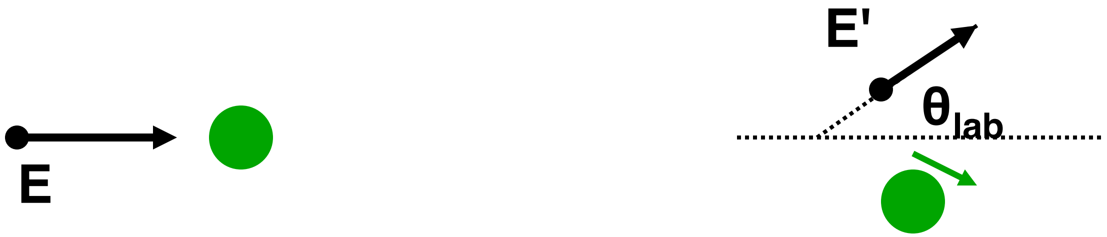
  - Piecewise linear PDF



Elastic Scatter - E' & μ_{lab}

- **Target-at-rest elastic scatter in lab system – kinematics**

  (from conservation of energy & momentum)



$\mu_{lab} = \cos\theta_{lab}$

$$E' = E \bullet \frac{A^2 + 2A\mu_{cm} + 1}{(A+1)^2}$$

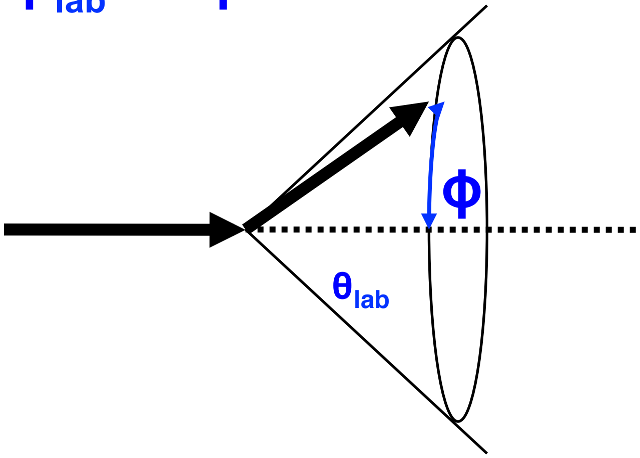
$$\mu_{lab} = \frac{1 + A\mu_{cm}}{\sqrt{A^2 + 2A\mu_{cm} + 1}}$$

Where A = (mass target)/(mass particle)

Exit Direction

- Rotation from (u,v,w) to (u',v',w') using μ_{lab} & φ

$\mu = \mu_{lab}$



$$\phi = 2\pi\xi$$

$$u' = \mu u + \frac{\sqrt{1-\mu^2}(uw\cos\phi - v\sin\phi)}{\sqrt{1-w^2}}$$

$$v' = \mu v + \frac{\sqrt{1-\mu^2}(vw\cos\phi + u\sin\phi)}{\sqrt{1-w^2}}$$

$$w' = \mu w - \sqrt{1-\mu^2}\sqrt{1-w^2}\cos\phi$$

If μ close to 1, special coding may be used to avoid roundoff

Inelastic Scattering - MCNP

– Law 1	ENDF law 1 - Equiprobable energy bins
– Law 2	Discrete photon energies
– Law 3	ENDF law 3 - Inelastic scatter from nuclear levels
– Law 4	ENDF law 4 - Tabular distribution
– Law 5	ENDF law 5 - General evaporation spectrum
– Law 7	ENDF law 7 - Simple Maxwell fission spectrum
– Law 9	ENDF law 9 - Evaporation spectrum
– Law 11	ENDF law 11 - Energy dependent Watt spectrum
– Law 22	UK law 2 - Tabular linear functions of incident energy out
– Law 24	UK law 6 - Equiprobable energy multipliers
– Law 44	ENDF law 1, lang 2, Kalbach-87 correlated energy-angle scatter
– Law 61	ENDF law 11, lang 0,12, or 14 - correlated energy-angle scatter
– Law 66	ENDF law 6 - N-body phase space distribution
– Law 67	ENDF law 7 - correlated energy-angle scatter

Other Collision Physics - MCNP

- **Emission from fission**
- **Delayed neutron emission**
- **S(α,β) scattering for thermal neutrons**
- **Free-gas scattering for neutrons**
- **Probability tables for the unresolved resonance energy range for neutrons**

- **Photoelectric effect**
- **Pair production**
- **Compton scattering (incoherent)**
- **Thomson scattering (coherent)**
- **Fluorescent emission**

- **Photonuclear reactions**

- **Electron interactions - condensed history approach**
  - Stopping power, straggling, angular deflections
  - Bremsstrahlung
  - K-shell impact ionization & Auger transitions
  - Knock-on electrons

Secondary Particle Creation

- **Consider a collision which results in fission**

  wgt • $\nu\Sigma_F/\Sigma_T$ = expected number of fission neutrons produced per collision

- **To sample the number of neutrons produced in the collision**

  – Let r = wgt • $\nu\Sigma_F/\Sigma_T$
  $n = \text{int}[\ r\ ]$

  – Then, Produce n fission neutrons with probability 1
  and an additional fission neutron with probability r-n

  – Example: wgt • $\nu\Sigma_F/\Sigma_T = 1.75$

  If $\xi < .75$, produce 2 neutrons, otherwise produce 1

  or

  Produce $\text{int}[\ 1.75 + \xi\ ]$ neutrons

Alternative Schemes for Flights/Collisions

- **Conventional scheme**
  - Particle weight constant during flight
  - Use Σ_T to determine distance-to-collision, $s = -\ln\xi / \Sigma_T$
  - Change weight only on collisions
  - For pathlength absorption estimator, tally $wgt \cdot s \cdot \Sigma_A$
  - Most common scheme for reactors & shielding applications

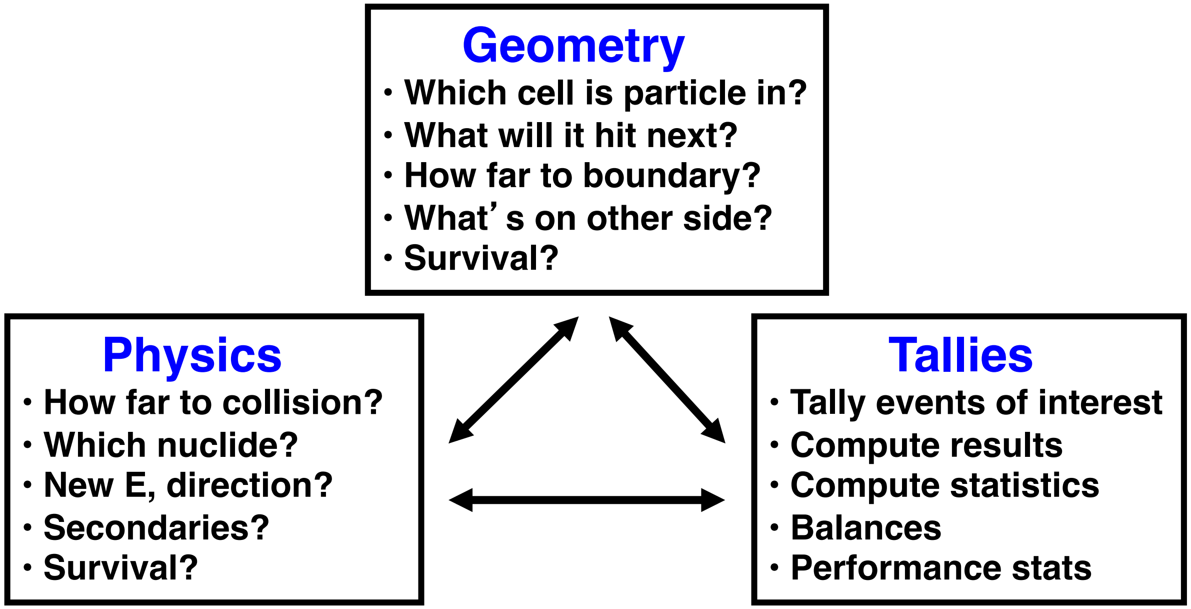
- **Continuous absorption**
  - Particle weight decreases continuously during flight, due to absorption

$$wgt(s) = wgt_0 \cdot e^{-\Sigma_A s}$$

  - Use Σ_S to determine distance-to-scattering, $s = -\ln\xi / \Sigma_s$
  - For pathlength absorption estimator, tally $wgt_0 \cdot (1 - e^{-\Sigma_A s})$
  - No absorption in collision
  - Typical use in astrophysics (Implicit Monte Carlo codes)

Tallies
&
Statistics

Monte Carlo Calculations



Geometry

- Which cell is particle in?
- What will it hit next?
- How far to boundary?
- What’ s on other side?
- Survival?

Physics

- How far to collision?
- Which nuclide?
- New E, direction?
- Secondaries?
- Survival?

Tallies

- Tally events of interest
- Compute results
- Compute statistics
- Balances
- Performance stats

mcnp, rcp, vim, racer, sam-ce, tart, morse, keno, tripoli, mcbend, monk, o5r, recap, andy,…..

- During a history, tally the events of interest
- Upon completing a history, accumulate total scores & squares
- After completing all histories, compute mean scores & standard deviations

Monte Carlo Estimates of Integrals

Given a function R(x), where x is a random variable with PDF f(x),

– Expected value of R(x) is

$$\bar{R} = \int R(x)\, f(x)\, dx$$

– Variance of R(x) is

$$\sigma^2 = \int R^2(x)\, f(x)\, dx - \mu^2$$

Monte Carlo method for estimating $\bar{R}$:

make N random samples $\hat{x}_j$ from f(x)

– Then

$$\bar{R} \approx \frac{1}{N} \sum_{j=1}^{N} R(\hat{x}_j)$$

– Central Limit Theorem states that for large N, the PDF of $\bar{R}$ approaches a Gaussian distribution

– That is, if the Monte Carlo problem is repeated, $\bar{R}$ will be normally distributed

Laws of Large Numbers

Let $x_1, x_2, \ldots, x_N$ be a sequence of independent, identically distributed random variables each with a finite mean $E[x_j] = \mu$ and let

$$\bar{x}_N = \frac{1}{N} \sum_{j=1}^{N} x_j$$

- Weak Law of Large Numbers

  For any $\varepsilon > 0$

$$\lim_{N \to \infty} P(|\bar{x}_N - \mu| > \varepsilon) = 0$$

Tells how a sequence of probabilities converges

- Strong Law of Large Numbers

$$P\left(\lim_{N \to \infty} |\bar{x}_N - \mu| > \varepsilon \right) = 0$$

Tells how the sequence of IID random variables behaves in the limit

Central Limit Theorem

- **Central Limit Theorem**

$$\lim_{N\to\infty} \text{Prob}\left\{ \mu - a\frac{\sigma}{\sqrt{N}} \le \bar{x} \le \mu + b\frac{\sigma}{\sqrt{N}} \right\} = \frac{1}{\sqrt{2\pi}} \int_{-a}^{b} e^{-t^2} dt$$

± 1 σ:

$$\text{Prob}\left\{ \mu - \frac{\sigma}{\sqrt{N}} \le \bar{x} \le \mu + \frac{\sigma}{\sqrt{N}} \right\} = 68\%$$

Note: 32% of the time, $\bar{x}$ should be outside range $\mu \pm \frac{\sigma}{\sqrt{N}}$

± 2 σ:

$$\text{Prob}\left\{ \mu - \frac{2\sigma}{\sqrt{N}} \le \bar{x} \le \mu + \frac{2\sigma}{\sqrt{N}} \right\} = 95\%$$

Note: 5% of the time, $\bar{x}$ should be outside range $\mu \pm \frac{2\sigma}{\sqrt{N}}$

Tallies & Statistics

- **For a given history, tally events of interest**
  - **Example - surface crossings**
    - For each particle crossing surface A, accumulate the weight each time a particle crosses that surface
    - A particular particle may cross the surface more than once
    - Progeny of that particle (e.g., another particle created by splitting) may also cross that surface one or more times

- **When the history is complete, add the score & score^2 to accumulators for the problem**

$$S1_{\text{problem}} = S1_{\text{problem}} + (S_{\text{history}})$$
$$S2_{\text{problem}} = S2_{\text{problem}} + (S_{\text{history}})^2$$

- **When all N histories are complete, compute final mean score & standard deviation**

$$\text{mean score} = \frac{1}{N} \bullet S1$$

$$\text{std dev of mean} = \sqrt{\frac{1}{N-1}\left[\frac{S2}{N} - \left(\frac{S1}{N}\right)^2\right]}$$

Variance of the Population vs. Mean

- Given a set of random samples, $x_1, x_2, \ldots, x_N,$
  - Mean $$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j$$
  - Population variance [what you normally see in statistics textbooks] $$\sigma^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \left(\frac{1}{N}\sum_{j=1}^{N} x_j\right)^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2$$
  - Variance of the mean [what you normally find in MC codes] $$\sigma_{\bar{x}}^2 = \frac{\sigma^2}{N} = \frac{1}{N}\cdot\left(\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2\right)$$ $$\sigma_{\bar{x}} \sim \frac{1}{\sqrt{N}}$$

Tally Bins

- Tallies can be made for selected events & portions of phase space:
  - Range of energies, E_1 - E_2
  - Range of particle times, t_1 - t_2
  - Specified cells
  - Specified surfaces
  - Specified range of $n \cdot \Omega$ for surface crossings
  - Specified reaction cross-sections Σ_x
  - Secondary particle production
  - Energy deposited in cell
  - Conditional events, e.g., absorption in cell B due to source in cell A
  - Energy of neutrons causing fission
  - Scattering from energy range E_1-E_2 to range E_3-E_4
  - Etc.

Flux & Current

- **Angular flux** $\Psi(\mathbf{r},\mathbf{E},\Omega)$

- **Flux** $\phi(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{4\pi} d\Omega\, \Psi(\mathbf{r},\mathbf{E},\Omega)$

  – Scalar quantity

  – Total distance traveled by all particles in a cm^3 per second

  – Units: distance / cm^3-sec = 1 / cm^2-sec

- **Current**

  – Number of particles crossing surface per second per unit area

  – Units: 1 / cm^2-sec

  – Partial current: in + or - direction only, J^+ or J^-

  – Net current = $J = J^+ - J^-$

$$J(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{4\pi} d\Omega\, \vec{n}\bullet\Omega\, \Psi(\mathbf{r},\mathbf{E},\Omega)$$

$$J^+(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{\vec{n}\bullet\Omega>0} d\Omega\, \vec{n}\bullet\Omega\, \Psi(\mathbf{r},\mathbf{E},\Omega) \qquad J^-(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{\vec{n}\bullet\Omega<0} d\Omega\, \vec{n}\bullet\Omega\, \Psi(\mathbf{r},\mathbf{E},\Omega)$$

Reaction Rates

- For a particular reaction "x"

$$R_x(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{4\pi} d\Omega\, \Psi(\mathbf{r},E,\Omega)\, \Sigma_x(\mathbf{r},E)$$

  – Reactions per cm^3 per sec

- Collision density

$$C(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{4\pi} d\Omega\, \Psi(\mathbf{r},E,\Omega)\, \Sigma_T(\mathbf{r},E)$$

- Energy deposition (average per collision)

$$E_{deposited}(\mathbf{r}) = \int_{E_1}^{E_2} dE \int_{4\pi} d\Omega\, \Psi(\mathbf{r},E,\Omega)\, \Sigma_T(\mathbf{r},E)\, K(\mathbf{r},E)$$

where $K(\mathbf{r},E) = \text{average E deposited per collision}$

Analog vs. Weighted Monte Carlo

- **Analog Monte Carlo**
  - Faithful simulation of particle histories
  - No alteration of PDFs (I.e., no biasing or variance reduction)
  - At collision, particle is killed if absorption occurs
  - Particle is born with weight = 1.0
  - Weight unchanged throughout history until particle is killed
  - Score 1.0 when tallying events of interest

- **Weighted Monte Carlo (non-analog)**
  - Alter the PDFs to favor events of interest
  - Particle is born with weight = 1.0
  - Weight is altered if biased PDF is used
  - Typically, particle always survives collision & weight is reduced by P_{surv}
  - Weight can also be changed by Russian roulette/splitting & other variance reduction techniques
  - Score wgt when tallying events of interest

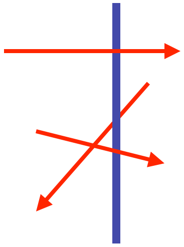
Tally Types

- Current tallies
  - Surface crossing estimator
- Flux tallies
  - Pathlength estimator
  - Collision estimator
  - Surface crossing estimator
  - Next event estimator (point detector)
- Reaction rate tallies
  - Any of the above flux estimators times a cross-section
- Energy deposition tallies
  - Any of the above flux estimators times Σ_T times energy deposited per collision

Basic Tallies

Current across surface

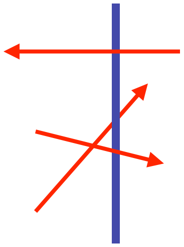
$$J=\frac{1}{W}\sum_{\substack{\text{all flights}\\ \text{crossing surface}}} wgt$$



W = total source weight

Flux on surface

$$\phi=\frac{1}{A\cdot W}\sum_{\substack{\text{all flights}\\ \text{crossing surface}}}\frac{\text{wgt}}{|\mu|}$$



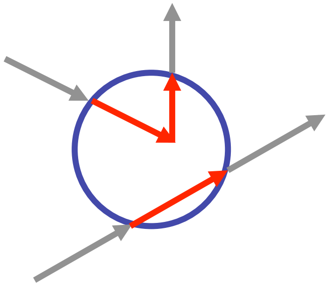
A = surface area

W = total source weight

μ = Ω • [surface normal]

Flux in a cell

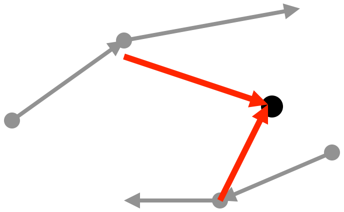
$$\phi=\frac{1}{V\cdot W}\sum_{\substack{\text{all flights}\\ \text{in cell}}}\text{wgt}\bullet\text{dist}$$



V = cell volume

W = total source weight

Flux at a point



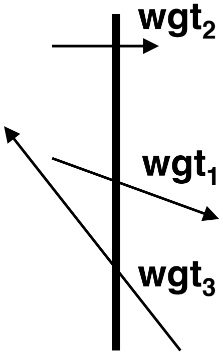
$$\phi=\frac{1}{W}\sum_{\substack{\text{all}\\ \text{collisions}}}\text{wgt}\cdot\frac{p(\mu)e^{-\Sigma_T R}}{2\pi R^2}$$

Current Tallies

- For each particle crossing surface, tally the particle weight

- Divide by total starting weight & surface area to get current

$$J = \frac{1}{W\,A} \sum_{\substack{\text{all}\\\text{particles}\\\text{crossing}\\\text{surface}}} wgt_j$$



W = total starting weight

A = surface area

- Typically, keep separate tally for outward partial current for each surface of a cell

- Can get net current by combining partial currents

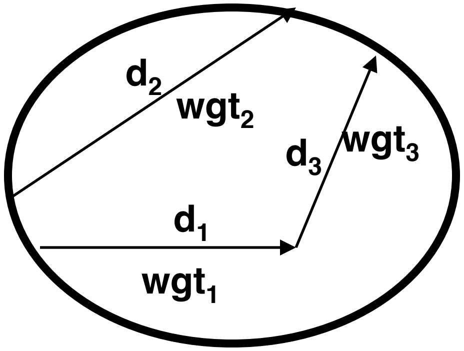
Flux Tally - Pathlength

- For each particle flight within a cell, tally (pathlength*weight)

- Divide by cell volume & total starting weight to get flux estimate

$$\phi = \frac{1}{W\,V} \bullet \sum_{\substack{\text{all}\\ \text{particle}\\ \text{flights}\\ \text{in cell}}} d_j \bullet wgt_j$$

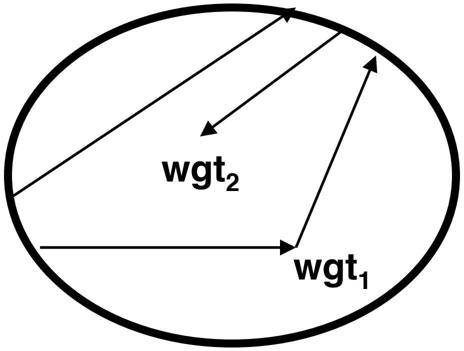
W = total starting weight
V = cell volume



Flux Tally - Collisions

- Since $(\Sigma_T \varphi)$ is collision rate, for each collision, tally (wgt/Σ_T) to estimate flux
- Divide by total starting weight & cell volume

$$\phi = \frac{1}{W\,V} \bullet \sum_{\substack{\text{all} \\ \text{collisions} \\ \text{in cell}}} \frac{wgt_j}{\Sigma_T(E_j)}$$



wgt_j = weight of particle entering collision

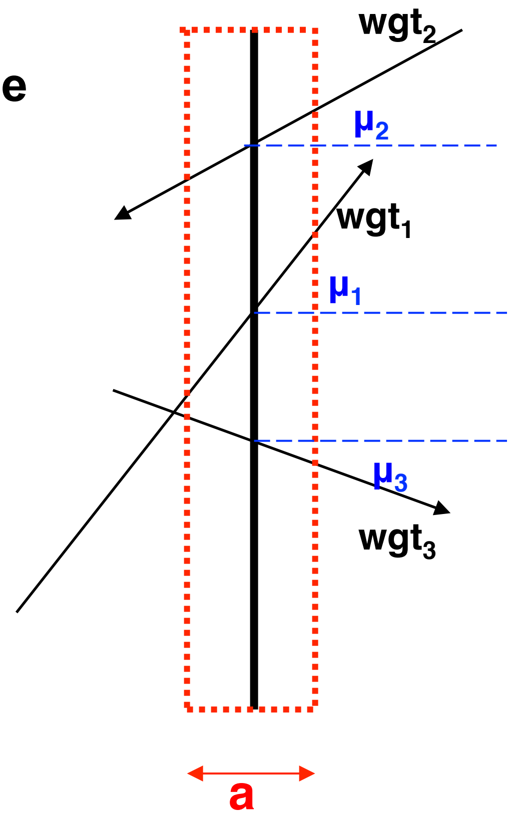
W = total starting weight
V = cell volume

Flux Tally - Surface Crossing

- Consider particles crossing a surface
  - Put a "box" of thickness a around the surface
  - Pathlength estimate of flux in the box

$$\phi = \frac{1}{W\,aA} \bullet \sum_{\substack{\text{all}\\\text{particles}\\\text{crossing}\\\text{surface}}} \text{wgt}_j \bullet \frac{a}{|\mu_j|}$$

$$\text{where} \quad \mu_j = \cos\theta_j$$



  - Note that a cancels out
  - Take the limit as a→0
- Surface crossing estimate of flux

$$\phi = \frac{1}{W\,A} \bullet \sum_{\substack{\text{all}\\\text{particles}\\\text{crossing}\\\text{surface}}} \frac{\text{wgt}_j}{|\mu_j|} \qquad \text{where} \quad \mu_j = \Omega_j \bullet \vec{S}$$

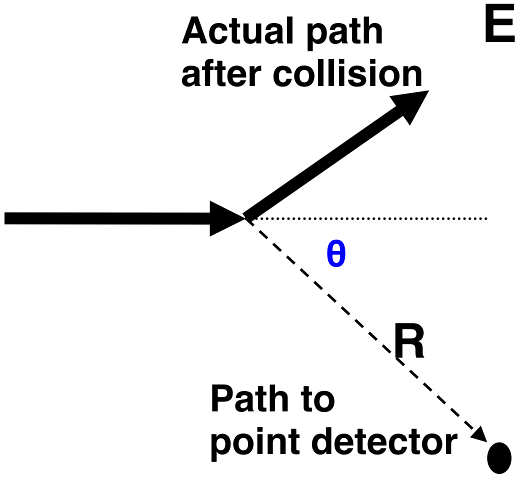
Flux Tally - Surface Crossing

- Complication: wgt_j/μ_j can be very large for small μ_j
  - Usual solution, based on theory from FH Clark, "Variance of Certain Flux Estimators Used in Monte Carlo Calculations", Nucl.Sci. Eng. 27, 235-239 (1967)
  - For small $|\mu|$, that is, $-\varepsilon < \mu < \varepsilon$, (where ε is small), if it is assumed that the flux is only isotropic or linearly anisotropic, then the expected value of $1/|\mu|$ is $2/\varepsilon$.
- Actual tally procedure:
  - If $|\mu|<\varepsilon$, then replace $|\mu|$ by $\varepsilon/2$ to score an expected flux.
  - This results in a reliable variance, without affecting the flux estimate significantly.
- MCNP uses ε=.1. Many other codes use ε=.001

Flux at a Point

- Instead of estimating flux for a cell or surface, it may be useful to estimate flux at a point
  - Probability of a history trajectory going through a particular point is zero

- Use a "next event estimator" to get flux at a point
  - Regardless of the actual outcome of simulating a collision, estimate what would happen if the particle scattered exactly in the direction of a point detector



$$\text{Expected}\ \phi\ \text{score} = \text{wgt}' \bullet \frac{p_{sc}(\mu)}{2\pi R^2} \bullet \exp\left\{ -\int_0^R \Sigma_T(E')ds \right\}$$

where

$\text{wgt}' =$ weight after collision

$p_{sc}(\mu) =$ scatter PDF evaluated at μ

$E' =$ energy corresponding to μ

Flux at a Point

- Expected score has 1/R^2 singularity - collisions close to detector can result in large scores
  - Point detector estimator has finite mean, but infinite variance due to 1/R^2 singularity

- To keep variance finite:
  - For collisions within radius $\mathfrak{R}$ of detector, replace the factor

$$\frac{\exp\left\{-\int_0^R \Sigma_T(E')ds\right\}}{R^2}$$

by volume average assuming uniform collisions inside sphere

$$\frac{\int_0^{\mathfrak{R}} e^{-\Sigma_T(E')s} ds}{\int_0^{\mathfrak{R}} s^2 ds} = \frac{1 - e^{\Sigma_T(E')\mathfrak{R}}}{\frac{1}{3}\mathfrak{R}^3 \Sigma_T(E')}$$

  - Typically choose $\mathfrak{R}$ to be ~half a mean free path

Reaction Rate Tallies

- Tally (flux-estimator)•(cross-section)
- Example - pathlength tallies

After each flight, tally

– Flux $\mathrm{wgt} \bullet d_j$

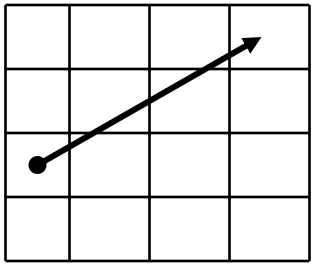
– Total absorption $\mathrm{wgt} \bullet d_j \bullet \Sigma_A$

– Nu-fission $\mathrm{wgt} \bullet d_j \bullet \nu\Sigma_F$

– U235 absorption $\mathrm{wgt} \bullet d_j \bullet N^{U^{235}} \sigma_A^{U^{235}}$

Mesh Tallies & Fission Matrix

- **Mesh Tallies**
  - Impose a grid over the problem & tally flux or reaction rates in each grid cell



- **Fission matrix**
  - Impose a grid over problem
  - Tally F(I→J) for source in cell I causing fission in cell J
  - For N cells in grid, N^2 tallies

Cautions

- Some codes (e.g., MCNP) report the mean score & relative error;

$$RE = \frac{\sigma_{\bar{x}}}{\bar{x}}$$

  - RE should decrease smoothly with 1/√N dependence as more histories are run

- Tallies are reliable only if "enough" histories traverse the portions of problem phase space being tallied
  - Undersampling can lead to questionable or erroneous values of the mean score & relative error
  - Indicators of undersampling:
    - Large RE, RE > .1
    - RE does not decrease smoothly as 1/√N
    - A few histories have very large scores

- MCNP performs statistical checks on selected tallies to try to detect undersampling effects
  - Large RE
  - Variance of the variance (VOV)
  - Tally fluctuation charts (distribution of scores)
  - Slope of tails in tally fluctuation charts
  - Etc.

RE & FOM

- Some codes (e.g., MCNP) report the mean score & relative error

$$\mathrm{RE} = \frac{\sigma_{\bar{x}}}{\bar{x}}$$

- Some codes report a Figure-of-Merit for selected tallies

$$\mathrm{FOM} = \frac{1}{\mathrm{RE}^2 \bullet T}$$

Where T = computer time used

– $\mathrm{RE}^2 \sim 1/N$, where N is the total number of histories

– $T \sim N$

– Therefore, FOM should be roughly constant

– Used for comparing effectiveness of different variance reduction schemes

Combining Independent MC Results

Given N sets of (mean,std-dev) for independent Monte Carlo calculations, (x_1, σ_1), (x_2, σ_2), … , how should the results be combined?

$$w_j = \frac{1}{\sigma_j^2} \qquad W = \sum_{j=1}^{N} \frac{1}{\sigma_j^2}$$

$$\bar{x} = \sum_{j=1}^{N} \frac{w_j}{W} x_j$$

$$\sigma_{\bar{x}}^2 = \sum_{j=1}^{N} \frac{w_j}{W^2} = \frac{1}{W}$$

Weighting factors ~ $1/\sigma^2$

Combining Correlated Tallies

- Suppose 2 estimators, x and y, are correlated, such as the path & collision estimator for Keff

$$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j \qquad \bar{y} = \frac{1}{N}\sum_{j=1}^{N} y_j$$

$$\sigma_x^2 = \frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2 \qquad \sigma_y^2 = \frac{1}{N}\sum_{j=1}^{N} y_j^2 - \bar{y}^2 \qquad \sigma_{xy}^2 = \frac{1}{N}\sum_{j=1}^{N} x_j y_j - \bar{x}\cdot\bar{y}$$

Minimum variance combination of x & y

$$\alpha = \frac{\sigma_y^2 - \sigma_{xy}^2}{\sigma_x^2 - 2\sigma_{xy}^2 + \sigma_y^2}$$

$$\text{mean}_{x,y} \;=\; \alpha\,\bar{x} \;+\; (1-\alpha)\,\bar{y}$$

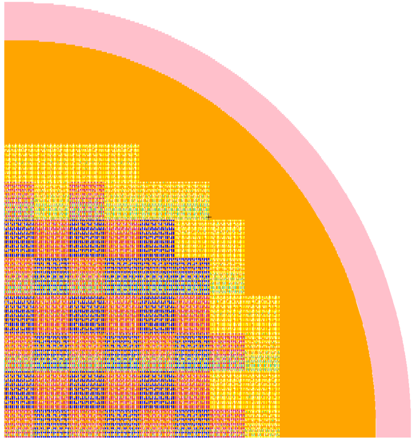
$$\text{std}-\text{dev}_{x,y} = \sqrt{\frac{\alpha^2\sigma_x^2 + 2\alpha\,(1-\alpha)\sigma_{xy}^2 + (1-\alpha)^2\sigma_y^2}{N-1}}$$

Eigenvalue Calculations - I

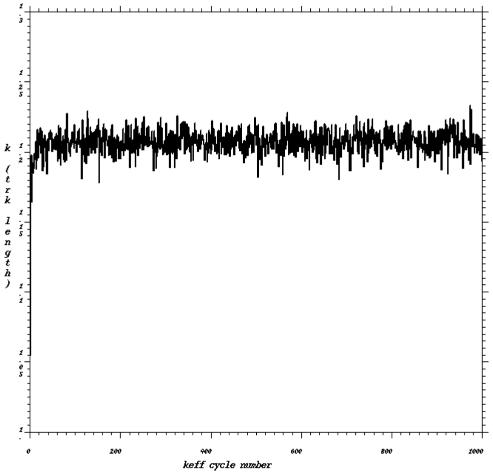
- k- and α- Eigenvalue Equations
- Power Iteration
- Convergence

Reactor Analysis with Monte Carlo

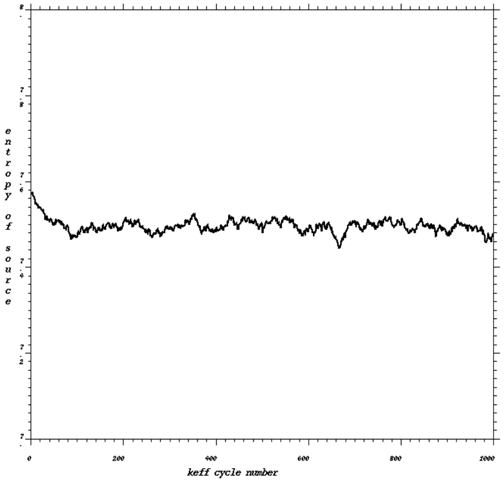
Geometry Model (1/4)



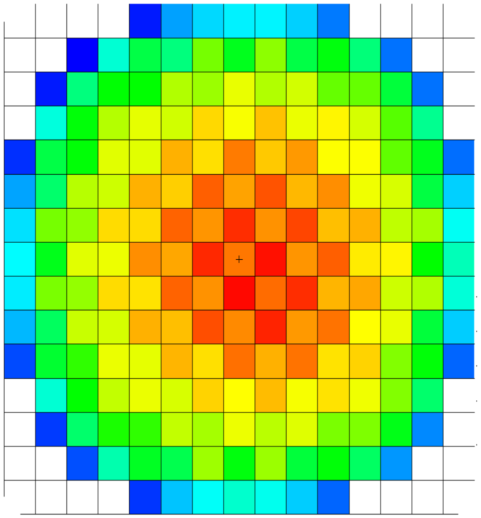
K vs cycle



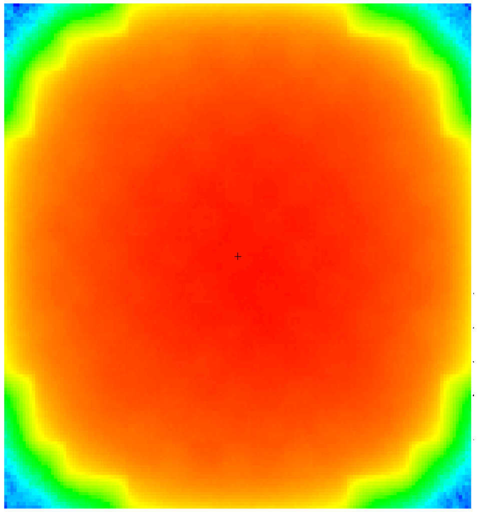
H_{src} vs cycle



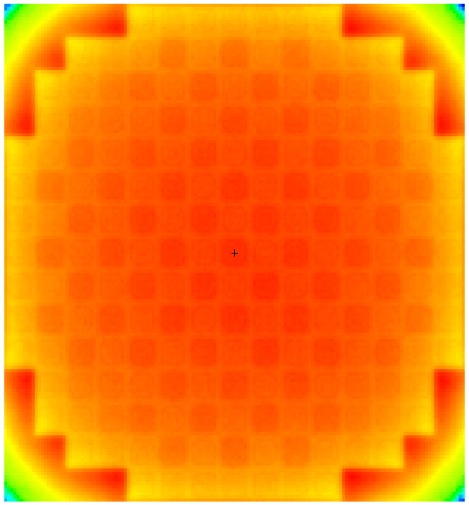
Assembly Powers



Fast Flux



Thermal Flux



The Challenge

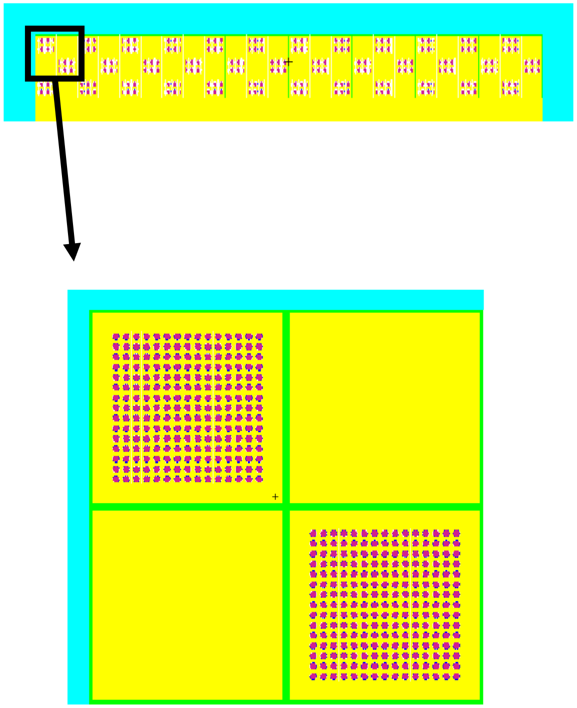
For Monte Carlo calculations of just K-effective,
plots of k_{cycle} vs cycle are adequate to judge convergence.

To compute power distributions, heating distributions, dose rates, production/depletion, & local reaction rates, new tools are needed to judge convergence of the source distribution

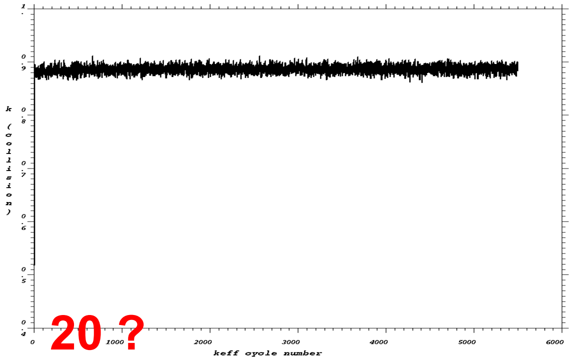
- The source distribution takes longer to converge than K-effective
- How do you tell if a 3D distribution has converged ?
- For the past 40 years, people calculating power distributions or production/depletion with Monte Carlo were "flying blind" -- no tools were available to assess source convergence

Source Distribution Convergence

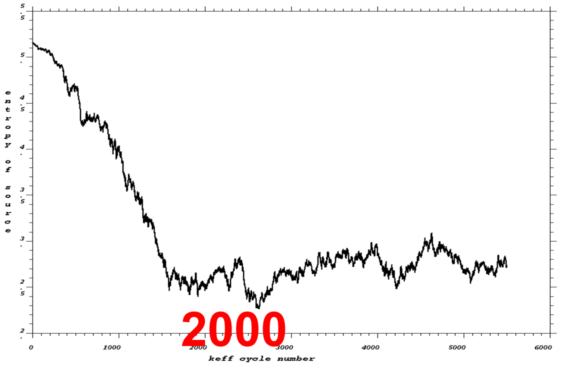
Fuel Storage Vault



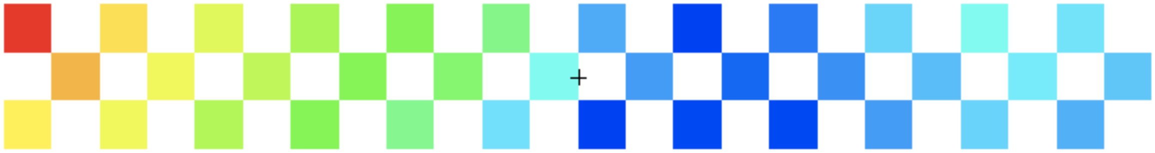
K vs cycle



H_{src} vs cycle



Assembly Heating Distribution



For this calculation,

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

K- and α- Eigenvalue Equations

Time-dependent Transport

- **Time-dependent linear Boltzmann transport equation for neutrons, with prompt fission source & external source**

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = Q(\vec{r},E,\vec{\Omega},t) + \iint \psi(\vec{r},E',\vec{\Omega}',t)\,\Sigma_S(\vec{r},E'\rightarrow E,\vec{\Omega}\cdot\vec{\Omega}')\,d\vec{\Omega}'dE'$$
$$+ \frac{\chi(\vec{r},E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\,\psi(\vec{r},E',\vec{\Omega}',t)\,d\vec{\Omega}'dE'$$
$$-\left[\,\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E)\,\right]\cdot\psi(\vec{r},E,\vec{\Omega},t)$$

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = Q + [S+M]\cdot\psi - [L+T]\cdot\psi$$

- **This equation can be solved directly by Monte Carlo, assuming:**
  - **Each neutron history is an IID trial (independent, identically distributed)**
  - **All neutrons must see same probability densities in all of phase space**
  - **Usual method: geometry & materials fixed over solution interval Δt**

Time-dependent Transport

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\vec{\Omega},t)}{\partial t} = Q + [S+M]\cdot\psi - [L+T]\cdot\psi$$

- **Monte Carlo solution (over Δt, with fixed geometry & materials)**
  - **Simulate time-dependent transport for a neutron history**
  - **If fission occurs, bank any secondary neutrons.**
  - **When original particle is finished, simulate secondaries till done.**
  - **Tallies for time bins, energy bins, cells, …**
- **At time t, the overall neutron level is** $N(t) = \iiint_{\vec{r},E,\hat{\Omega}} \frac{\psi(\vec{r},E,\hat{\Omega},t)}{v} d\vec{r}dEd\hat{\Omega}$
- **Alpha & T (reactor period) can be defined by:**

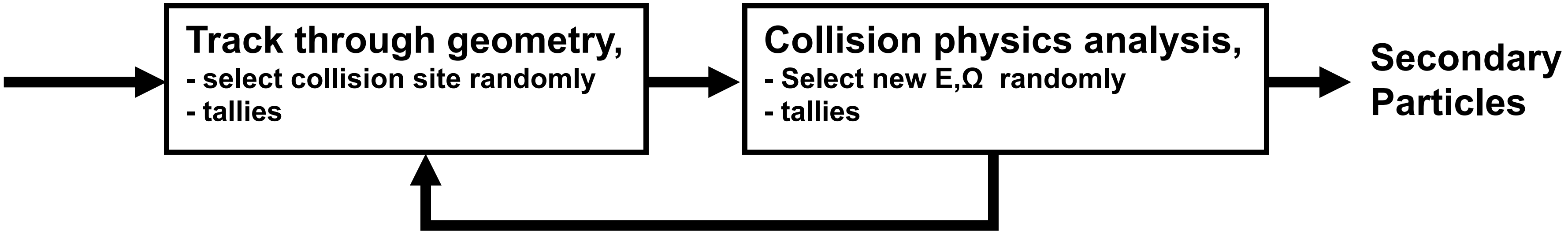
$$N(t) = N_0\ e^{\alpha t} = N_0\, e^{t/T}$$

$$\alpha = \frac{1}{T} \approx \frac{\ln N(t) - \ln N_0}{t - t_0}$$

This is the "dynamic alpha", NOT an eigenvalue !

Particle Histories

- Random Walk for particle

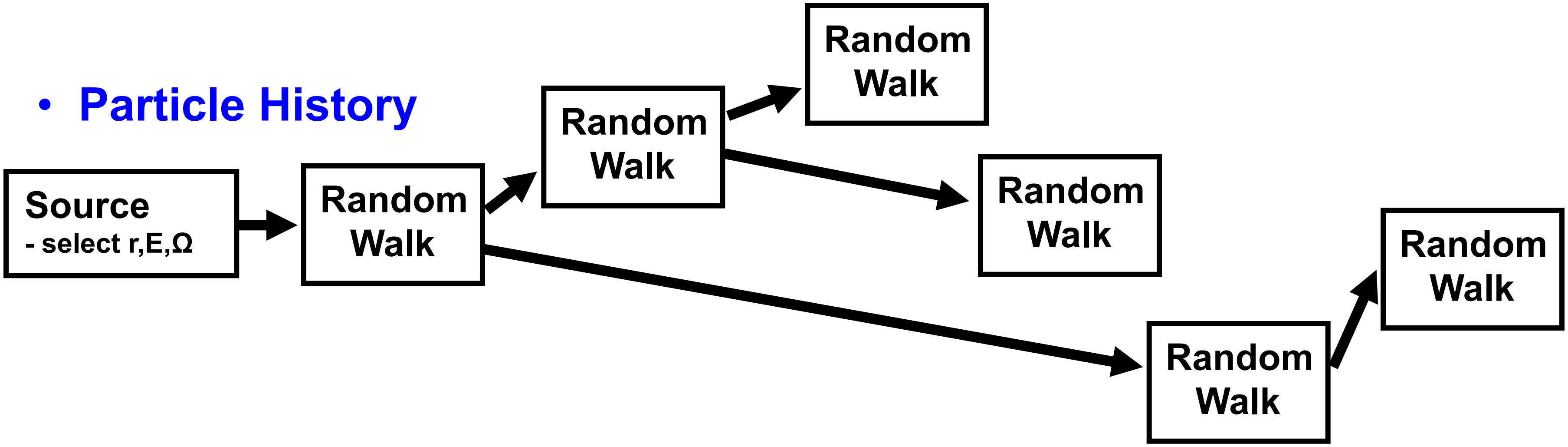


Track through geometry,
- select collision site randomly
- tallies

Collision physics analysis,
- Select new E,Ω randomly
- tallies

Secondary Particles

- Particle History



Source
- select r,E,Ω

Random Walk

Random Walk

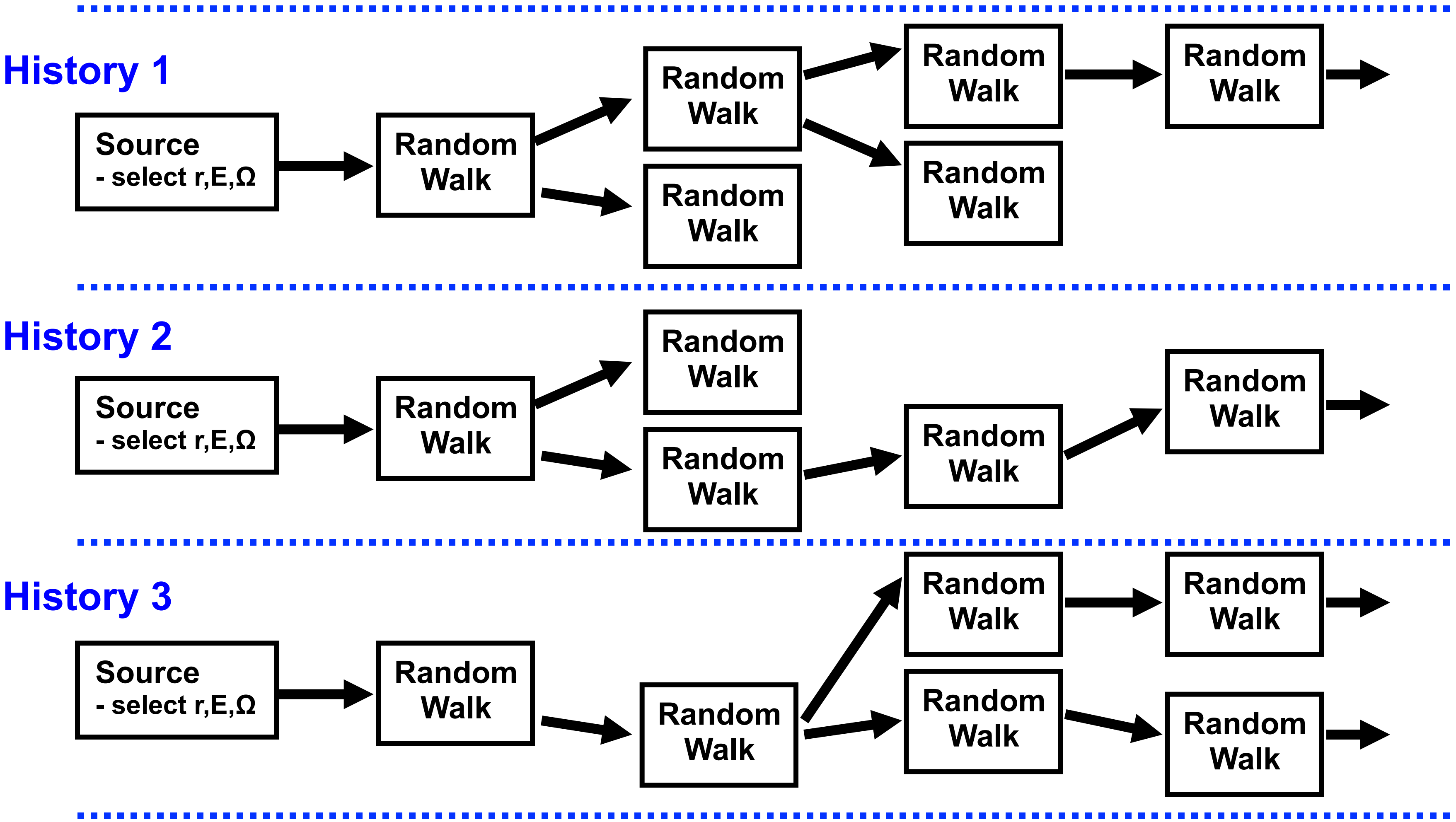
Random Walk

Random Walk

Random Walk

Random Walk

Fixed-source Monte Carlo Calculation



History 1

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

History 2

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

History 3

Source
- select r,E,Ω

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

Random Walk

Alpha Eigenvalue Equations

- For problems which are separable in space & time, it may be advantageous to solve a **static eigenvalue problem**, rather than a fully time-dependent problem

- **Assume:**
  1. **Fixed geometry & materials**
  2. **No external source:** **$Q(r,E,\Omega,t) = 0$**
  3. **Separability:** **$\Psi(r,E,\Omega,t) = \Psi_\alpha(r,E,\Omega)\, e^{\alpha t}$,**

- **Substituting Ψ into the time-dependent transport equation yields**

$$\left[L + T + \frac{\alpha}{v} \right] \Psi_\alpha(\vec{r},E,\vec{\Omega}) \ = \left[S + M \right] \Psi_\alpha$$

  - **This is a static equation, an eigenvalue problem for α and Ψ_α without time-dependence**
  - **α is often called the time-eigenvalue or time-absorption**
  - **α -eigenvalue problems can be solved by Monte Carlo methods**

K_{eff} Eigenvalue Equations

- **Another approach to creating a static eigenvalue problem from the time-dependent transport equation is to introduce K_{eff}, a scaling factor on the multiplication (ν)**

- **Assume:**
  1. **Fixed geometry & materials**
  2. **No external source:** $Q(r,E,\Omega,t) = 0$
  3. **$\partial\Psi/\partial t = 0$:** $\nu \rightarrow \nu / k_{eff}$

- **Setting $\partial\Psi/\partial t = 0$ and introducing the K_{eff} eigenvalue gives**

$$\left[L+T\right]\Psi_k(\vec{r},E,\vec{\Omega}) = \left[S+\frac{1}{K_{eff}}M\right]\Psi_k$$

  - **This is a static equation, an eigenvalue problem for K_{eff} and Ψ_k without time-dependence**
  - **K_{eff} is called the effective multiplication factor**
  - **K_{eff} and Ψ_k should never be used to model time-dependent problems.**
  - **K_{eff}-eigenvalue problems can be solved by Monte Carlo methods**

Comments on K_{eff} and α Equations

- **Criticality**

Supercritical:	$\alpha > 0$	**or**	$K_{eff} > 1$
Critical:	$\alpha = 0$	**or**	$K_{eff} = 1$
Subcritical: $\alpha < 0$	**or**	$K_{eff} < 1$	

- **K_{eff} vs. α eigenvalue equations**
  - $\Psi_k(r,E,\Omega) \neq \Psi_\alpha(r,E,\Omega)$, **except for a critical system**
  - α **eigenvalue &** Ψ_α **eigenfunction used for time-dependent problems**
  - K_{eff} **eigenvalue &** Ψ_k **eigenfunction used for reactor design & analysis**
  - **Although** $\alpha = (K_{eff}-1)/\Lambda$, **where** Λ **= lifetime,**
    there is no direct relationship between $\Psi_k(r,E,\Omega)$ **and** $\Psi_\alpha(r,E,\Omega)$

- K_{eff} eigenvalue problems can be solved **directly** using Monte Carlo

- α eigenvalue problems are solved by Monte Carlo **indirectly**
  using a series of K_{eff} calculations

Comments on K_{eff} and α Equations

K equation $[\,L + T\,]\,\Psi_k = [S + 1/k\; M\,]\,\Psi_k$

α equation $[\,L + T + \alpha/v\,]\,\Psi_\alpha = [S + M\,]\,\Psi_\alpha$

- The factor 1/k changes the relative level of the fission source
- The factor α/v changes the absorption & neutron spectrum
  - For $\alpha > 0$, more absorption at low E ➜ harder spectrum
  - Double-density Godiva, average neutron energy causing fission:

    k calculation: 1.30 MeV

    α calculation: 1.68 MeV
- For separable problems, $\Psi(r,E,\Omega,t) = \Psi_\alpha(r,E,\Omega)\, e^{\alpha t}$
- No similar equation for k, since not used for time-dependence

Power Iteration
&
Convergence

K-eigenvalue equation

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

where

L = leakage operator S = scatter-in operator

T = collision operator M = fission multiplication

operator

- Rearrange

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

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

$$\Psi = \frac{1}{K_{eff}} \cdot F\Psi$$

➜ This eigenvalue equation will be solved by power iteration

$$\Psi^{(n+1)} = \frac{1}{K_{eff}^{(n)}} \cdot F\Psi^{(n)}$$

Power Iteration

Diffusion Theory or Discrete-ordinates Transport

1. Initial guess for K_{eff} and Ψ

   $K_{eff}^{(0)}, \Psi^{(0)}$

2. Solve for $\Psi^{(n+1)}$

   Inner iterations over space or space/angle to solve for $\Psi^{(n+1)}$

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

3. Compute new K_{eff}

$$K_{eff}^{(n+1)} = K_{eff}^{(n)} \cdot \frac{1 \bullet M\Psi^{(n+1)}}{1 \bullet M\Psi^{(n)}}$$

4. Repeat 1-3 until both $K_{eff}^{(n+1)}$ and $\Psi^{(n+1)}$ have converged

Monte Carlo

1. Initial guess for K_{eff} and Ψ

   $K_{eff}^{(0)}, \Psi^{(0)}$

2. Solve for $\Psi^{(n+1)}$

   Follow particle histories to solve for $\Psi^{(n+1)}$

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

   During histories, save fission sites to use for source in next iteration

3. Compute new K_{eff}

   During histories for iteration (n+1), estimate $K_{eff}^{(n+1)}$

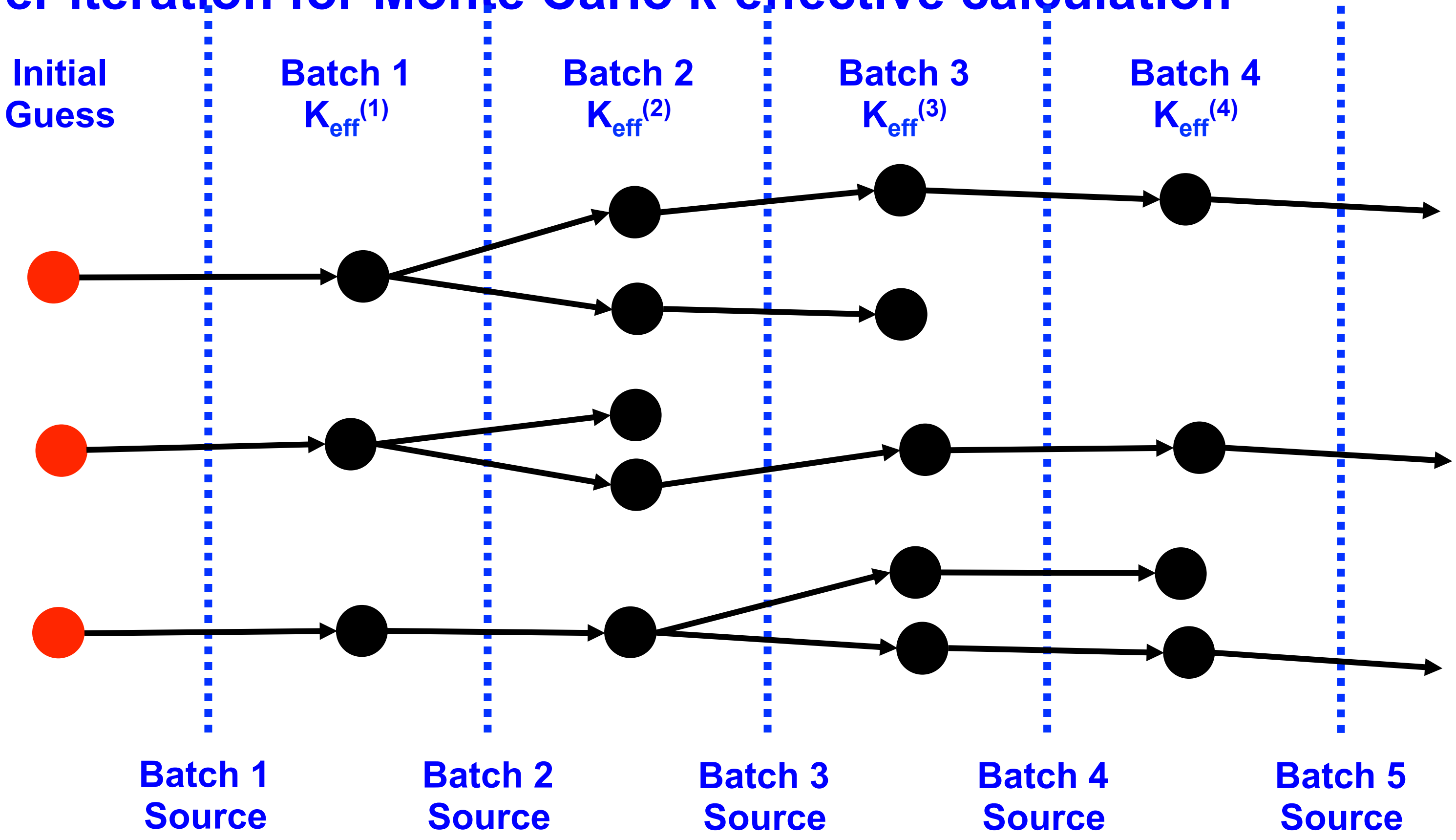
$$K_{eff}^{(n+1)} = K_{eff}^{(n)} \cdot \frac{\int M\Psi^{(n+1)} d\vec{r}}{\int M\Psi^{(n)} d\vec{r}}$$

4. Repeat 1-3 until both $K_{eff}^{(n+1)}$ and $\Psi^{(n+1)}$ have converged

5. **Continue iterating, to compute tallies**

Power Iteration

- Power iteration for Monte Carlo k-effective calculation



● Source particle generation

● Monte Carlo random walk

↗ Neutron

α-Eigenvalue Calculations

- **Eigenvalue equation with** both **K_{eff} & α**
  - **α is a fixed number, not a variable or eigenvalue**
  - **Find the k-eigenvalue as function of α, K(α)**

$$\left[L + T + \frac{\alpha}{v} \right] \Psi_\alpha(\vec{r},E,\vec{\Omega}) = \left[S + \frac{1}{K_{eff}} M \right] \Psi_\alpha$$

- Note: If α < 0
  - Real absorption plus time absorption could be negative
  - Move α/v to right side to prevent negative absorption,
  - -α/v term on right side is treated as a delta-function scatter

- **Select a fixed value for α**
- **Solve the K-eigenvalue equations, with fixed time-absorption α/v**
- **Select a different α and solve for a new Keff**
- **Repeat, searching for value of α which results in Keff = 1**

K- and α-Eigenvalue Calculations

- K-eigenvalue solution

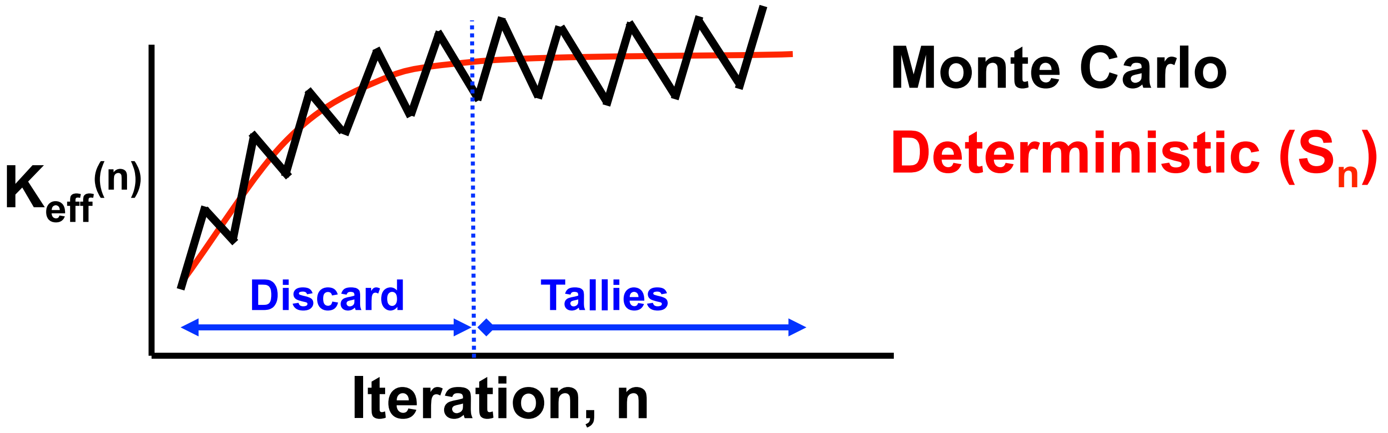
```
Loop for Power Iteration for K
•       Loop over neutrons in cycle
•       •         neutron history
•       • • •                Monte Carlo
• • •
```

- α-eigenvalue solution

```
Loop for α search iterations
•  Loop for Power Iteration for K
•  •       Loop over neutrons in cycle
•  •       •         neutron history
•  •       • • •                Monte Carlo
•  • • •
• • •
```

➜ Find K(α), then search for α that gives K(α)=1

K-Calculations



- Guess an initial source distribution
- Iterate until converged (How do you know ???)
- Then
  - For S_n code: done, print the results
  - For Monte Carlo: start tallies, keep running until uncertainties small enough

- Details? Bias? Statistics?

Monte Carlo Solution of K_{eff} Problems

Note: batch = cycle = iteration = generation

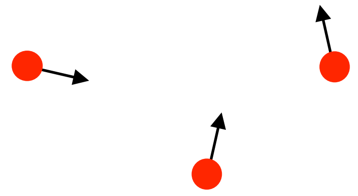
- **Initialize**
  - **Assume a value for the initial K_{eff} (usually, $K_0 = 1$)**
  - **Sample M fission sites from the initial source distribution**
- **For each cycle n, $n = 1 \dots N+D$**
  - **Follow histories for all source particles in cycle**
    - If fissions occur, bank the sites for use as source in next cycle
    - Make tallies for $K_{cycle}^{(n)}$ using path, collision, & absorption estimators
    - If $n \le D$, discard any tallies
    - If $n > D$, accumulate tallies
  - **Estimate $K_{cycle}^{(n)}$**
- **Compute final results & statistics using last N cycles**

K-Calculations -- Power Iteration

- **Power iteration procedure:**

1. **Initial guess for K_{eff} and Ψ**
   $K_{eff}^{(0)}$, $\Psi^{(0)}$

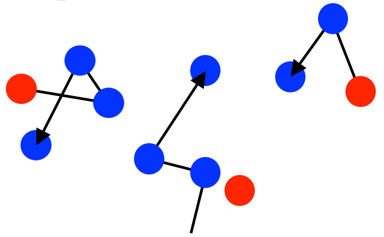
Source points
For $\Psi^{(0)}$



2. **Solve for $\Psi^{(n+1)}$ [Monte Carlo random walk for N particles]**

$$\Psi^{(n+1)} = \frac{1}{K_{eff}^{(n)}} \cdot F\Psi^{(n)}$$

Source points
For $\Psi^{(n+1)}$



3. **Compute new K_{eff}**

$$K_{eff}^{(n+1)} = K_{eff}^{(n)} \cdot \frac{\int M\Psi^{(n+1)} d\vec{r}}{\int M\Psi^{(n)} d\vec{r}}$$

4. **Repeat 1-3 until both $K_{eff}^{(n+1)}$ and $\Psi^{(n+1)}$ have converged**

K-Calculations -- Banking Fission Sites

- During a particle random walk,

$$\text{wgt} \cdot \frac{\nu\Sigma_F}{\Sigma_T} \quad = \text{expected number of fission neutrons created at collision point}$$

- Averaged over all collisions for all histories, the expected value for $\text{wgt} \cdot \nu\Sigma_F / \Sigma_T$ is K_{eff}.

- In order to bank approximately the same number of fission sites in each cycle, the current value of Keff is used to bias the selection of fission sites at a collision:

$$R = \text{wgt} \cdot \frac{\nu\Sigma_F}{\Sigma_T} \cdot \frac{1}{K}, \qquad n = \lfloor R \rfloor$$

If $\xi < R - n$, store $n+1$ sites in bank with $\text{wgt}' = K$

Otherwise, store n sites in bank with $\text{wgt}' = K$

K-Calculations -- Renormalization

- N_J = number of particles starting cycle J,
  N'_J = number of particles created by fission in cycle J (number of particles stored in fission bank)
  - The expected value for N'_J is: $E[\, N'_J \,] = K_{eff} \bullet N_J$
  - (N'_J/N_J) is a single-cycle estimator for K_{eff}

- To prevent the number of particles per cycle from growing exponentially (for K>1) or decreasing to 0 (for K<1), the particle population is renormalized at the end of each cycle:
  - In some Monte Carlo codes, the number of particles starting each cycle is a constant N. Russian roulette or splitting are used to sample N particles from the N' particles in the fission bank. (All particles in fission bank have a weight of 1.0)
  - In other codes, the total weight W starting each cycle is constant. The particle weights in the fission bank are renormalized so that the total weight is changed from W' to W. (Particles in fission bank have equal weights, but not necessarily 1.0)

Single-cycle Keff Estimators

- Pathlength estimator for Keff

$$K_{path} = \left(\sum_{\substack{\text{all}\\ \text{flights}}} wgt_j \cdot d_j \cdot \nu\Sigma_F \right) \Big/ W$$

W = total weight starting each cycle

- Collision estimator for Keff

$$K_{collision} = \left(\sum_{\substack{\text{all}\\ \text{collisions}}} wgt_j \cdot \frac{\nu\Sigma_F}{\Sigma_T} \right) \Big/ W$$

- Absorption estimator for Keff

$$K_{absorption} = \left(\sum_{\substack{\text{all}\\ \text{absorptions}}} wgt_j \cdot \frac{\nu\Sigma_F}{\Sigma_A} \right) \Big/ W$$

K-Calculations -- Bias

- **The renormalization procedure used at the end of each cycle introduces a small bias into the computed Keff**
  - **Renormalization involves multiplying particle weights by (W/W'), where W = total weight starting a cycle,**
    W'= total weight at the end of a cycle.
  - **W' is a random variable, due to fluctuations in particle random walks.**

- **Theoretical analysis of the MC iteration process & propagation of history fluctuations gives**

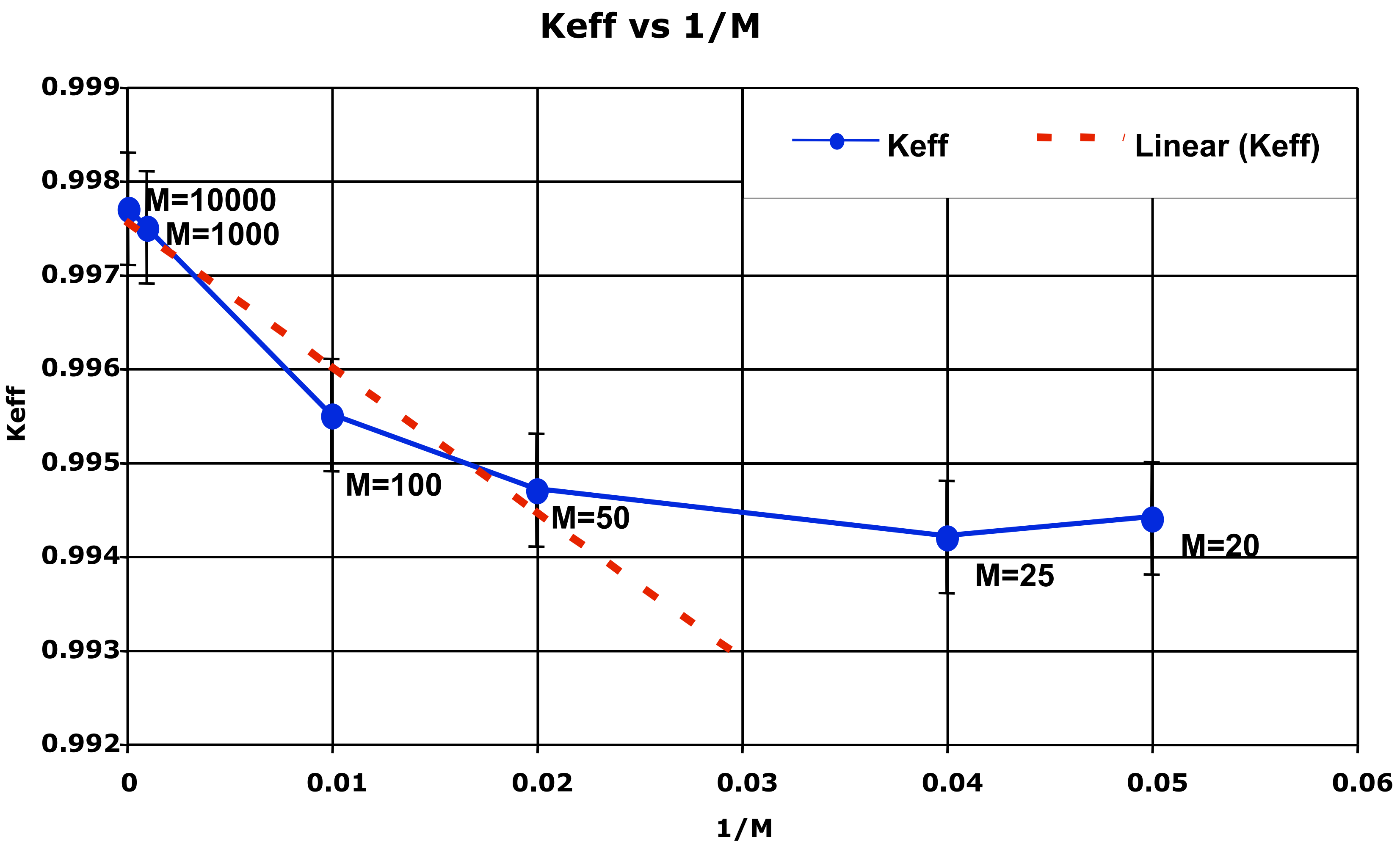
$$\text{bias in } K_{eff} \;=\; -\frac{\sigma_k^2}{K_{eff}} \cdot \left(\begin{matrix} \text{sum of correlation coeff's} \\ \text{between batch K's} \end{matrix} \right)$$

  - **M = histories/cycle**
  - **Bias in Keff ~ 1/M**
    - Smaller M ➜ larger cycle correlation ➜ larger bias in Keff & source
    - Larger M ➜ smaller cycle correlation ➜ smaller bias

[T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations**", Nucl. Sci. Eng. (2002)]**

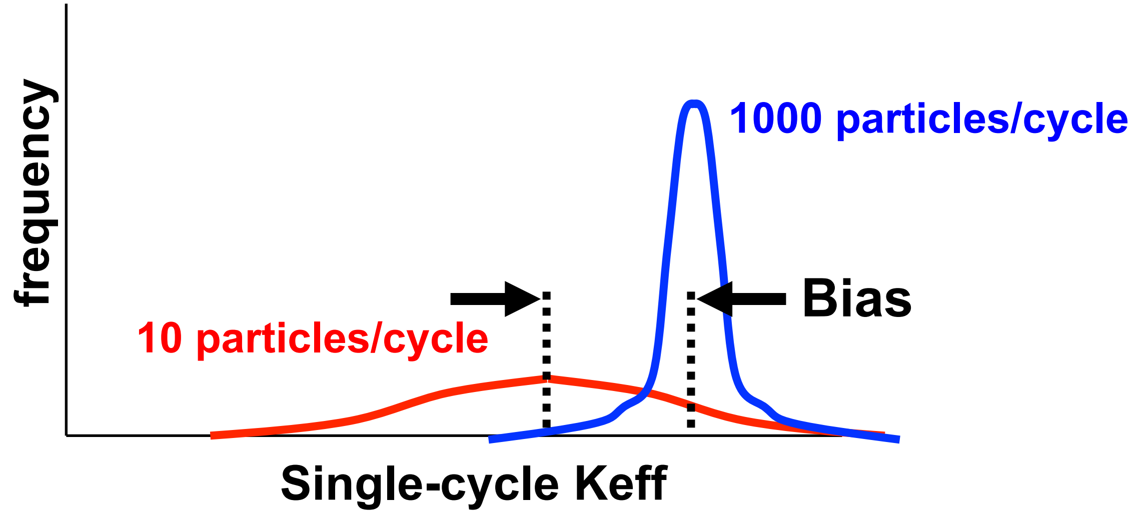
K-Calculations -- Bias

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



K-Calculations -- Bias

- Observed PDF for single-cycle Keff, for varying M

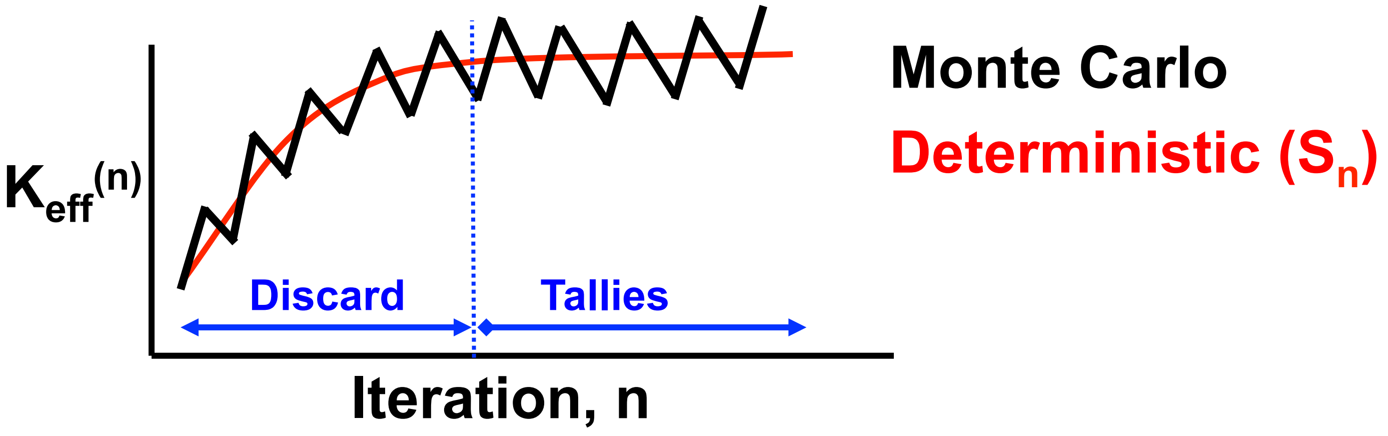


- Bias in Keff is negative: $K_{calc} < K_{true}$

Bias is	significant	for	$M < 10$	particles/cycle
	small	for	$M \sim 100$	
	negligible	for	$M > 1000$	
	0	for	$M \rightarrow \infty$	

- Recommendation: Always use 10,000 or more particles/cycle

Power Iteration & Convergence



- Guess an initial source distribution
- Iterate until converged (How do you know ???)
- Then
  - – For S_n code: done, print the results
  - – For Monte Carlo: start tallies, keep running until uncertainties small enough

- Convergence? Stationarity?

K-eigenvalue equation

- Use operator (or matrix) form to simplify notation

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

where

L = leakage operator S = scatter-in operator

T = collision operator M = fission multiplication operator

- Rearrange

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

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

$$\Psi = \tfrac{1}{K_{eff}} \cdot F\Psi$$

➜ This eigenvalue equation will be solved by power iteration

Power Iteration - Convergence

- **Expand Ψ in terms of eigenfunctions $u_j(r,E,\Omega)$**

$$\Psi = \sum_{j=0}^{\infty} a_j \vec{u}_j = a_0\vec{u}_0 + a_1\vec{u}_1 + a_2\vec{u}_2 + a_3\vec{u}_3 + ...$$

$$\int \vec{u}_j \vec{u}_k dV = \delta_{jk} \qquad a_j = \int \Psi \cdot \vec{u}_j dV$$

$$\vec{u}_j = \frac{1}{k_j} F \cdot \vec{u}_j \qquad k_0 > k_1 > k_2 > ... \qquad k_0 \equiv k_{\text{effective}}$$

- **Expand the initial guess in terms of the eigenmodes**

$$\Psi^{(0)} = \sum_{j=0} a_j^{(0)} \vec{u}_j$$

- **Substitute the expansion for $\Psi^{(0)}$ into power iteration equation**

$$\Psi^{(n+1)} = \frac{1}{K^{(n)}} F \cdot \Psi^{(n)} = \frac{1}{k^{(n)}} \cdot \frac{1}{k^{(n-1)}} \cdots \frac{1}{k^{(0)}} \cdot F^n \cdot \Psi^{(0)}$$

$$= \left[\prod_{m=0}^{n} \frac{k_0}{K^{(m)}} \right] \cdot a_0^{(0)} \cdot \left[\vec{u}_0 + \sum_{j=1} \left(\frac{a_j^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_j}{k_0} \right)^{n+1} \cdot \vec{u}_j \right]$$

Power Iteration - Convergence

$$\Psi^{(n+1)} \approx [\text{constant}] \cdot \left[\vec{u}_0 + \left(\frac{a_1^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_1}{k_0} \right)^{n+1} \cdot \vec{u}_1 + \ldots \right]$$

$$K^{(n+1)} \approx k_0 \cdot \left[1 + \left(\frac{a_1^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_1}{k_0} \right)^{n} \cdot \left(\frac{k_1}{k_0} - 1 \right) \cdot G_1 + \ldots \right]$$

- **Because $k_0 > k_1 > k_2 > \ldots$, all of the red terms vanish as $n \rightarrow \infty$**
  - **$\Psi^{(n+1)}$ ➜ constant · u_0**
  - **$K^{(n+1)}$ ➜ k_0**

- **After the initial transient, error in $\Psi^{(n)}$ is dominated by first mode**
  - **(k_1 / k_0) is called the dominance ratio, DR or ρ**
  - **Errors in $\Psi^{(n)}$ die off as ~ $(DR)^n$**

- **For problems with a high dominance ratio (e.g., DR ~ .99), the error in K_{eff} may be small, since the factor (k_1/k_0 - 1) is small.**
  - **K_{eff} may appear converged,
even if the source distribution is not converged**

Power Iteration - Convergence

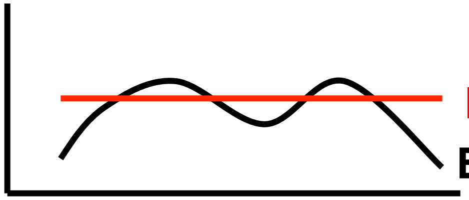
- After n iterations, J^{th} mode error component is reduced by the factor $(k_J / k_0)^n$

- Since $1 > k_1/k_0 > k_2/k_0 > k_3/k_0 > \ldots$,
after the initial transient, error in $\Psi^{(n)}$ is dominated by first mode:

$$\Psi^{(n)} \approx [\text{constant}] \bullet \left[\vec{u}_0 + \left(\frac{a_1^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_1}{k_0} \right)^n \cdot \vec{u}_1 + \ldots \right]$$

- (k_1 / k_0) is called the dominance ratio, DR or ρ
  - Errors die off as ~ $(DR)^n$
  - To reduce 10% error → .1% error

DR~.9 → 44 iterations
DR~.99 → 458 iterations
DR~.999 → 2301 iterations

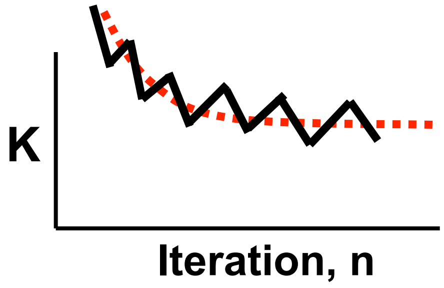


Initial guess
Exact solution

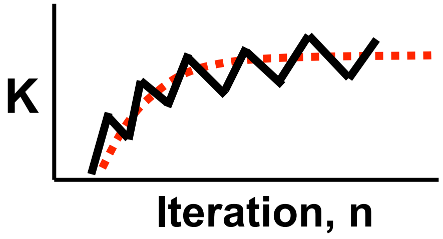
Power Iteration - Convergence

Typical K-effective convergence patterns

- Higher mode error terms die out as $(k_J / k_0)^n$, for n iterations
- When initial guess is concentrated in center of reactor, initial K_{eff} is too high **(underestimates leakage)**



- When initial guess is uniformly distributed, initial K_{eff} is too low **(overestimates leakage)**

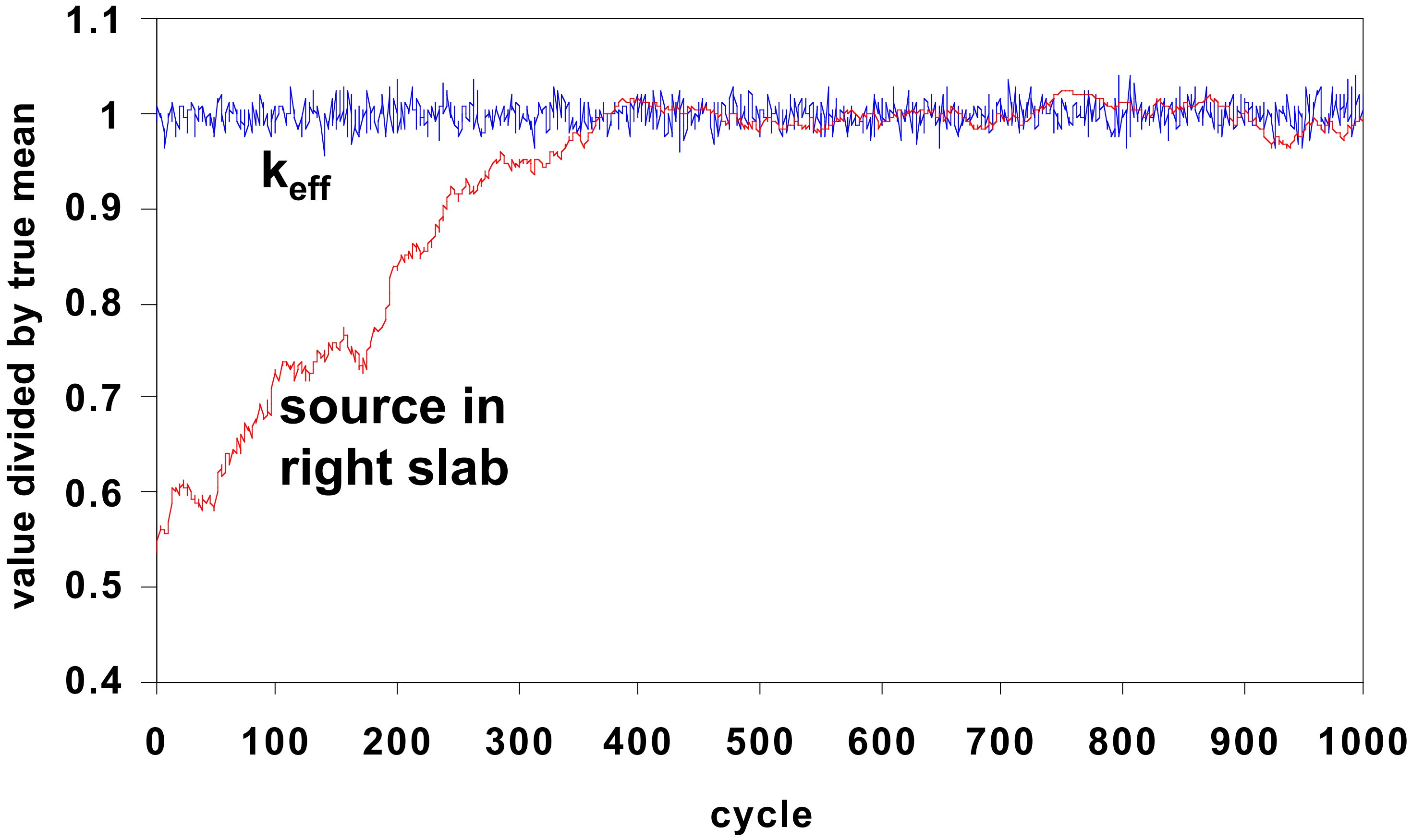


- **The Sandwich Method uses 2 K_{eff} calculations - one starting too high & one starting too low. Both calculations should converge to the same result.**

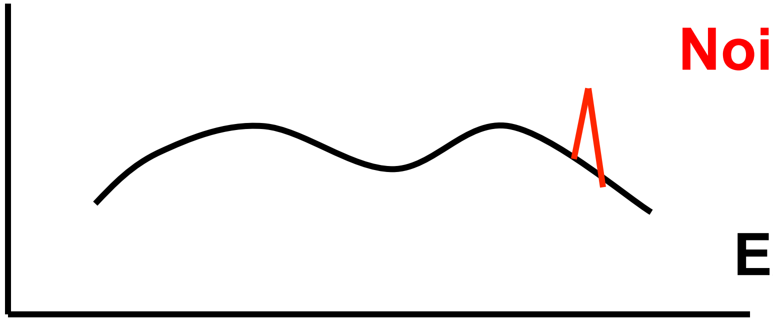
Power Iteration - Convergence

- Keff is an integral quantity - converges faster than source shape

Keff calculation for 2 nearly symmetric slabs, with Dominance Ratio = .9925



Power Iteration - Convergence



Noise (fluctuation)

Exact solution

- **For Monte Carlo power iteration, statistical fluctuations in source shape die out gradually over a number of successive iterations.**
  - **Persistence of the noise over successive iterations gives correlation among source distributions in successive iterations. (Positive correlation)**
  - **Correlation directly affects confidence intervals:**
    Serial correlation in the source distribution ➔ larger confidence intervals

➜ Most Monte Carlo codes ignore these correlation effects & incorrectly underestimate the confidence intervals

Power Iteration - Convergence

Summary

- Local errors in the source distribution decay as $(k_J/k_0)^n$
  - Higher eigenmodes die out rapidly, convergence dominated by k_1/k_0
  - High DR ➜ slow convergence
  - High DR ➜ large correlation ➜ large error in computed variances
- Errors in K_{eff} decay as $(k_J/k_0 – 1) * (k_J/k_0)^n$
  - High DR ➜ $k_J/k_0 \sim 1$ ➜ small error
- K_{eff} errors die out faster than local source errors
  - K_{eff} is an integral quantity - positive & negative fluctuations cancel
- High DR is common for
  - Large reactors, with small leakage
  - Heavy-water moderated or reflected reactors
  - Loosely-coupled systems

➜ If local tallies are important (e.g., assembly power, pin power, …), examine their convergence - not just K_{eff} convergence

Eigenvalue Calculations - II

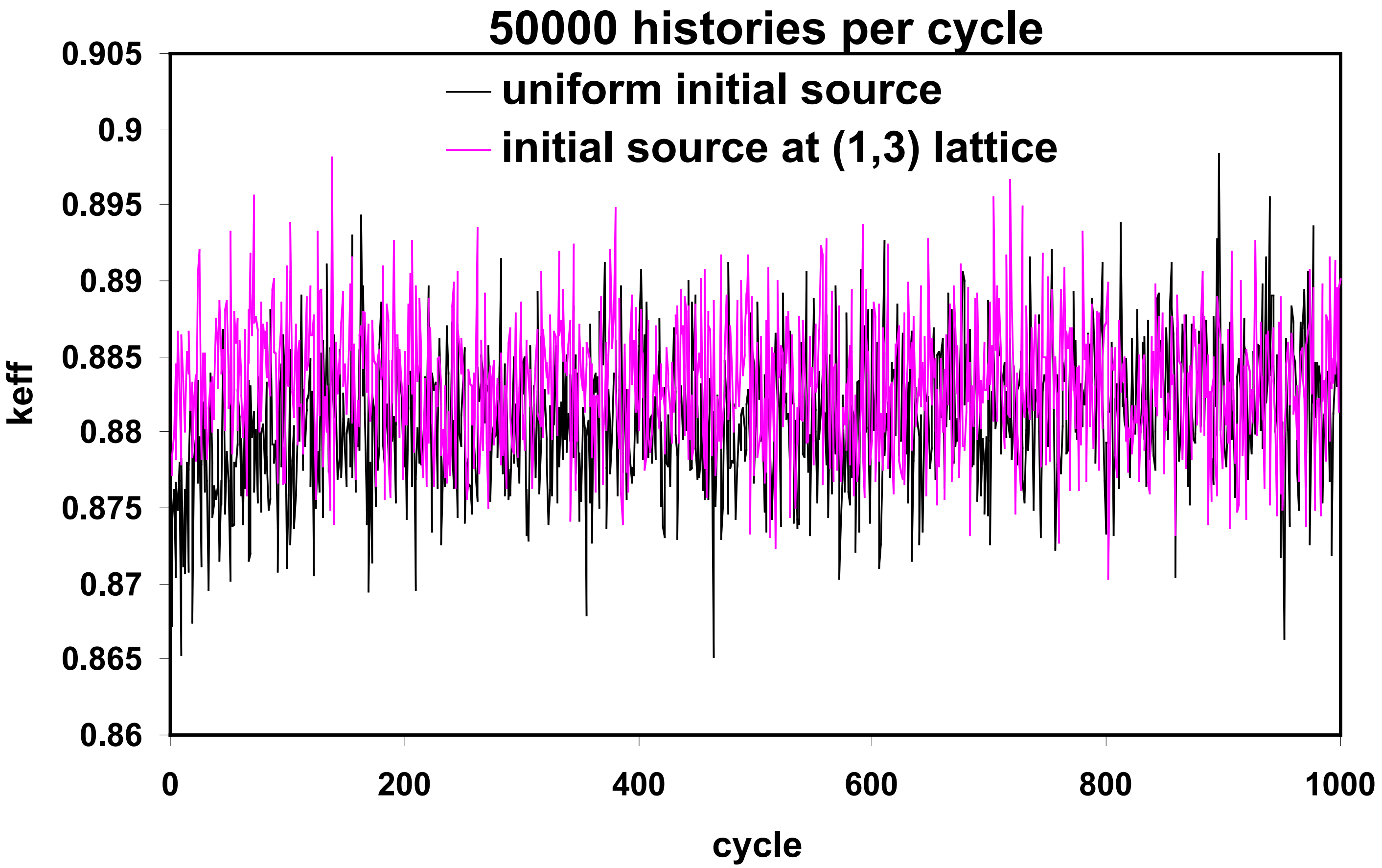
- Stationarity Diagnostics

- Wielandt & Superhistory Methods
- Dominance Ratio

Keff Calculations

- Plots of single-cycle Keff or cumulative Keff are sometimes difficult to interpret when assessing convergence

Cycle k_{eff}



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
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}.**

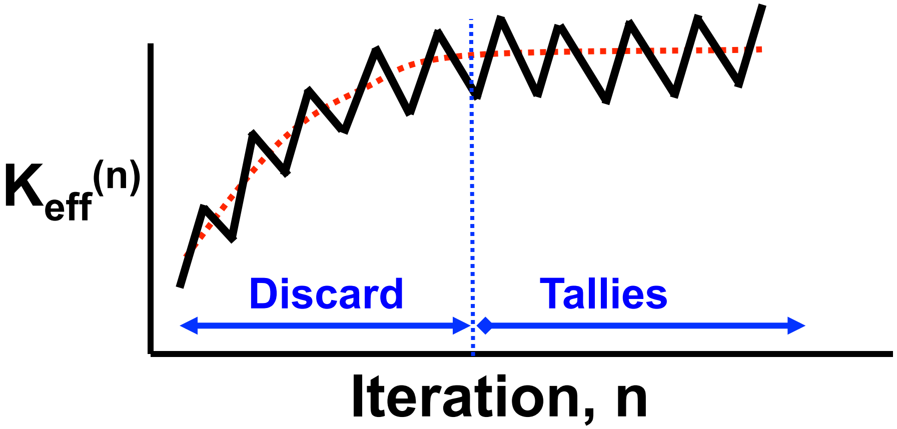
Source Convergence

&

Shannon Entropy

Keff Calculations

- Initial cycles of a Monte Carlo K-effective calculation should be discarded, to avoid contaminating results with errors from initial guess
  - **How many cycles should be discarded?**
  - **How do you know if you discarded enough cycles?**

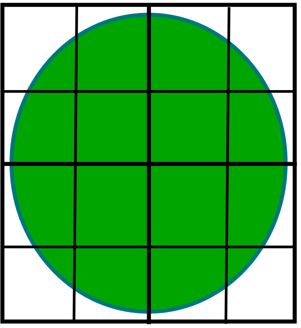


- Analysis of the power iteration method shows that Keff is not a reliable indicator of convergence **-- K_{eff} can converge faster than the source shape**

- Based on concepts from information theory,
  Shannon entropy of the source distribution is useful for characterizing the convergence of the source distribution

K_{eff} Calculations - Stationarity Diagnostics

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



  - **Rule-of-thumb for number of spatial bins:**

    N_S ~ (histories/batch) / 25 or less

    Why?

    - Would like to have >25 fission source sites per bin to get good statistics
    - If source distribution were uniform, ~25 sites would be in each bin

- **Shannon entropy of the source distribution**

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

K_{eff} Calculations - Stationarity Diagnostics

- **Shannon entropy of the source distribution**

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

– **$0 \leq H(S) \leq \ln_2(N_S)$**

– **Note that $p_J \ln_2(p_J) = 0$ if $p_J = 0$**

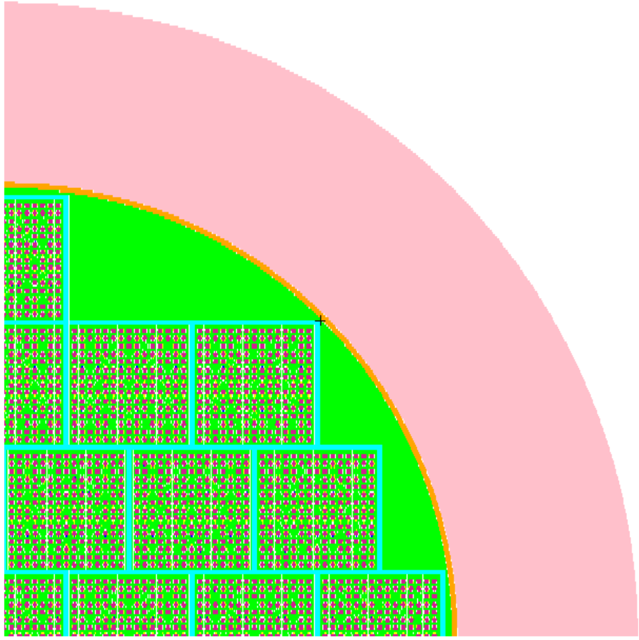
– **For a uniform source distribution,**	**$H(S) = \ln_2(N_S)$**
– **For a point source (in a single bin),**	**$H(S) = 0$**
– **For any general source,**	**$0 \leq H(S) \leq \ln_2(N_S)$**

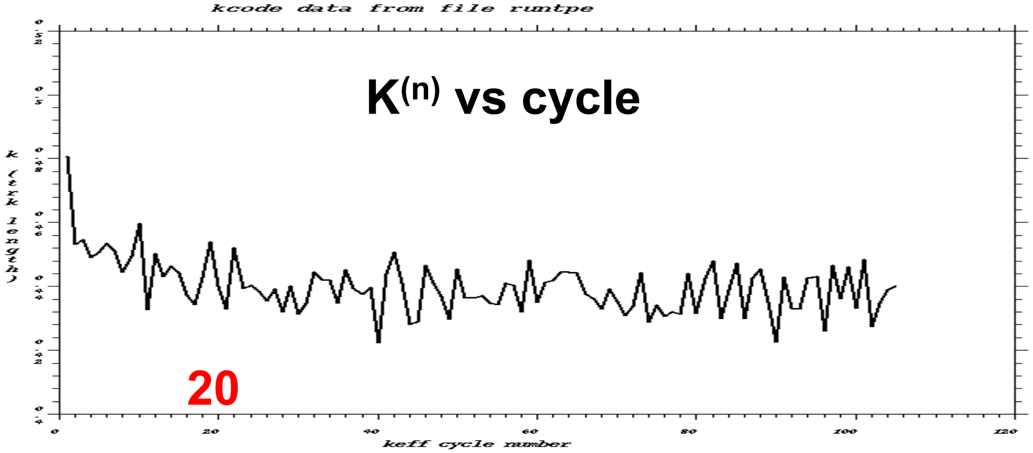
- **$H(S^{(n)})$ provides a single number to characterize the source distribution for iteration n (no physics!)**

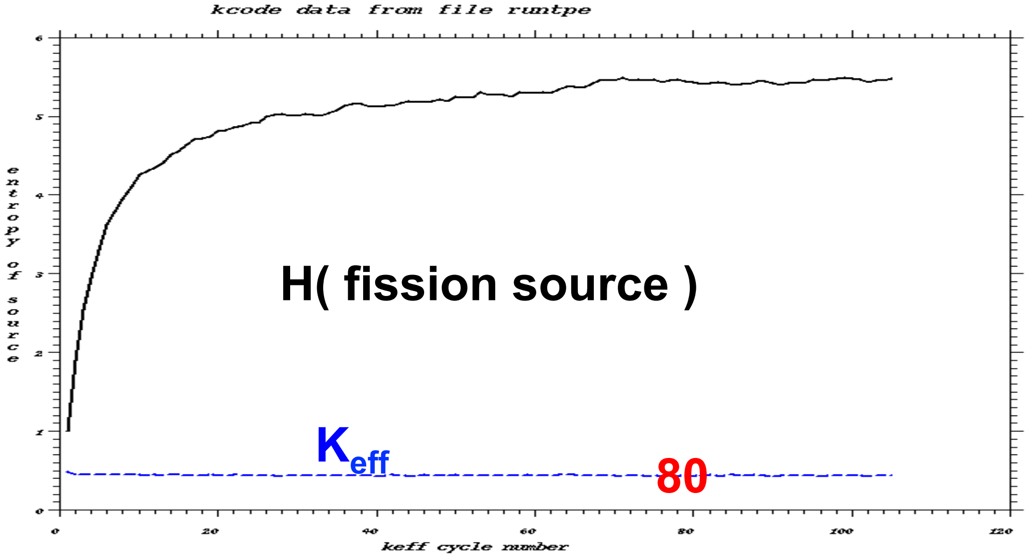
➜ As the source distribution converges in 3D space, a line plot of $H(S^{(n)})$ vs. n (the iteration number) converge

Criticality Calculations - Convergence

- Reactor core (Problem inp24)



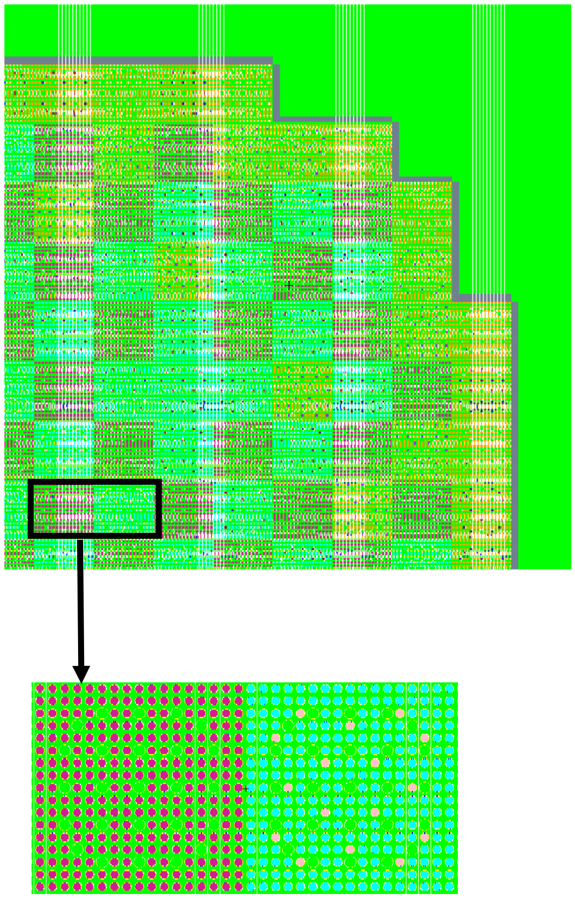




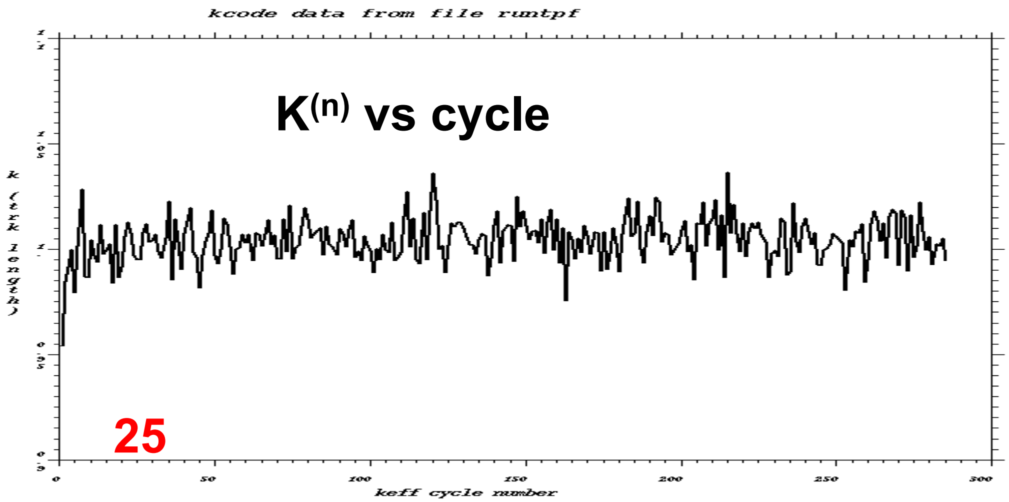
DR = .98

Criticality Calculations - Convergence

- PWR 1/4-Core (Napolitano)

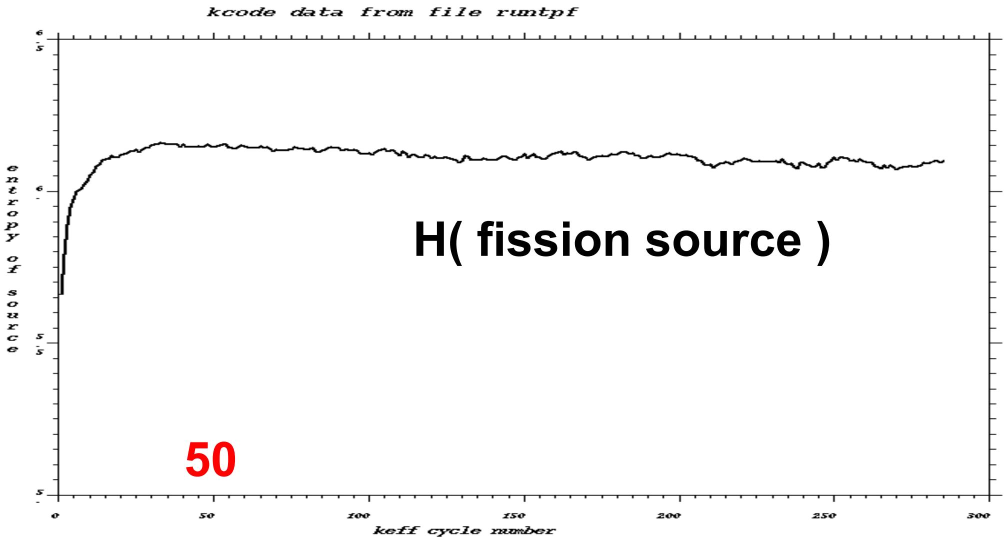


DR = .95



K$^{(n)}$ vs cycle

25

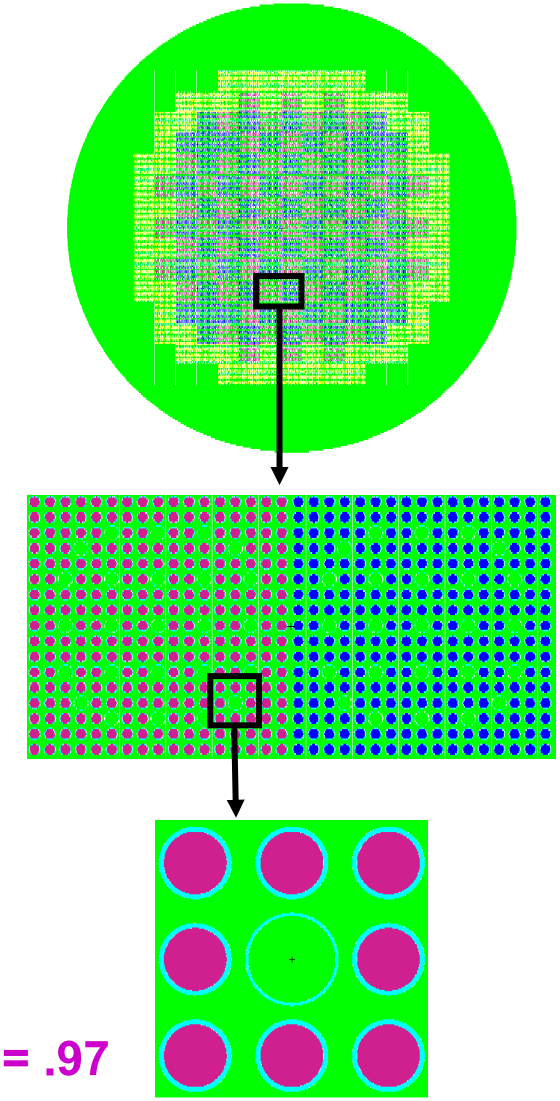


H(fission source)

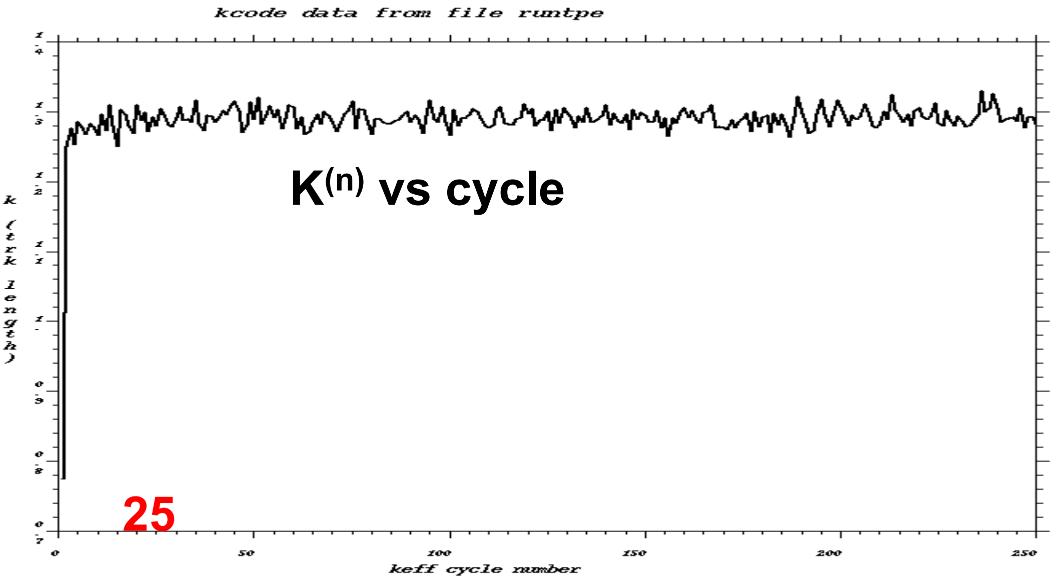
50

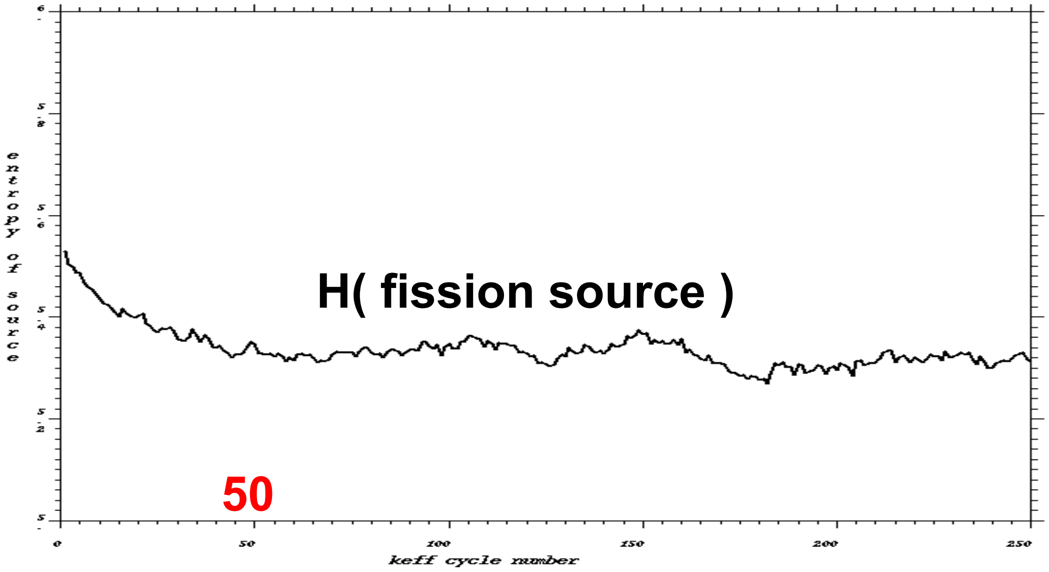
Criticality Calculations - Convergence

- 2D PWR (Ueki)



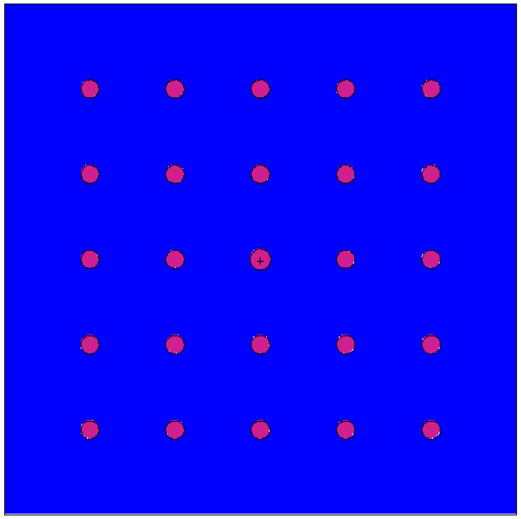
DR = .97

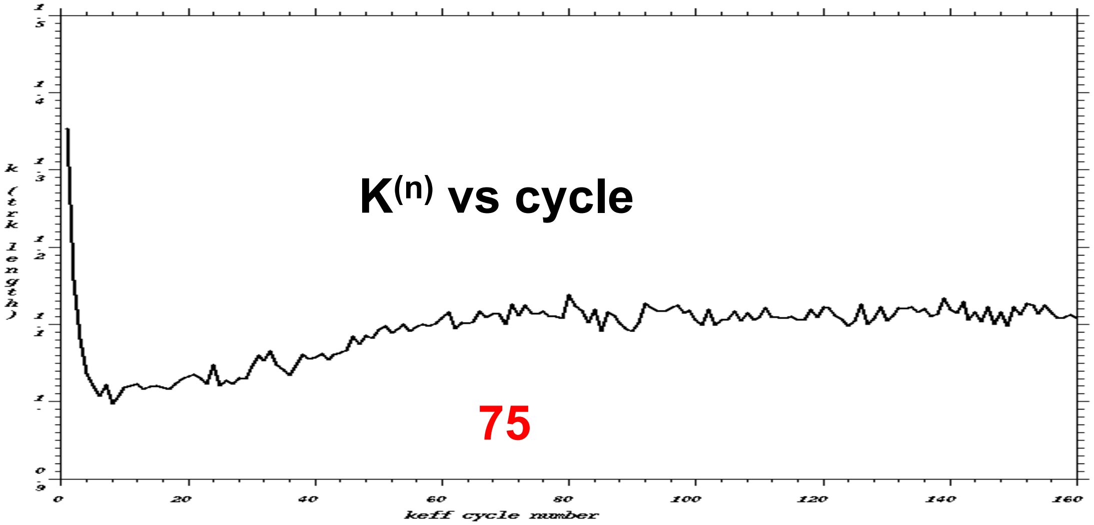




Criticality Calculations - Convergence

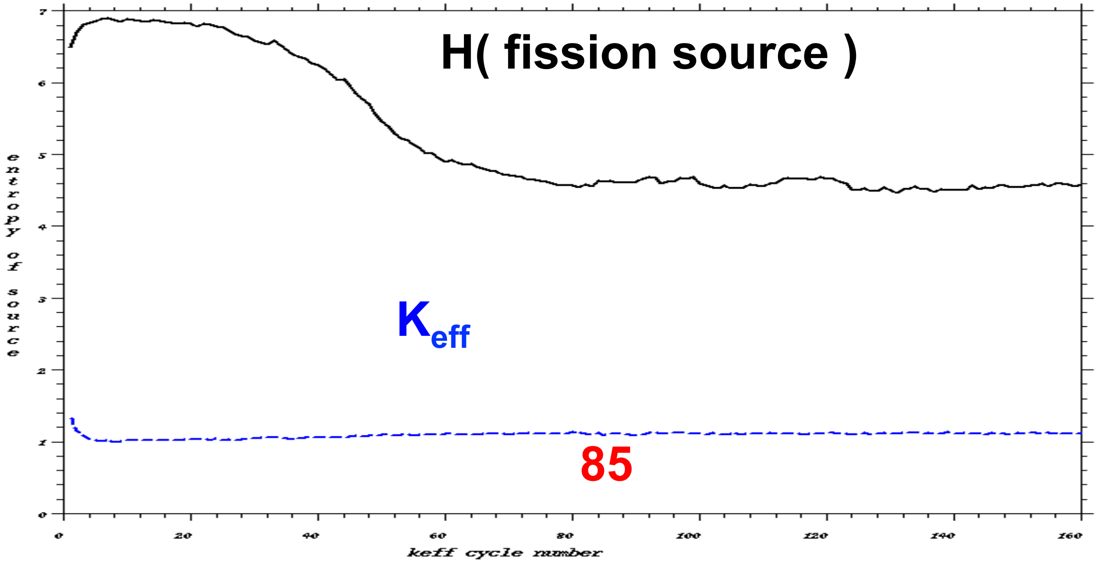
- **Loosely-coupled array of spheres (Problem test4s)**





$K^{(n)}$ vs cycle

75



H(fission source)

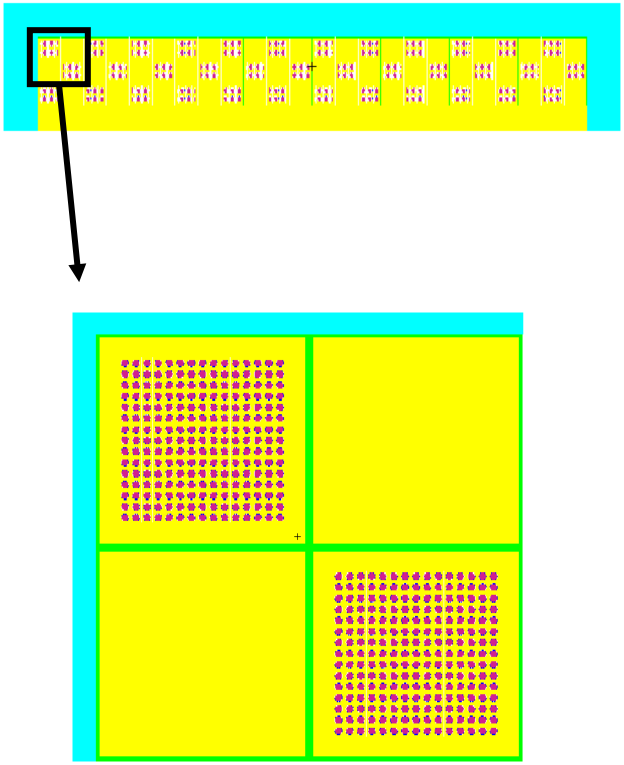
K_{eff}

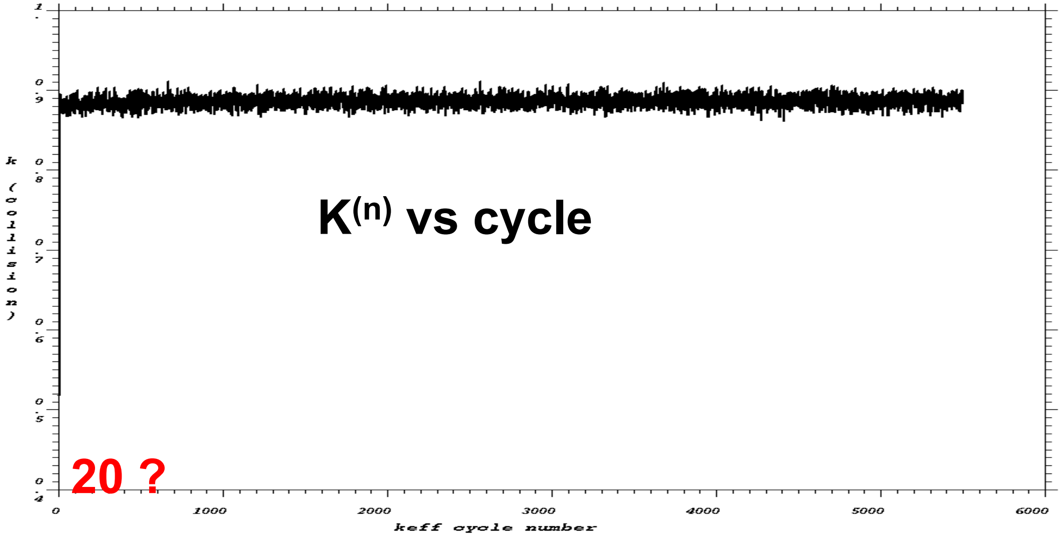
85

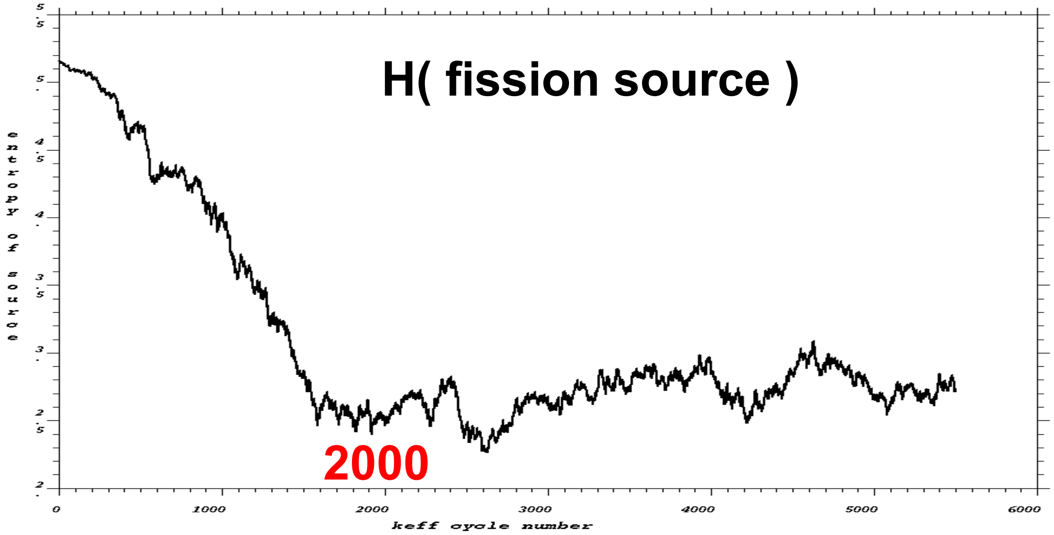
DR = .91

Criticality Calculations - Convergence

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



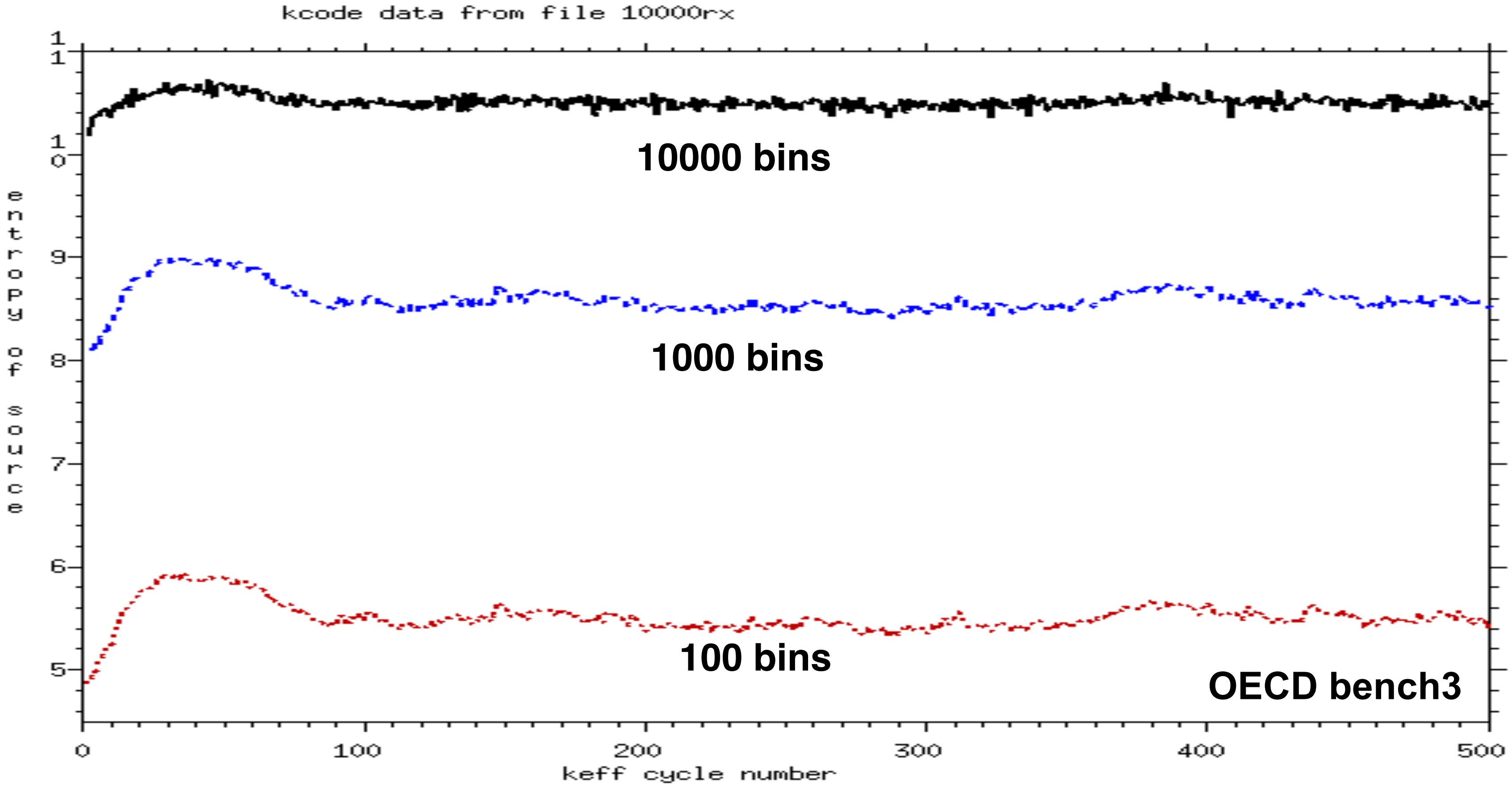




DR = .99+

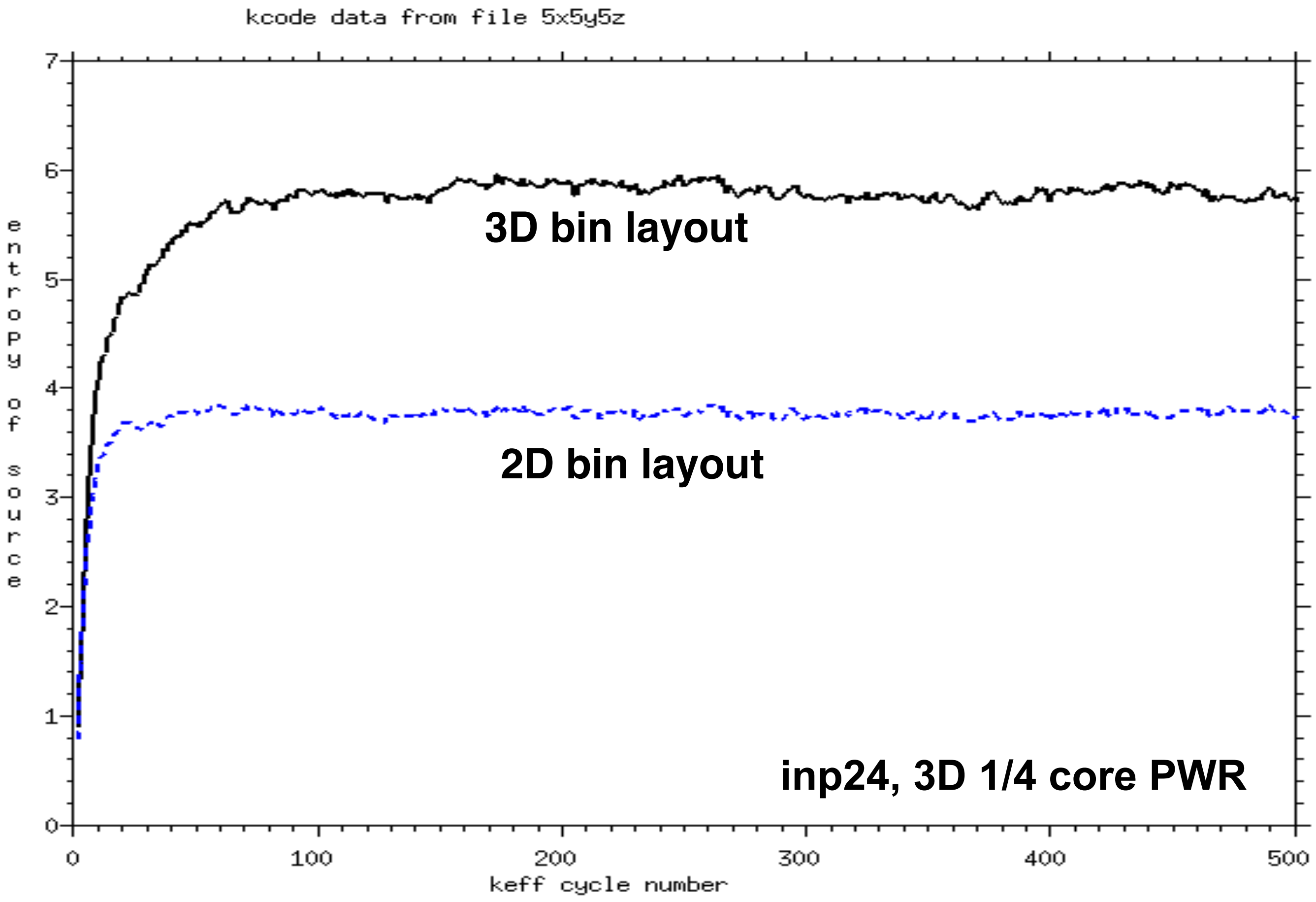
H_{src} Convergence vs Number of Spatial Bins

- For large number of bins, H_{src} approaches uniform upper limit
- Use 10s or 100s of bins, not 1000s or more



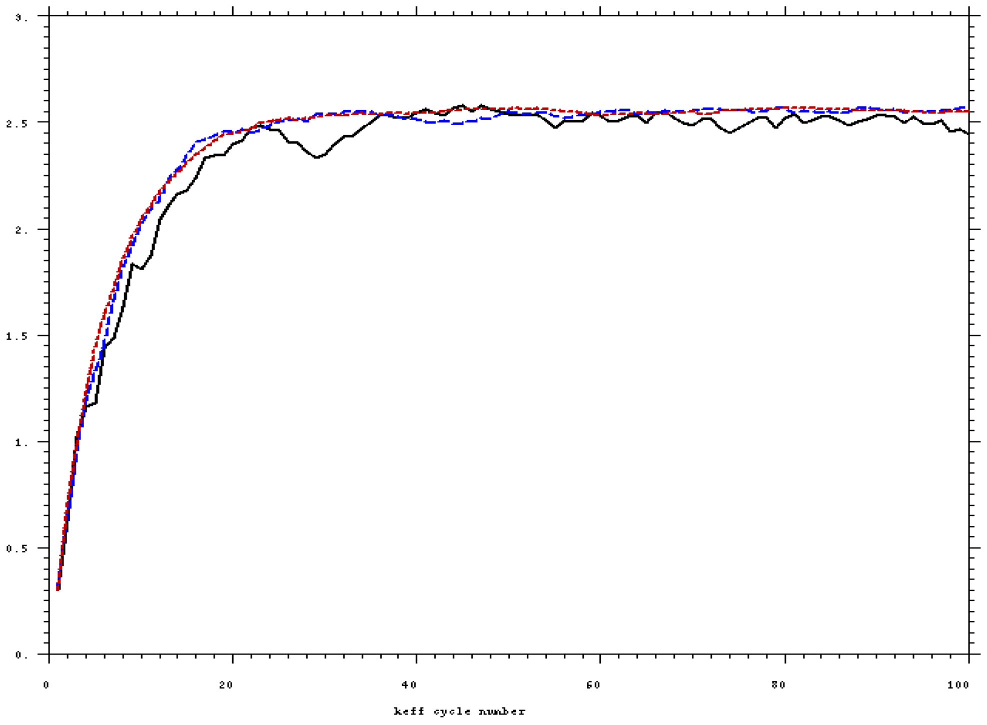
H_{src} and 2D vs 3D Spatial Bins

- For 3D problems, using a 2D bin layout for H_{src} may incorrectly assess convergence
- Important to use 3D bin layout for 3D problems



H_{src} Convergence vs Neutrons per Cycle

- Problems converge at the same rate, for any number of neutrons/cycle. (The rate depends on dominance ratio, ie, physics & geom)
- More neutrons/cycle does <u>not</u> make problems converge faster
- More neutrons/cycle ➔ less noise in convergence plots



Shannon Entropy
Of the Fission Source

<u>for different neutrons / cycle</u>

1000 - black
5000 - blue
20000 - red

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

- MCNP6 will compute & plot H_{src} as an important new tool for assessing problem convergence.

- The recommended MCNP6 procedures for defining spatial tally bins and computing H_{src} are effective for a variety of typical criticality problems.

Wielandt Acceleration

(For future versions of MCNP)

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

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

Wielandt Method

- **Power iteration for modified transport equation**

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

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

$$\Psi^{(n+1)} = \tfrac{1}{\tilde{K}^{(n)}}\cdot\tilde{F}\Psi^{(n)}$$

$$\text{where}\quad \tilde{K}^{(n)} = (\tfrac{1}{K_{eff}^{(n)}}-\tfrac{1}{k_e})^{-1}\quad \text{or}\quad K_{eff}^{(n)} = (\tfrac{1}{\tilde{K}^{(n)}}+\tfrac{1}{k_e})^{-1}$$

- **How to choose k_e**
  - **k_e must be larger than k_0 (but, don't know k_0!)**
  - **k_e must be held constant for all of the histories in a batch, but can be adjusted between batches**
    - Typically, guess a large initial value for k_e, such as k_e=5 or k_e=2
    - Run a few batches, keeping k_e fixed, to get an initial estimate of K_{eff}
    - Adjust k_e to a value slightly larger than the estimated K_{eff}
    - Run more batches, possibly adjusting k_e if the estimated K_{eff} changes

Wielandt Method

- **Convergence**
  - **Eigenfunctions for the Wielandt method are same as for basic power iteration**
  - **Eigenvalues are shifted:**

$$\tilde{k}_J = \left[\frac{1}{k_J} - \frac{1}{k_e} \right]^{-1} \qquad\qquad k_e > k_0 > k_1 > \ldots$$

  - **Expand the initial guess, substitute into Wielandt method, rearrange to:**

$$\Psi^{(n+1)} \approx [\text{cons tan t}] \cdot \left[\vec{u}_0 + \left(\frac{a_1^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_e - k_0}{k_e - k_1} \cdot \frac{k_1}{k_0} \right)^{n+1} \cdot \vec{u}_1 + \ldots \right]$$

$$K^{(n+1)} \approx k_0 \cdot \left[1 + \left(\frac{a_1^{(0)}}{a_0^{(0)}} \right) \cdot \left(\frac{k_e - k_0}{k_e - k_1} \cdot \frac{k_1}{k_0} \right)^{n} \cdot \left(\frac{k_e - k_0}{k_e - k_1} \cdot \frac{k_1}{k_0} - 1 \right) \cdot G_1 + \ldots \right]$$

  - **Additional factor $(k_e\text{-}k_0)/(k_e\text{-}k_1)$ is less than 1 and positive, so that the red terms die out faster than for standard power iteration**

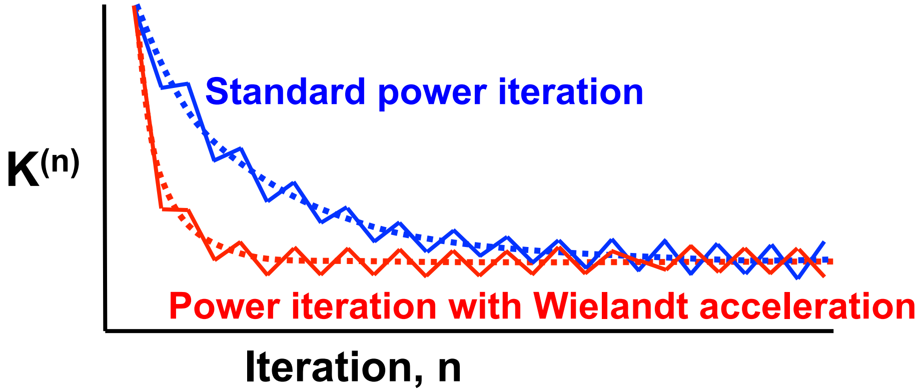
Convergence

- 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

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

➜ Wielandt method will converge in fewer iterations



Monte Carlo Interpretation

- Power iteration with Wielandt acceleration

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

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

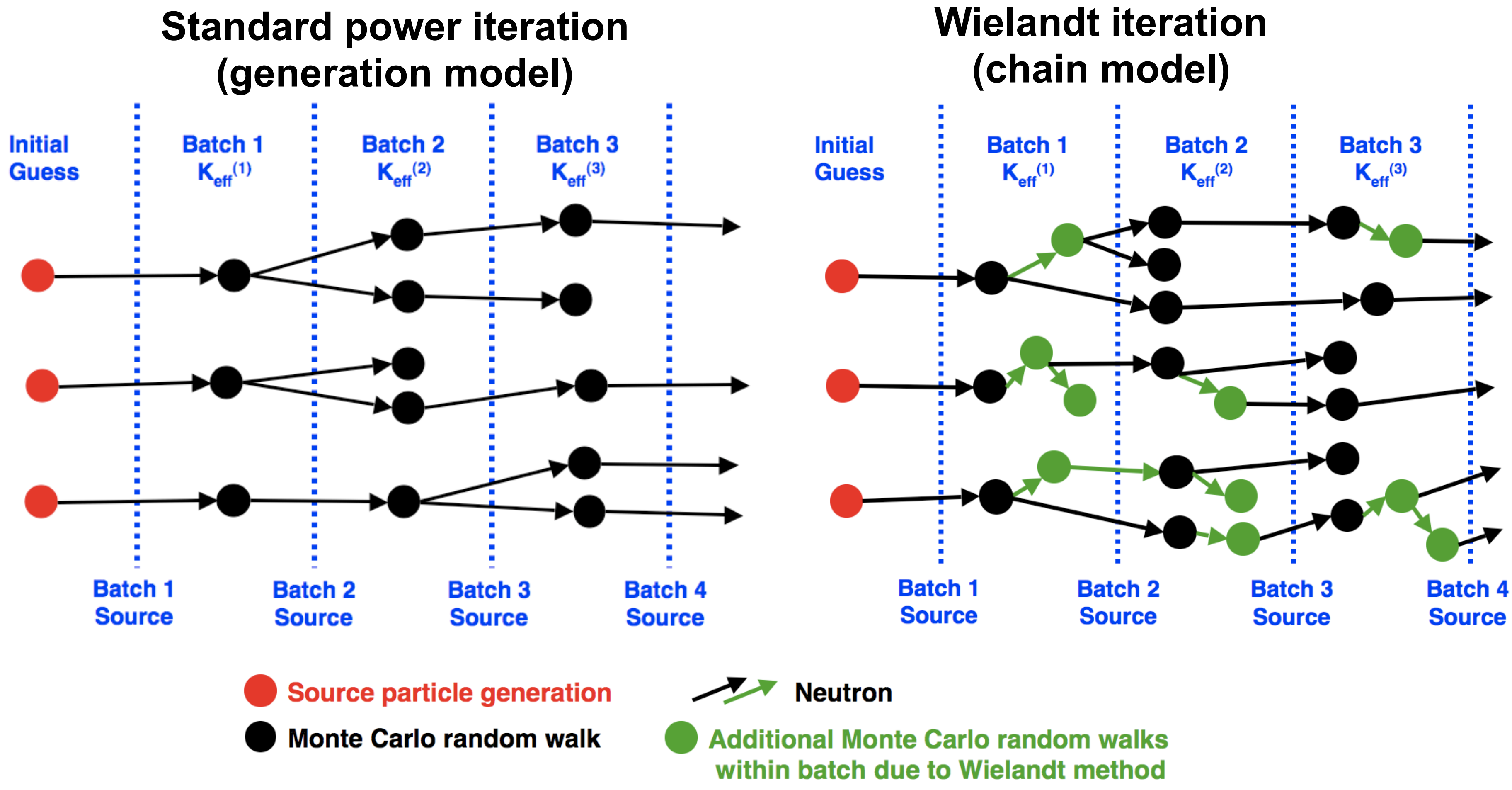
$$n'_e = \left\lfloor wgt \cdot \frac{\nu\Sigma_F}{\Sigma_T} \cdot \frac{1}{k_e} + \xi \right\rfloor$$

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



Standard power iteration (generation model)

Wielandt iteration (chain model)

● Source particle generation

● Monte Carlo random walk

→ Neutron

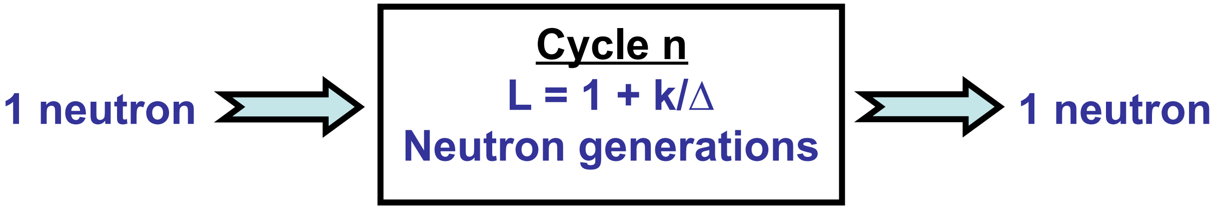
● Additional Monte Carlo random walks within batch due to Wielandt method

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



1 neutron

Cycle n

$L = 1 + k/\Delta$

Neutron generations

1 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

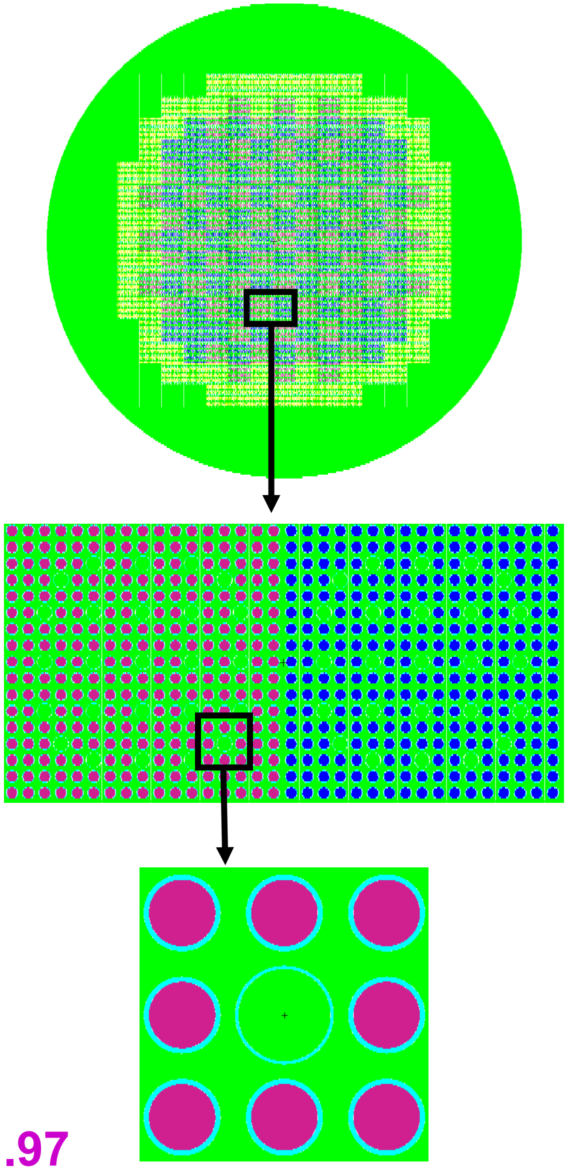
Typical: $\Delta = .1$, .05, or .025

Smaller Δ ➜ larger average chain length, L

➜ more spread in fission sites each cycle

➜ faster convergence

Numerical Testing



DR = .97

2D whole-core PWR test problem (Ueki)

- Ran with different shifts, Δ:
  ∞, 1.0, 0.5, 0.2, 0.1
- Examined convergence of source entropy, H_{src} vs Δ(plots next page)
- Examined FOM = $1 / \sigma^2 T$ vs Δ

Δ	FOM
∞	168 K
1.0	188 K
0.5	212 K
0.2	188 K
0.1	184 K

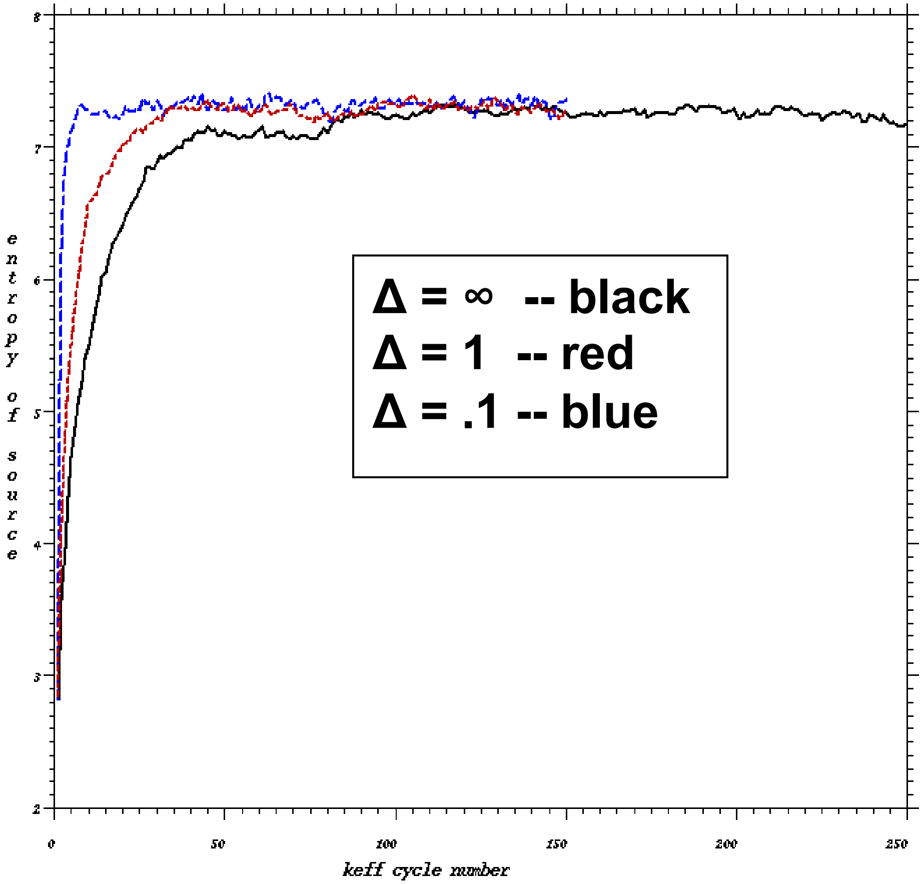
For this problem, FOM was about the same for a range of Δ's

Numerical Testing

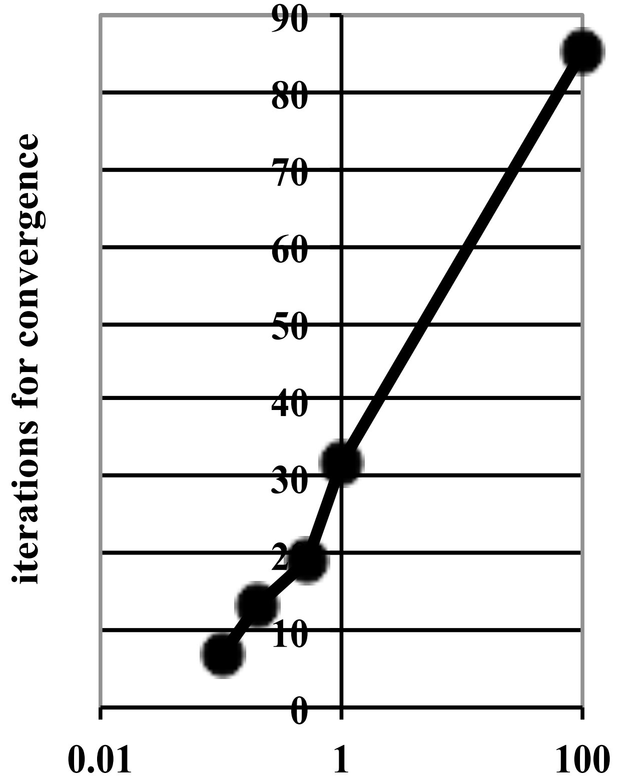
2D PWR test problem

– **Wielandt shift parameter:** $K_e^{(n)} = K^{(n-1)}_{collision} + \Delta$

Convergence of H_{src} vs Δ

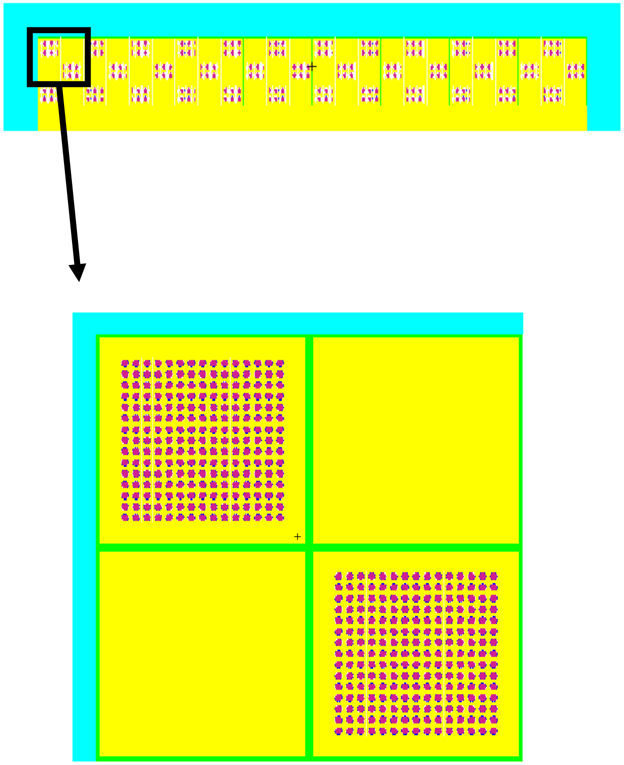


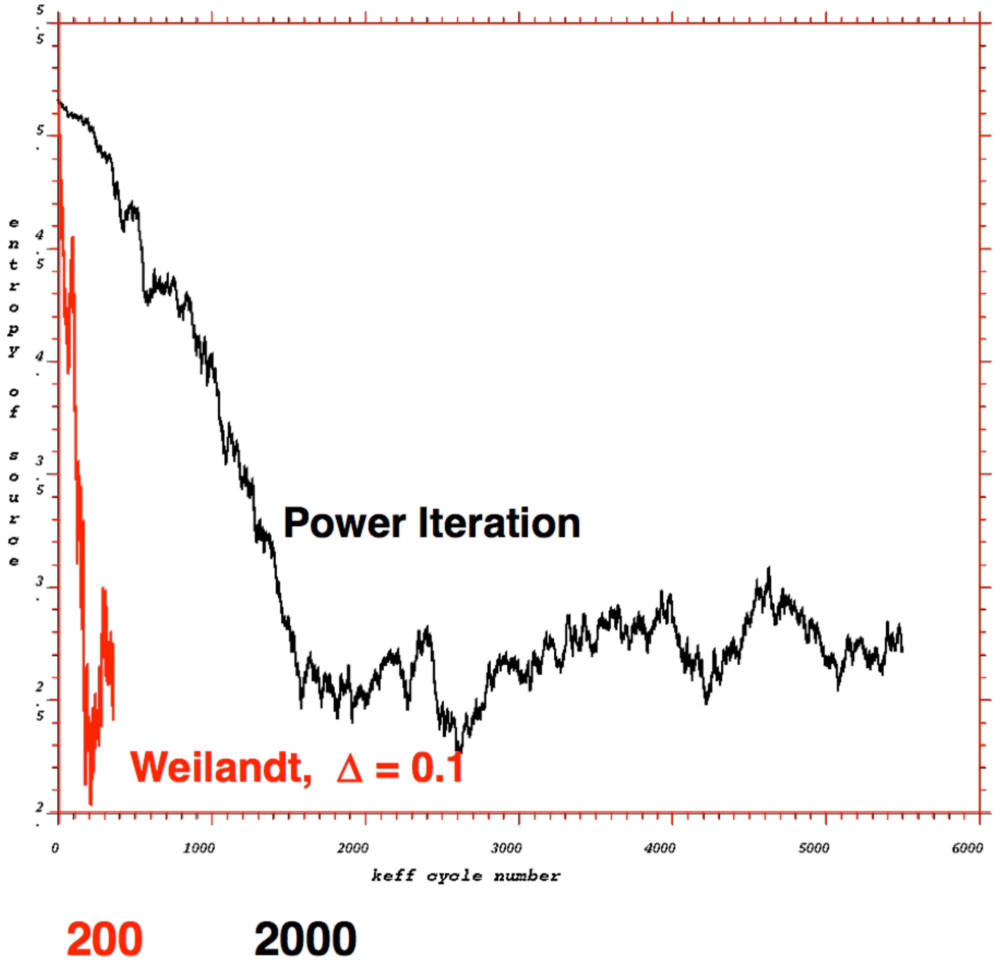
Iterations for convergence vs



Numerical Testing

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





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 MCNP

Superhistory Method

- **Standard generation model, solved by power iteration**

$$\Psi^{(n+1)} = \frac{1}{K_{eff}^{(n)}} \cdot F\Psi^{(n)}$$

- **Superhistory method**
  - **Follow several generations (L) before recomputing K_{eff} and renormalizing**

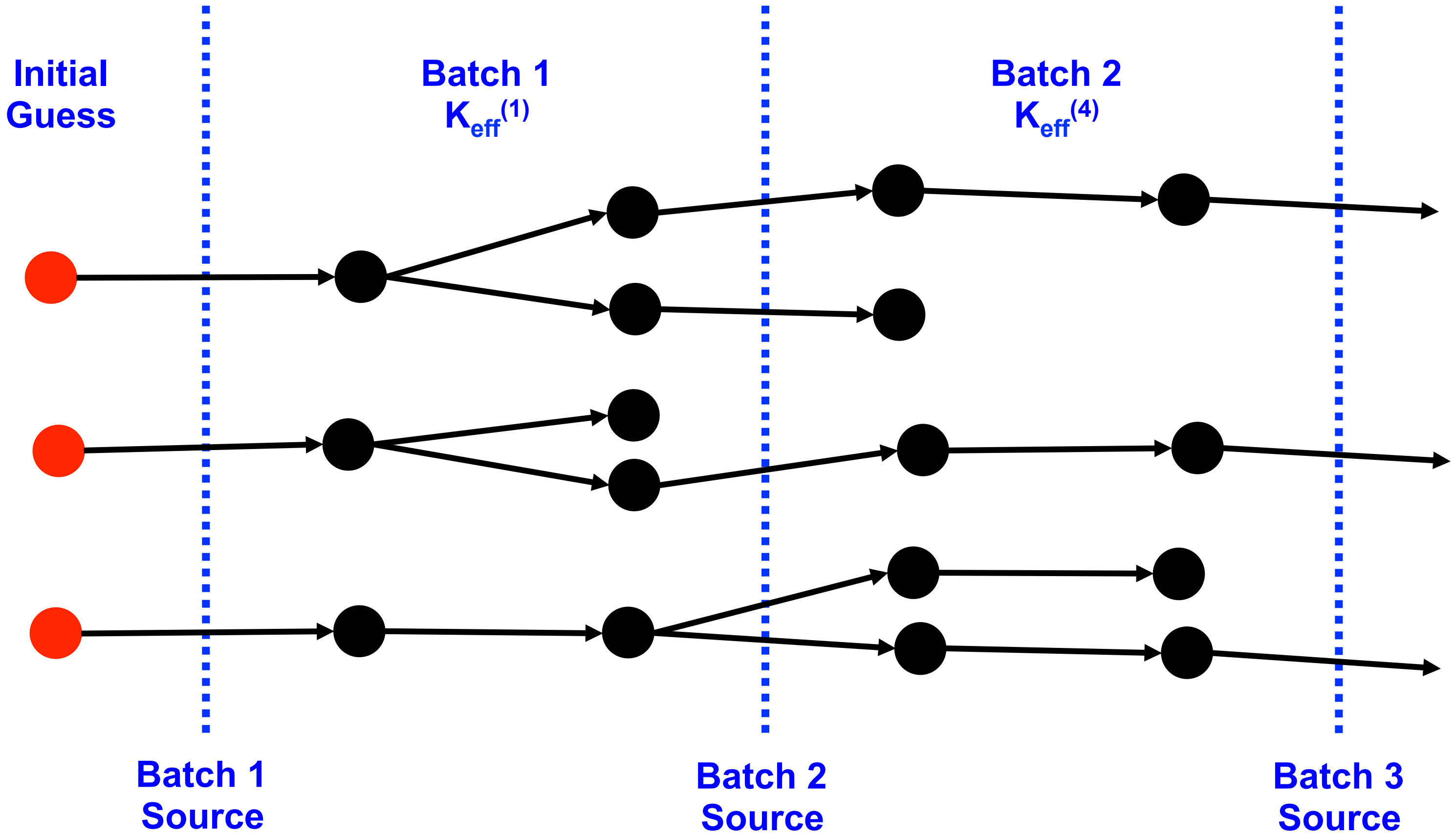
$$\Psi^{(n+1)} = \frac{1}{\tilde{K}^{(n)}} \cdot \tilde{F}\Psi^{(n)}, \qquad \text{with} \quad \tilde{F} = F^L, \quad \tilde{K}^{(n)} = (K_{eff}^{(n)})^L$$

- **Convergence**
  - **Same eigenfunctions as standard power iteration**
  - **Eigenvalues are k_0^L, k_1^L, k_2^L, …**
  - **DR' = DR^L, where DR = dominance ratio for power iteration**
  - **Fewer iterations, but L generations per iteration ➜ same work as power iteration**
  - **Same convergence rate as power iteration**
- **Advantages**
  - **Reduced correlation between iterations**
  - **Fewer renormalizations**

Superhistory Method

- Superhistory Method for Monte Carlo k-effective calculation

Example with L = 2 generations/batch



● Source particle generation

● Monte Carlo random walk

↗ Neutron

Dominance Ratio Calculations

(For future versions of MCNP5)

DR - Overview

- Time-series methods for computing DR
  - Ueki developed a method

    T. Ueki, F.B. Brown, D.K. Parsons, and D.E. Kornreich, "Autocorrelation and Dominance Ratio in Monte Carlo Criticality Calculations," Nuclear Science and Engineering, 145, 279-290 (2003)
  - Recent extensions by Nease & Ueki provide a practical method

    B.R. Nease and T. Ueki, "Time Series Analysis of Monte Carlo Fission Sources – III: Coarse Mesh Projection," Nuclear Science and Engineering, 157, 51-64 (2007)
  - Recent work by Nease & Brown for MCNP5

    B. Nease & F. Brown, "Implementing the Coarse Mesh Method into MCNP for Dominance Ratio Calculation", LA-UR-07-5462 (2007)
  - Accurate, regardless of mesh used for collecting statistics
  - Can be used only after source has converged

- Fission Matrix method
  - $\vec{S} = \frac{1}{k}\bar{F} \cdot \vec{S}$ 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

    G. W. Morrison, J. T. Mihalczo, & D. C. Irving, "REACT and CONVERG Fortran Subroutines for Determining Source Convergence for the O5R Monte Carlo Neutron Transport Code", ORNL-TM-1325, (1966)
  - Approximate, results are very sensitive to mesh
  - Can be used before source has converged

Comparison of Methods

- **Fission matrix method:**
  - Accurate only for fine mesh, large number of mesh cells, N
  - Fission matrix storage varies as N^2

    10 x 10 x 10 mesh - pretty coarse, but requires 10^6 storage locations
  - Need to find eigenvalues/vectors of nonsymmetric NxN matrix

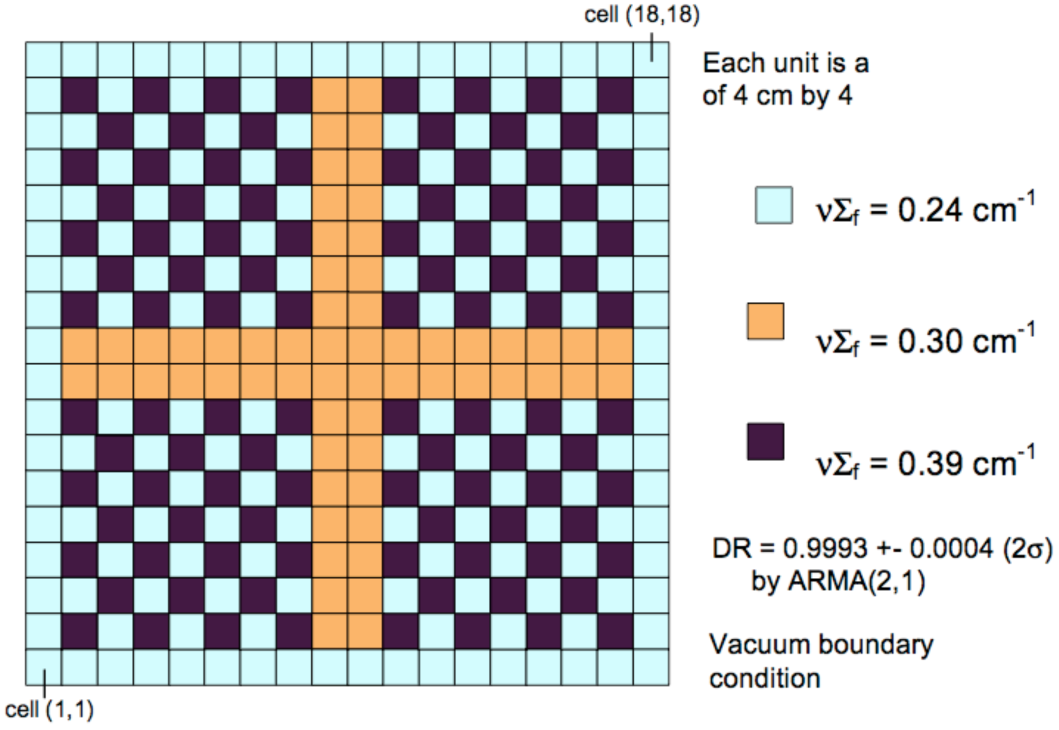
- **Godiva problem example**
  - Fission matrix

mesh size	F-matrix size	DR
2 x 2 x 2	8 x 8	.560
4 x 4 x 4	64 x 64	.602
8 x 8 x 8	512 x 512	.646

  - Coarse Mesh & time series: .677 +- .033

Example

- **From Nease & Ueki (NSE, Sept 2007)**
  - 1-group, 2D problem
  - DR from previous work (Ueki) = .9993 +- .0004
  - DR fission matrix using $(4x4x1)^2$ = .988
    using $(9x9x1)^2$ = .993
    using $(18x18x1)^2$ = .997
  - DR using CMM + time series method = .998 +- .002


cell (18,18)
cell (1,1)
$\nu\Sigma_f = 0.24\ \mathrm{cm}^{-1}$
$\nu\Sigma_f = 0.30\ \mathrm{cm}^{-1}$
$\nu\Sigma_f = 0.39\ \mathrm{cm}^{-1}$

Each unit is a of 4 cm by 4

DR = 0.9993 +- 0.0004 (2σ) by ARMA(2,1)

Vacuum boundary condition

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 Method with time series analysis for DR
  - Can only be used after convergence
  - Independent of mesh size
  - Provides accurate DR

Conclusions

- **Shannon entropy of the fission distribution is a highly effective means of characterizing convergence of the fission distribution**
  - MCNP5 (version 1.40) computes & plots Shannon entropy as an important new tool for assessing problem convergence.
  - It is highly recommended that both k_{eff} and H_{src} be carefully checked for convergence in all Monte Carlo criticality calculations.

- **Wielandt's method improves convergence & reduces inter-cycle correlation, without significant changes in CPU time**
  - Helps to prevent false convergence assessment
  - Eliminates nonconservative underprediction of confidence intervals

- **Can now reliably calculate the dominance ratio using Monte Carlo**
  - Fission matrix for early, approximate DR
  - Coarse-mesh method with time-series for later, accurate DR

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Eigenvalue Calculations – III
Case Studies

F.B. Brown, "K_{eff} of the World" & Other Concerns for Monte Carlo Eigenvalue Calculations", SNA +MC 2010 conference, Tokyo, 17-21 Oct [also LA-UR-10-06874] (2010)

Concerns for MC Eigenvalue Calculations

- **Monte Carlo Criticality Calculations**
  - Methodology
  - Concerns
- **Numerical Results**
  - K_{eff} of the World Problem
  - 1/4-Core PWR Problem
  - Criticality Safety Problem
- **Best Practices**
  - Discussion
  - Conclusions

MC Criticality Calculations

-

Methodology & Concerns

Introduction

- **Several fundamental problems with MC criticality calculations were identified in the 1960s - 1980s:**
  - **Convergence of K_{eff} & source distribution**
  - **Bias in K_{eff} & tallies**
  - **Underprediction bias in tally statistics**

(see Lieberoth, Gelbard & Prael, Gast & Candelore, Brissenden & Garlick)

- **These problems are well-understood & can be readily avoided, if some simple "best practices" guidelines are followed**

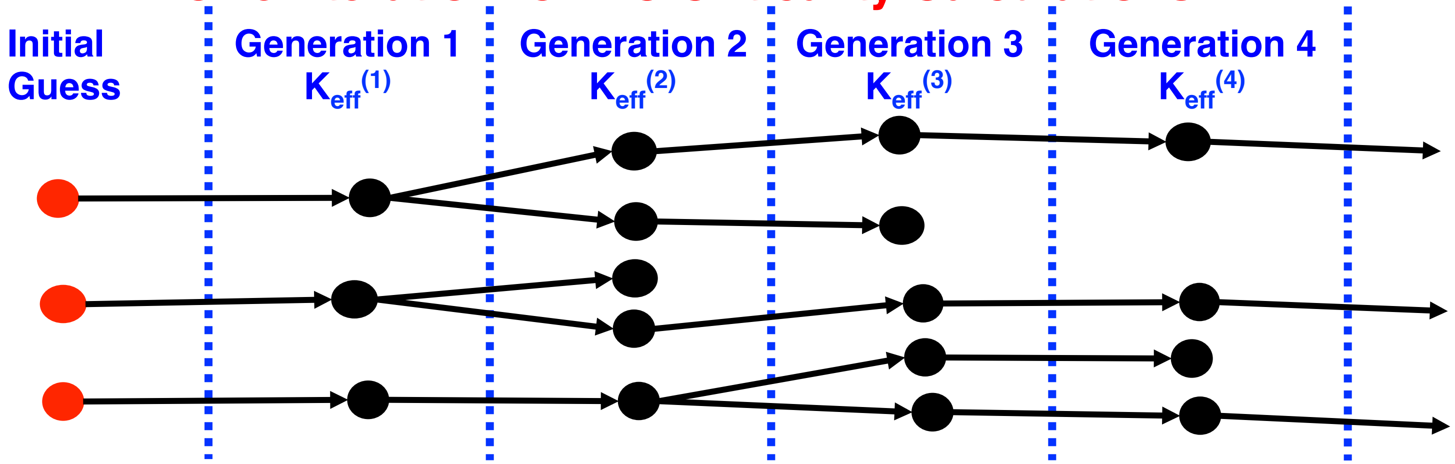
- **Previous discussion of details:**
  - **2008 - PHYSOR - Monte Carlo workshop**
  - **2009 - M&C - Monte Carlo workshop**
  - **2009 - NCSD - 'Best Practices' paper**
  - **2010 - PHYSOR - Monte Carlo workshop**

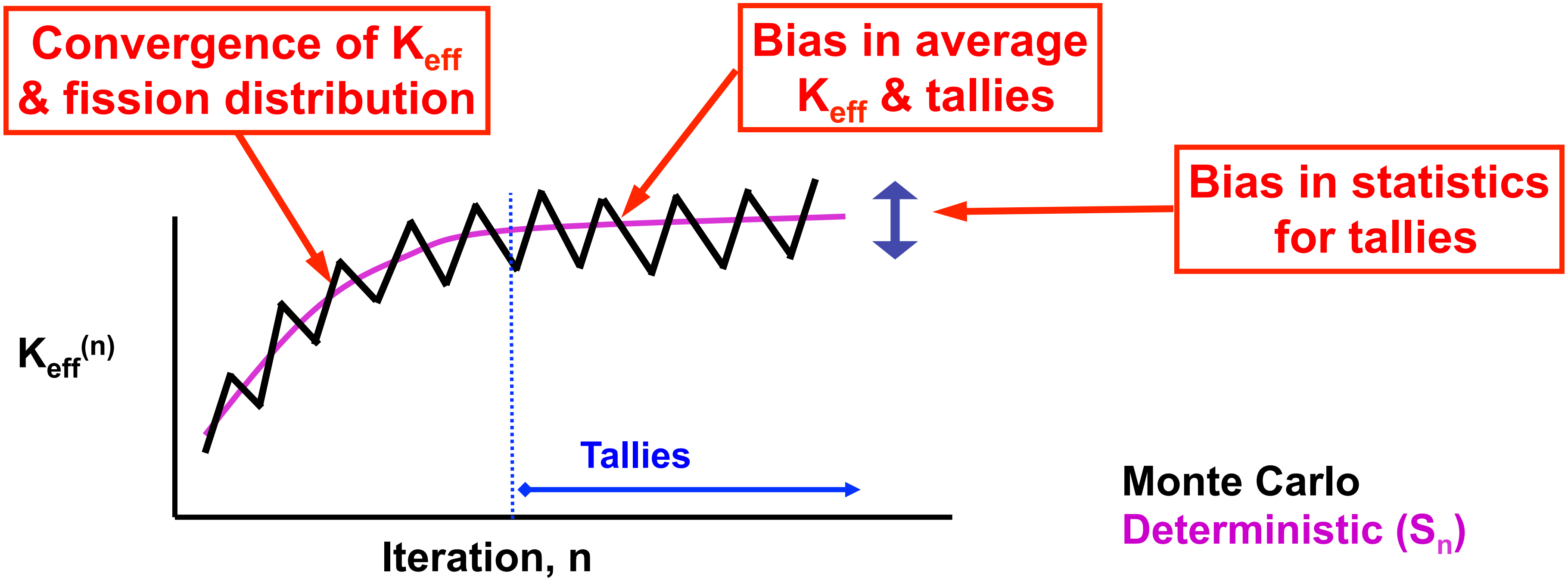
Presentations available at

http://mcnp.lanl.gov/publication/mcnp_publications.html

Concerns

Power Iteration for MC Criticality Calculations





Convergence of K_{eff} & fission distribution

Bias in average K_{eff} & tallies

Bias in statistics for tallies

Convergence

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

- Power iteration convergence is well-understood:

n = cycle number, k_0, u_0 - fundamental, k_1, u_1 - 1st higher mode

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

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

  - 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}.

Bias in K_{eff} & Tallies

- **Power iteration is used for Monte Carlo K_{eff} calculations**
  - **For one cycle (iteration):**
    - $\mathbf{M_0}$ neutrons start
    - $\mathbf{M_1}$ neutrons produced, $E[\,\mathbf{M_1}\,] = K_{eff} \cdot \mathbf{M_0}$
  - **At end of each cycle, must renormalize by factor M_0 / M_1**
  - **Dividing by stochastic quantity (M_1) introduces bias in K_{eff} & tallies**
- **Bias in Keff, due to renormalization**

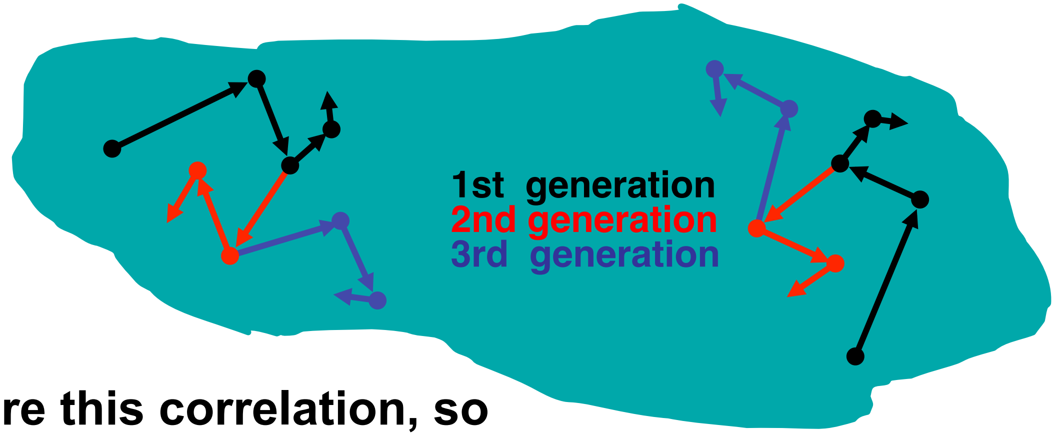
$$\text{Bias in } K_{eff} \propto \frac{1}{M}$$

M = neutrons / cycle

  - **Power & other tally distributions are also biased, produces "tilt"**

Bias in Statistics

- **MC eigenvalue calculations are solved by power iteration**



– **Tallies for one generation are spatially correlated with tallies in successive generations**

– **The correlation is positive**

– **MCNP & other MC codes ignore this correlation, so computed statistics are smaller than the real statistics**

– **Errors in statistics are small/negligible for K_{eff}, may be significant for local tallies (eg, fission distribution)**

– **Running more cycles or more neutrons/cycle does not reduce the underprediction bias in statistics**

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

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

Numerical Results

-

K_{eff} of the World Problem

Introduction

Elliot Whitesides, 1971:

… if one attempts to calculate the k_{eff} of the world using a Monte Carlo calculation, what keff would be computed assuming that there are several critical assemblies located around the world?

The answer would likely be the k_{eff} of the world with no critical assemblies present. …

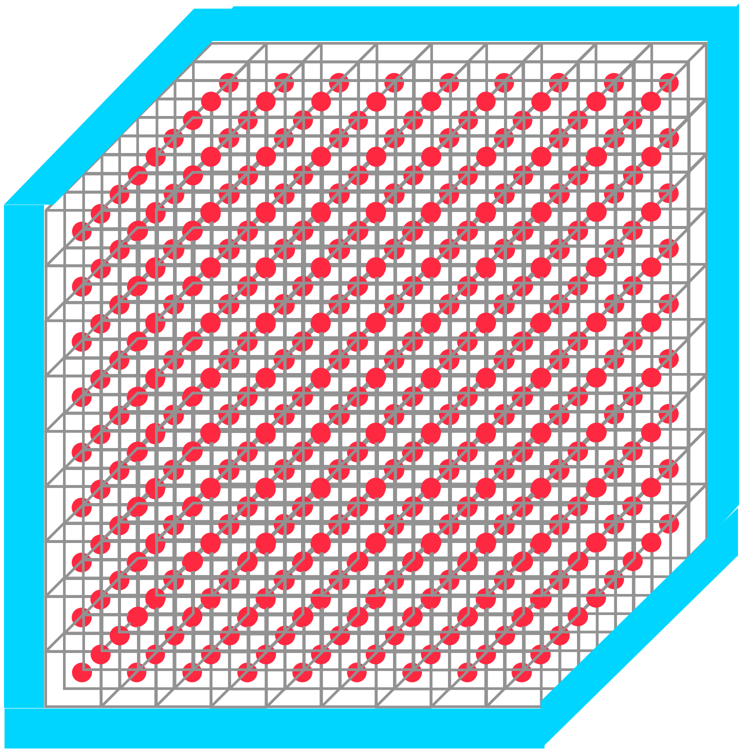
… The erroneous results for these types of problems are the result of the failure of the calculation to converge the source to the fundamental source mode. …

… unless the correct fission distribution is achieved, the results will most likely be nonconservative.

Whitesides' Model Problem

9 x 9 x 9 array of Pu-239 spheres

- 729 spheres
- Void between spheres
- Surrounded by 30 cm water
- Sphere radii ~ 4 cm
- Pitch = 60 cm



- MCNP5-1.60 + ENDF/B-VII.0 data
- For uniform array of identical spheres with surrounding water, sphere radii adjusted to r = 3.9 cm, so that

  Keff = .9328 ± .0002

- Single bare sphere, r=4.928 cm,

  Keff = 1.0001 ± .0002

- Whitesides' model problem:

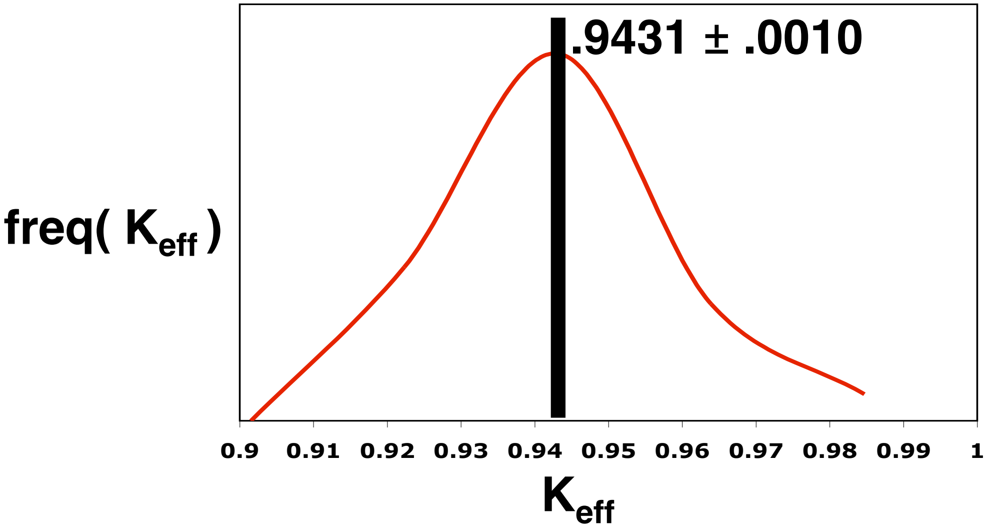
  Replace center sphere of array by larger (critical) sphere

Should be supercritical - is it ?

Whitesides' Problem, circa 1971

- Due to severe computer limitations ~1971, KENO defaults were:
  - 300 neutrons/cycle
  - Discard first 3 cycles
  - Run 100 more cycles

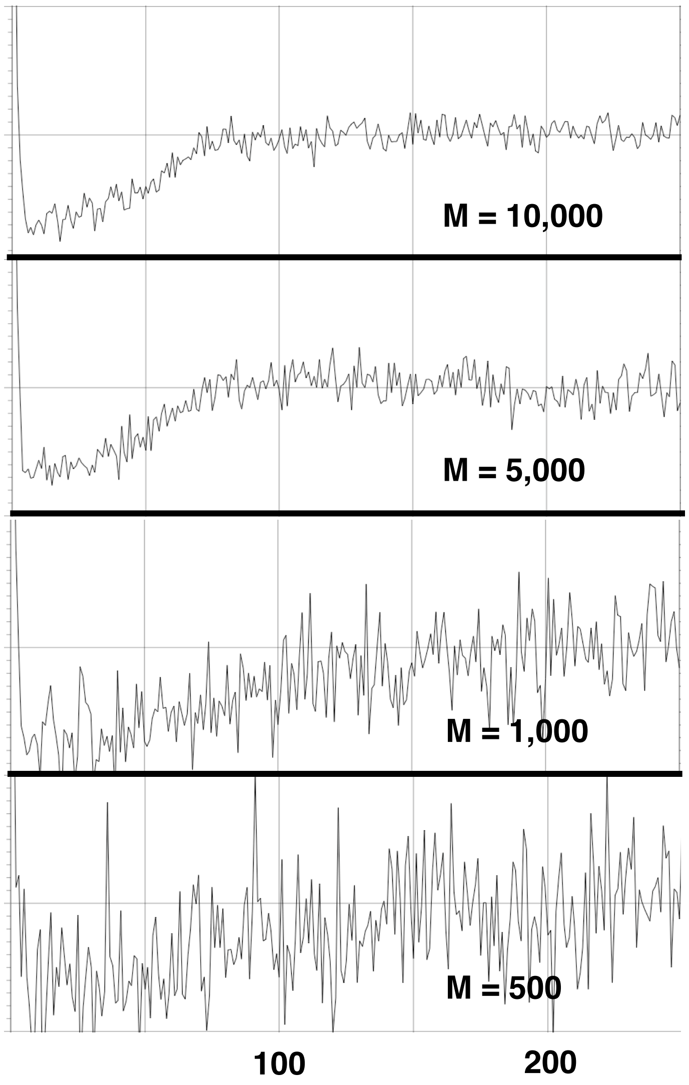
- If MCNP5 is run using the 1971 KENO defaults, 200 independent replica calculations give:
  - Average of 200 replicas: K_{eff} = .9431 ± .0010
  - None of the 200 calculations produced K_{eff} > 1
  - Distribution of replica results:



Convergence

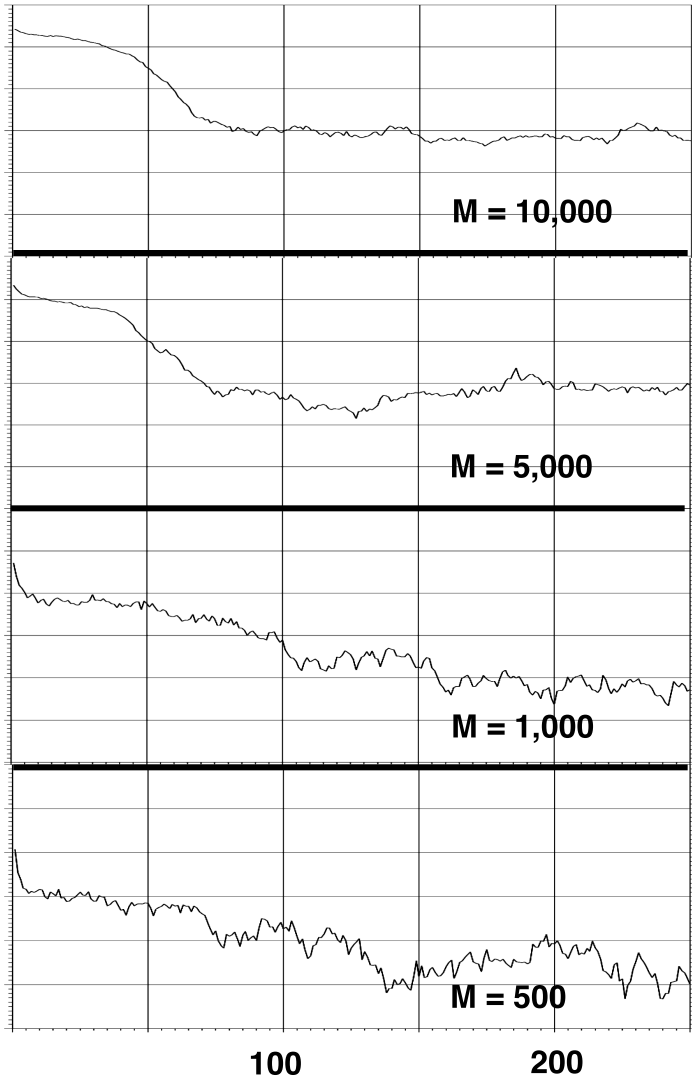
K_{eff} vs cycle, various M

M = neutrons/cycle



H_{src} vs cycle, various M

M = neutrons/cycle



Initial source guess = uniform sampling of points at sphere centers

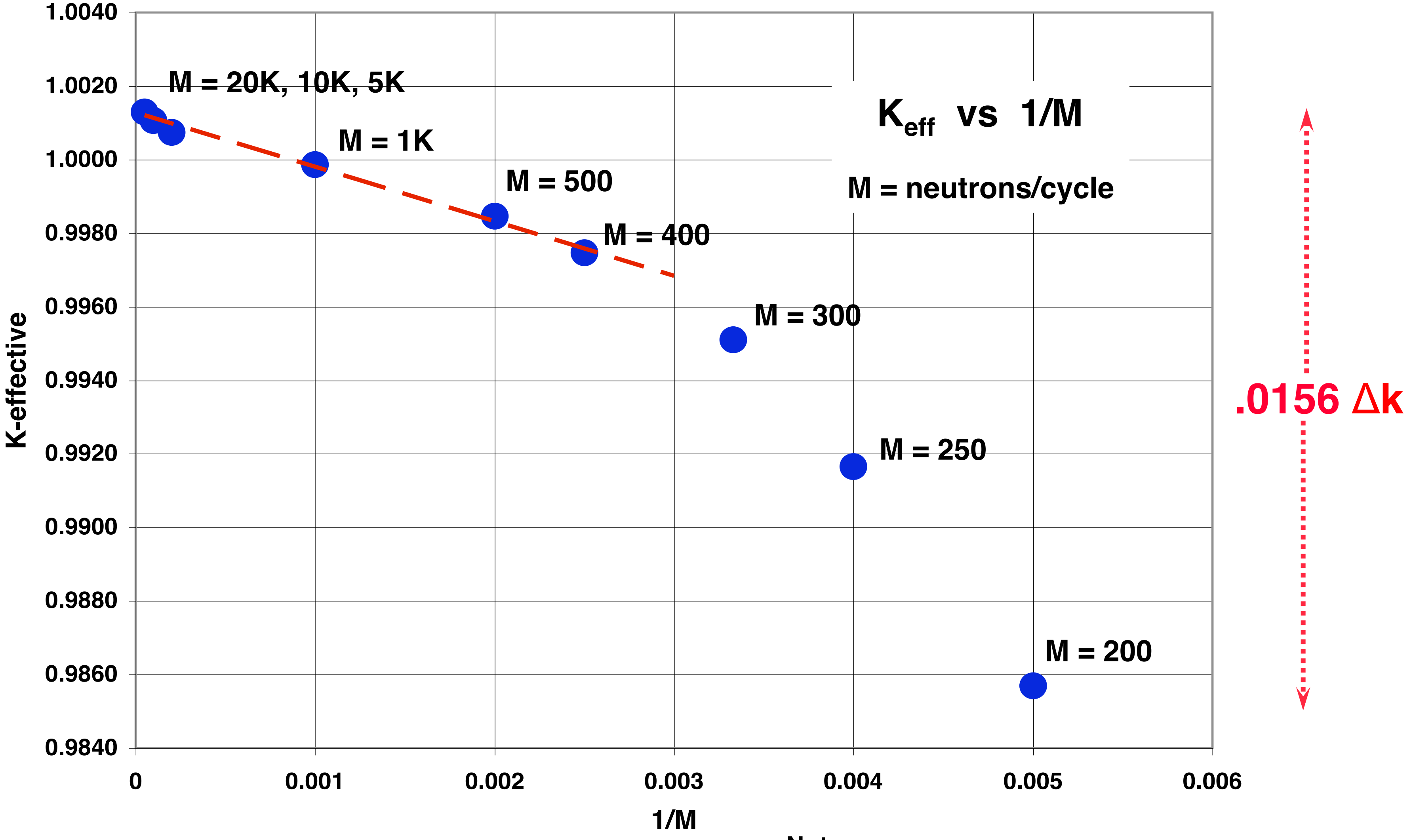
K_{eff} converges in 75-100 cycles

H_{src} converges in 100-150 cycles

Must discard 150 or more initial cycles

Convergence depends on the dominance ratio & source guess, NOT on neutrons/cycle

K_{eff} Bias



Notes:

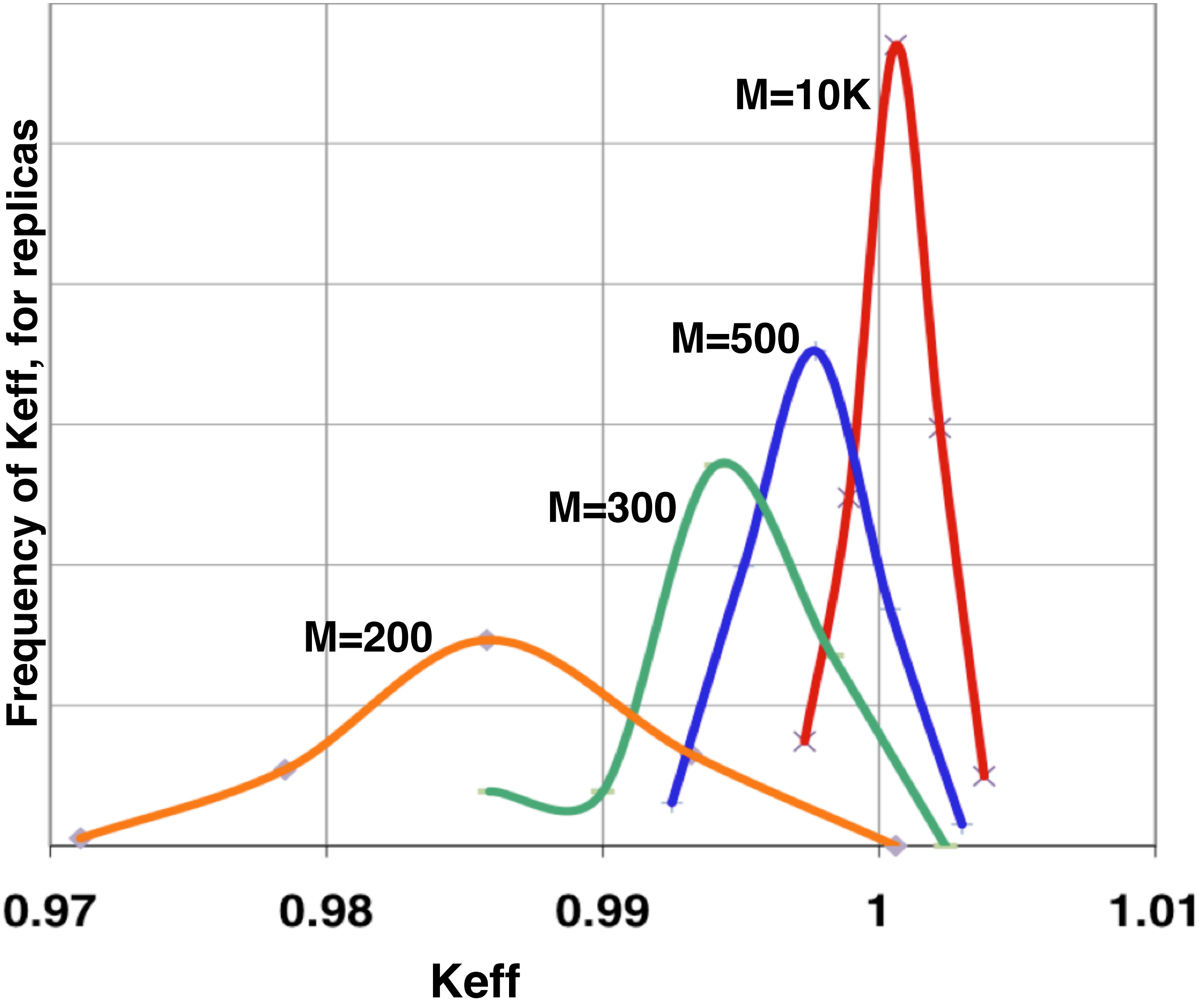
- All cases discarded the first 150 cycles
- All cases used 10M neutrons in active cycles
- All cases: σ ~ .00025, smaller than plot markers

Historical note:

When this problem was first proposed in 1971,
the default batch size for KENO was 300 neutrons/cycle

K_{eff} Bias

Distribution of K_{eff} for 200 replicas, various M = neuts/cycle



Discussion & Conclusions

- **The original 1971 version suffered from:**
  - Computers: small memory & slow
  - Discard only 3 cycles: not converged
  - 300 neutrons/cycle: K_{eff} bias - too low, nonconservative
  - 300 neutrons/cycle: undersampled the source (729 spheres)
  - No tools were available for diagnosing fission distribution convergence (today, we have Shannon entropy & other diagnostics)

- **If (1) enough initial cycles are discarded (150 or more), and**
  (2) enough neutrons/cycle are used (10K or more),

  then the "K-effective of the World" problem is actually not a difficult problem to solve

Numerical Results

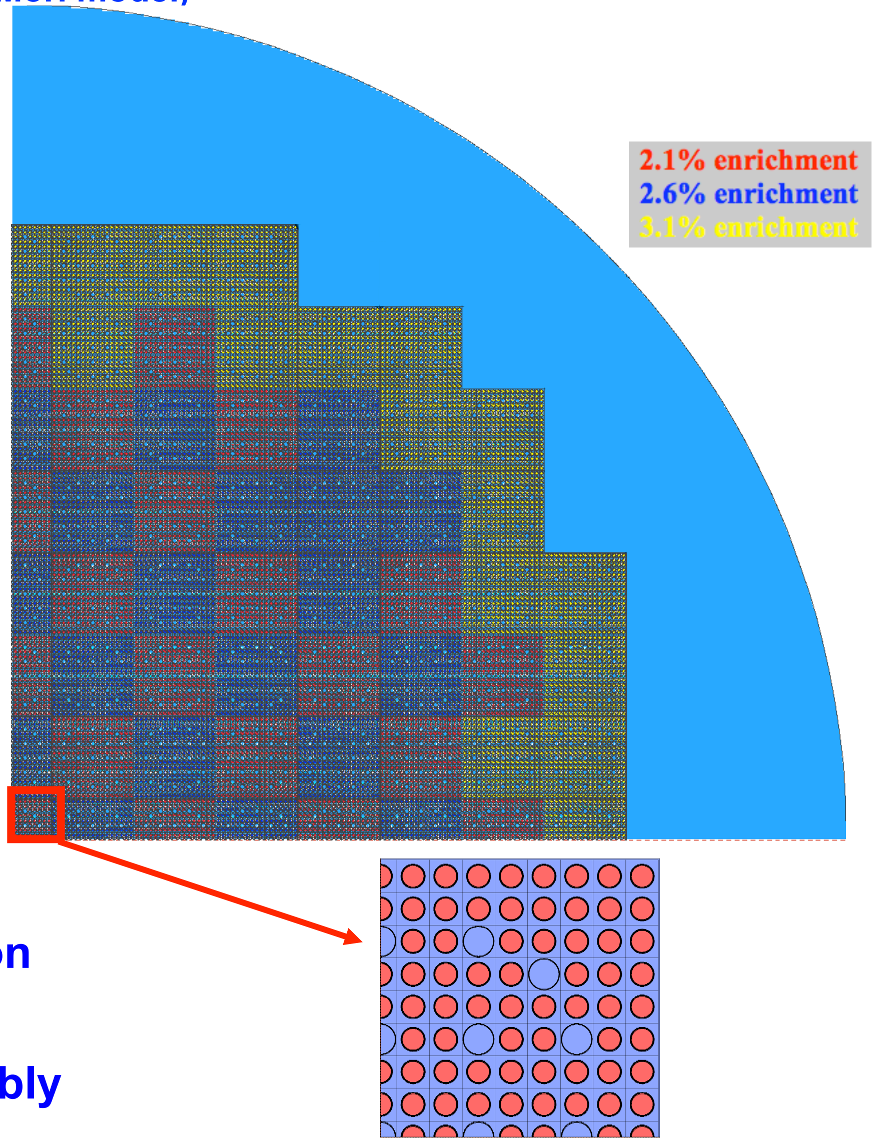
-

1/4-Core PWR

Example Problem - Reactor

2D quarter-core PWR

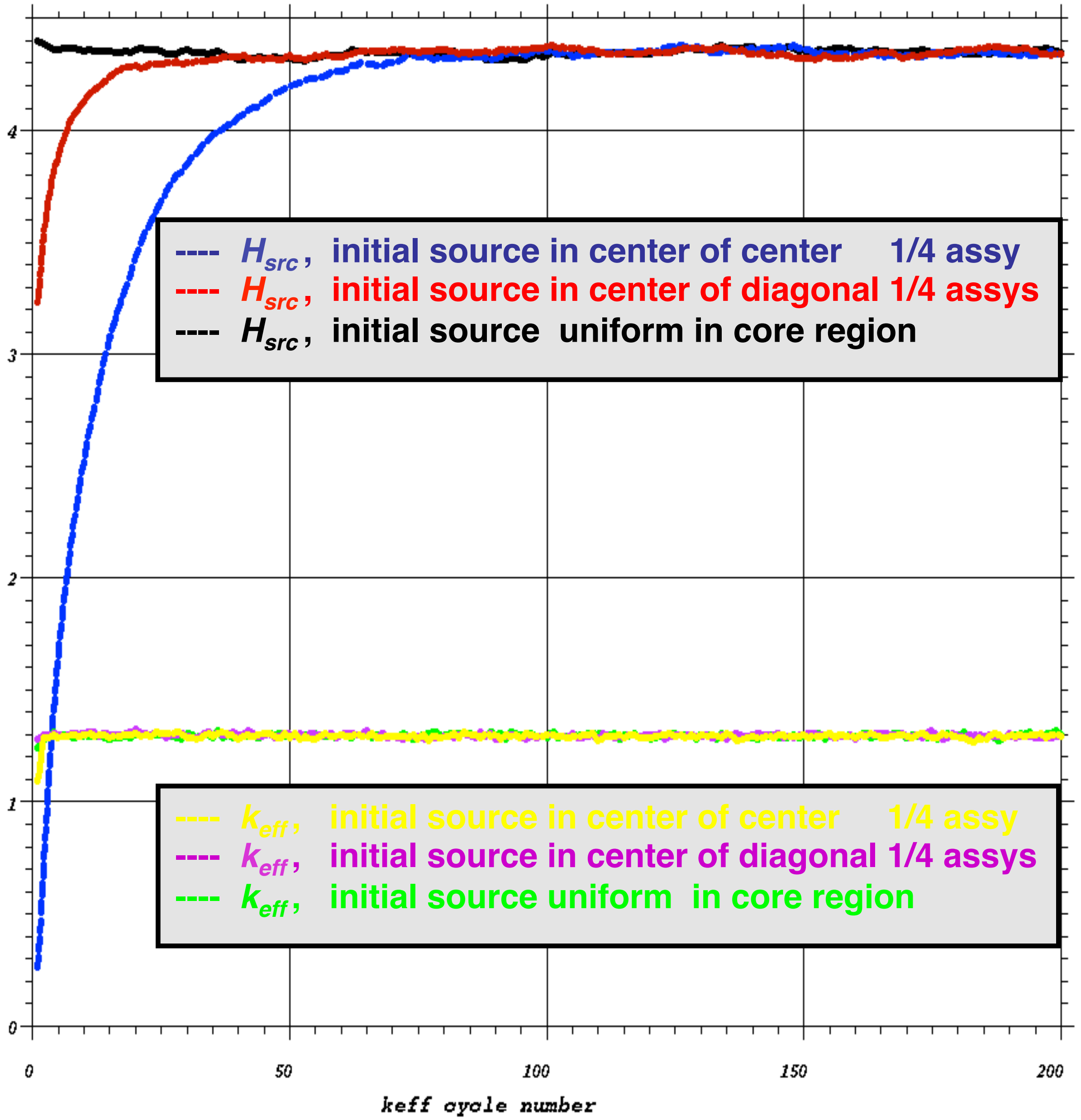
(Nakagawa & Mori model)

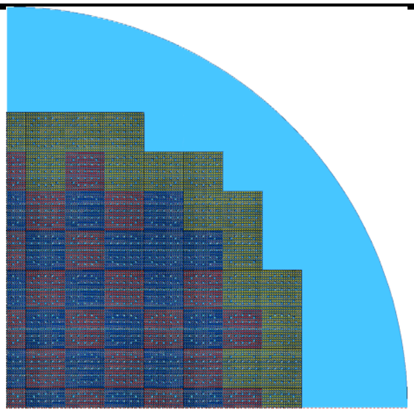


- **48 1/4 fuel assemblies:**
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes for control rods or detectors
- **Each assembly:**
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- **Dominance ratio ~ .96**

- 125 M active neutrons for each calculation
- ENDF/B-VII data, continuous-energy
- Tally fission rates in each quarter-assembly

Convergence



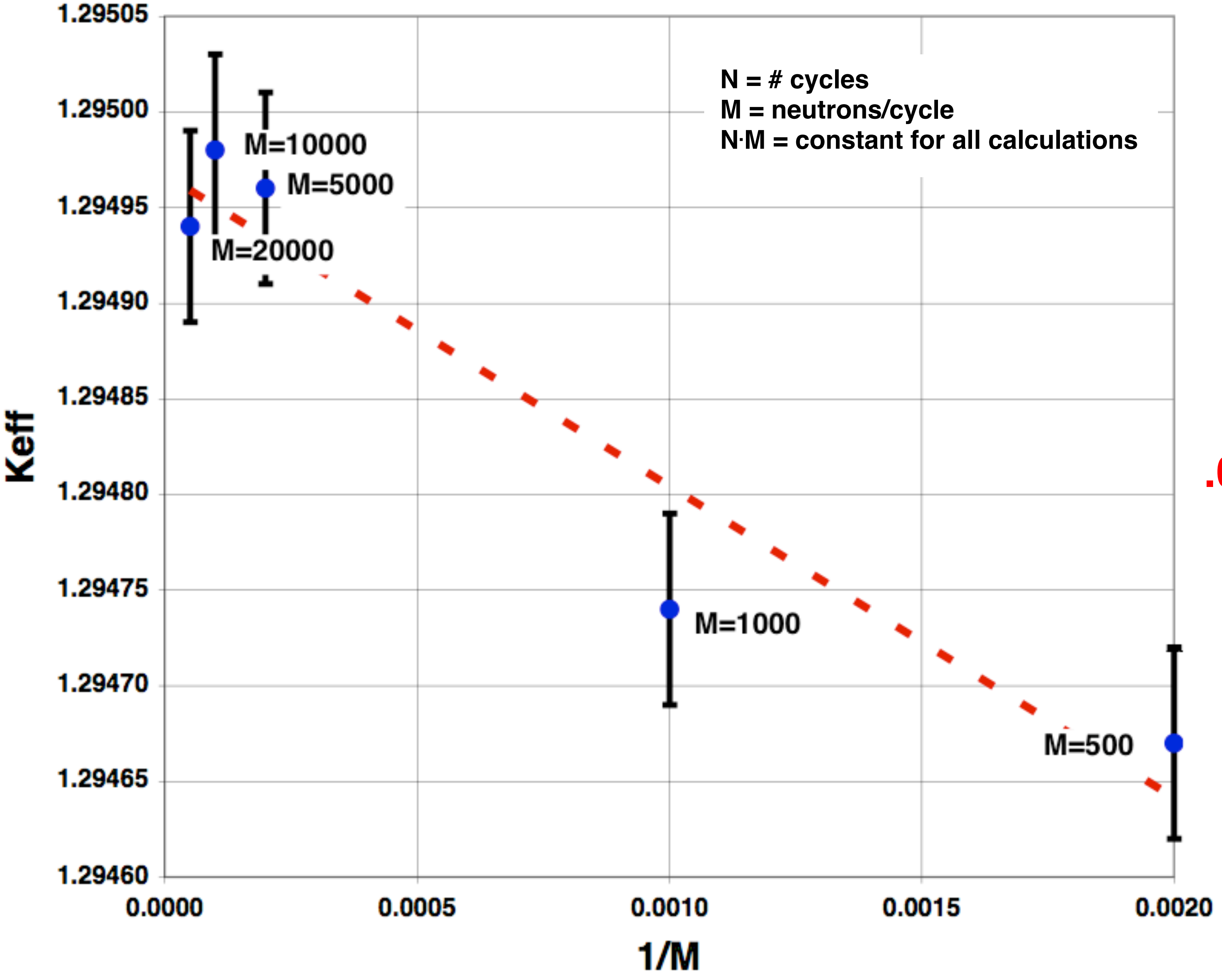


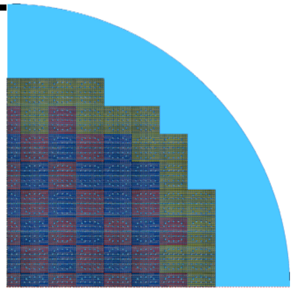
K_{eff} **converges sooner than the fission distribution**

H_{src} **=**

- **Shannon entropy of fission source distribution**
- **A metric for assessing convergence of the distribution**
- **Computed/plotted by MCNP**

Bias in K_{eff}





.0003 Δk

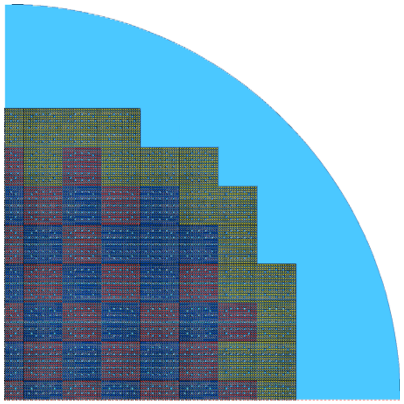
Bias in Tallies

0.0	-0.5	-0.6	-0.2	-0.3	0.5	0.8								
-0.2	-0.7	-0.8	0.1	0.3	0.7	0.6								
-0.5	-0.7	-0.7	0.0	0.3	0.7	1.0	1.3	1.2	1.6	2.0				
-0.1	-0.7	-0.8	0.2	0.3	0.8	1.1	1.2	1.2	1.3	2.4				
-0.4	-0.6	-0.5	0.0	-0.1	0.2	0.7	0.6	1.4	2.0	1.9	2.7	3.2		
-0.7	-0.9	-0.8	-0.4	0.2	0.5	0.4	1.0	1.2	1.6	2.0	1.6	2.6		
-0.6	-0.3	-0.7	-0.6	-0.6	0.3	0.8	1.1	1.2	1.5	1.1	1.7	1.8		
-0.5	-0.8	-1.0	-0.8	-0.5	0.2	0.8	0.9	1.2	1.2	1.4	1.3	1.9		
-0.5	-0.9	-0.8	-1.0	-0.6	0.2	0.2	0.6	0.9	1.1	0.8	0.7	1.1	0.9	1.5
-0.9	-0.9	-1.1	-1.0	-0.9	-0.1	0.2	0.6	0.8	0.6	0.6	0.6	1.3	1.2	1.1
-1.2	-1.3	-1.2	-1.0	-0.6	-0.5	-0.3	0.2	0.9	0.7	1.1	0.9	1.3	1.2	1.1
-1.3	-1.5	-1.0	-0.9	-0.7	-0.5	-0.6	0.3	0.4	0.5	1.3	1.4	2.1	1.9	1.6
-1.7	-1.5	-1.1	-1.1	-0.6	-0.5	-0.2	-0.1	0.3	0.6	1.0	1.7	2.0	2.1	1.9
-1.5	-1.5	-1.4	-1.0	-1.1	-0.8	0.0	0.1	0.3	0.4	1.0	1.0	1.5	3.1	2.3
-1.6	-1.6	-1.2	-1.2	-0.6	-0.7	-0.4	-0.2	0.1	0.2	0.5	1.6	2.1	2.4	2.3

Percent errors in 1/4-assembly fission rates using 500 neutrons/cycle

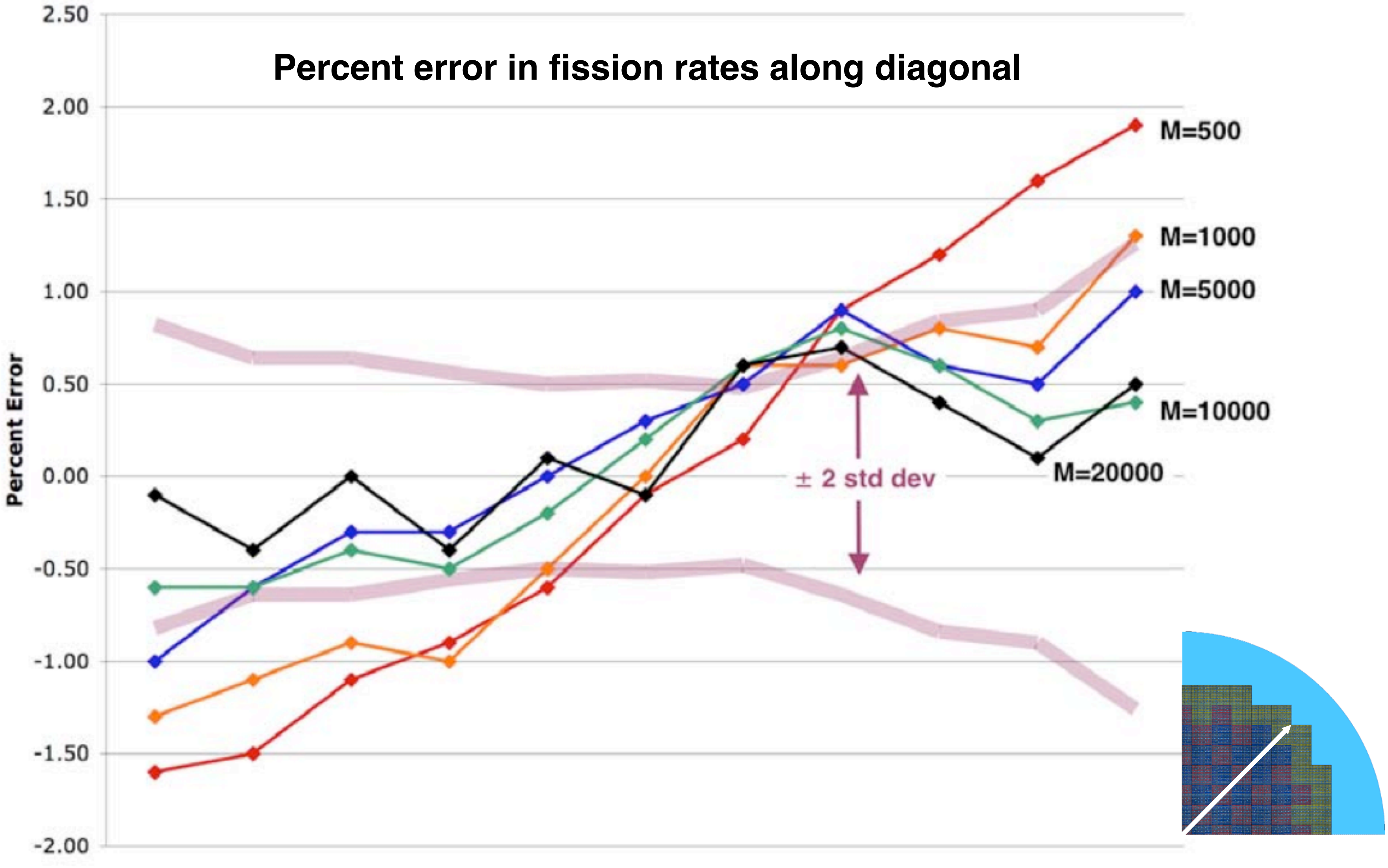
Errors of -1.7% to +3.2%

Statistics ~ .1% to .3%



Reference: ensemble-average of 25 independent calculations, with 25 M neutrons each & 20K neutrons/cycle

Bias in Tallies



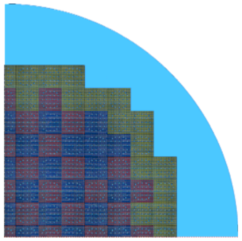
Bias in σ's

True relative errors in 1/4-assembly fission rates, as multiples of calculated relative errors, $\sigma_{TRUE} / \sigma_{MCNP}$

3.4	3.1	2.7	2.7	2.6	2.3	2.7								
3.3	3.7	3.6	3.7	3.7	2.7	2.9								
3.8	3.8	3.9	4.0	3.6	3.3	3.0	2.9	2.5	2.5	2.2				
3.8	3.9	4.2	3.3	3.5	3.4	3.2	3.6	3.0	3.0	2.8				
3.9	3.6	3.5	3.3	3.4	3.4	4.0	3.9	3.5	3.2	3.1	2.5	1.7		
4.1	3.8	3.5	3.2	2.9	2.6	2.9	3.2	3.1	2.8	2.7	1.9	1.7		
3.4	3.4	3.2	3.5	2.6	2.4	2.6	3.0	2.9	2.9	2.8	2.3	2.1		
4.2	3.5	3.4	3.1	2.7	2.3	2.0	2.4	2.5	2.5	2.1	2.3	2.3		
3.9	3.6	3.1	2.9	2.3	1.9	1.9	2.3	2.4	2.9	2.7	2.7	2.2	2.8	2.3
3.7	3.3	3.6	2.4	2.2	2.2	2.5	1.8	2.2	2.6	2.7	2.9	2.5	2.4	2.5
3.0	3.1	3.0	2.2	2.2	2.1	2.4	2.5	2.4	2.6	2.7	2.6	2.7	3.0	2.6
2.9	3.7	3.3	2.6	2.5	2.8	3.0	2.9	3.5	3.2	3.3	3.1	3.1	3.2	3.3
3.2	3.1	2.9	3.1	3.2	3.3	3.5	3.5	3.6	3.9	3.7	3.9	3.5	3.4	2.9
3.4	3.0	3.1	3.6	3.4	3.5	3.9	3.7	4.0	4.3	4.0	4.3	3.8	4.2	3.5
3.5	3.2	2.8	3.5	3.8	3.9	3.9	3.9	4.1	4.1	4.6	4.4	4.7	4.5	3.8

Average factor = 3.1

Calculated uncertainties are 1.7 to 4.7 times smaller than true uncertainties



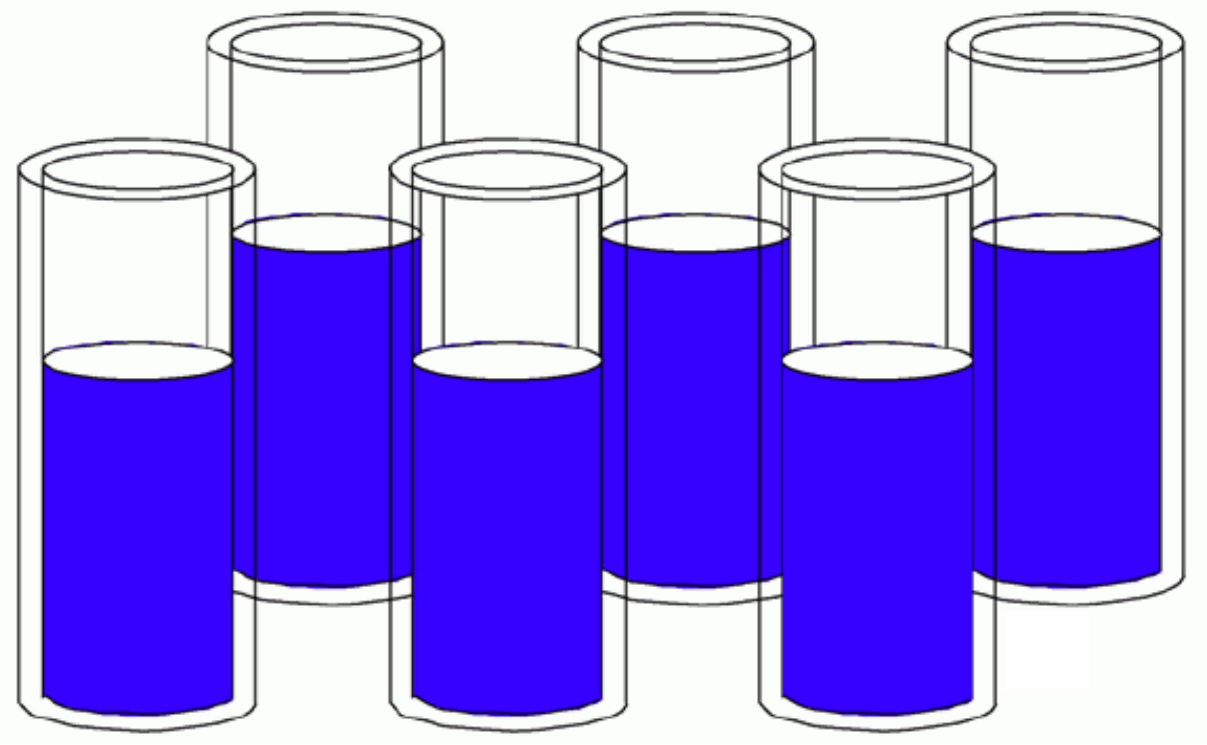
Numerical Results

-

Crit-Safety Problem

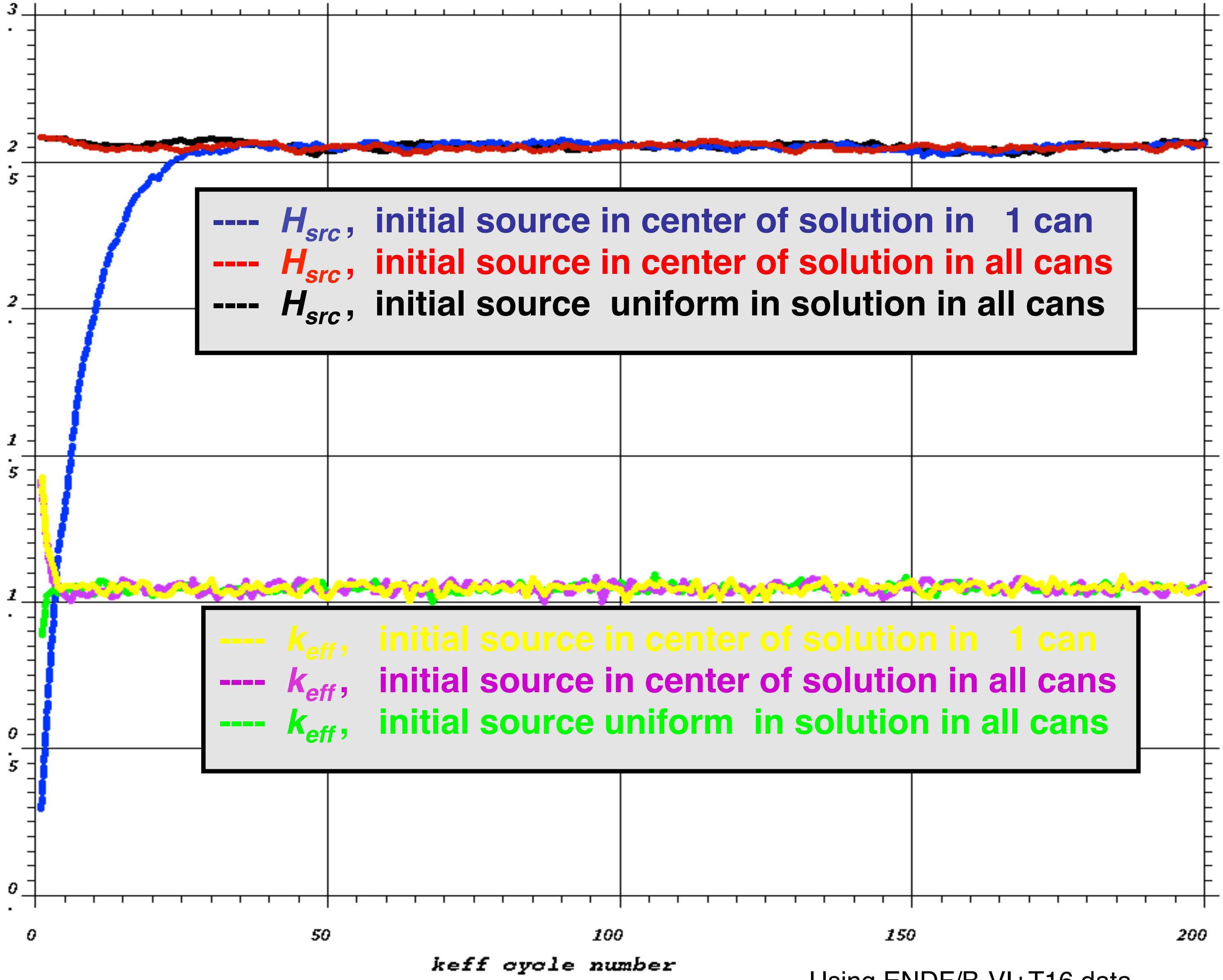
Example Problem - Criticality Safety

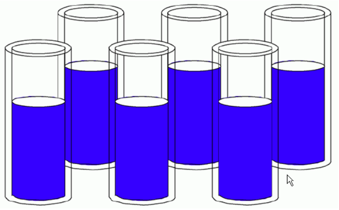
2 x 3 array of steel cans containing plutonium nitrate solution



From MCNP Criticality Primer (chap 5) & MCNP Criticality Classes

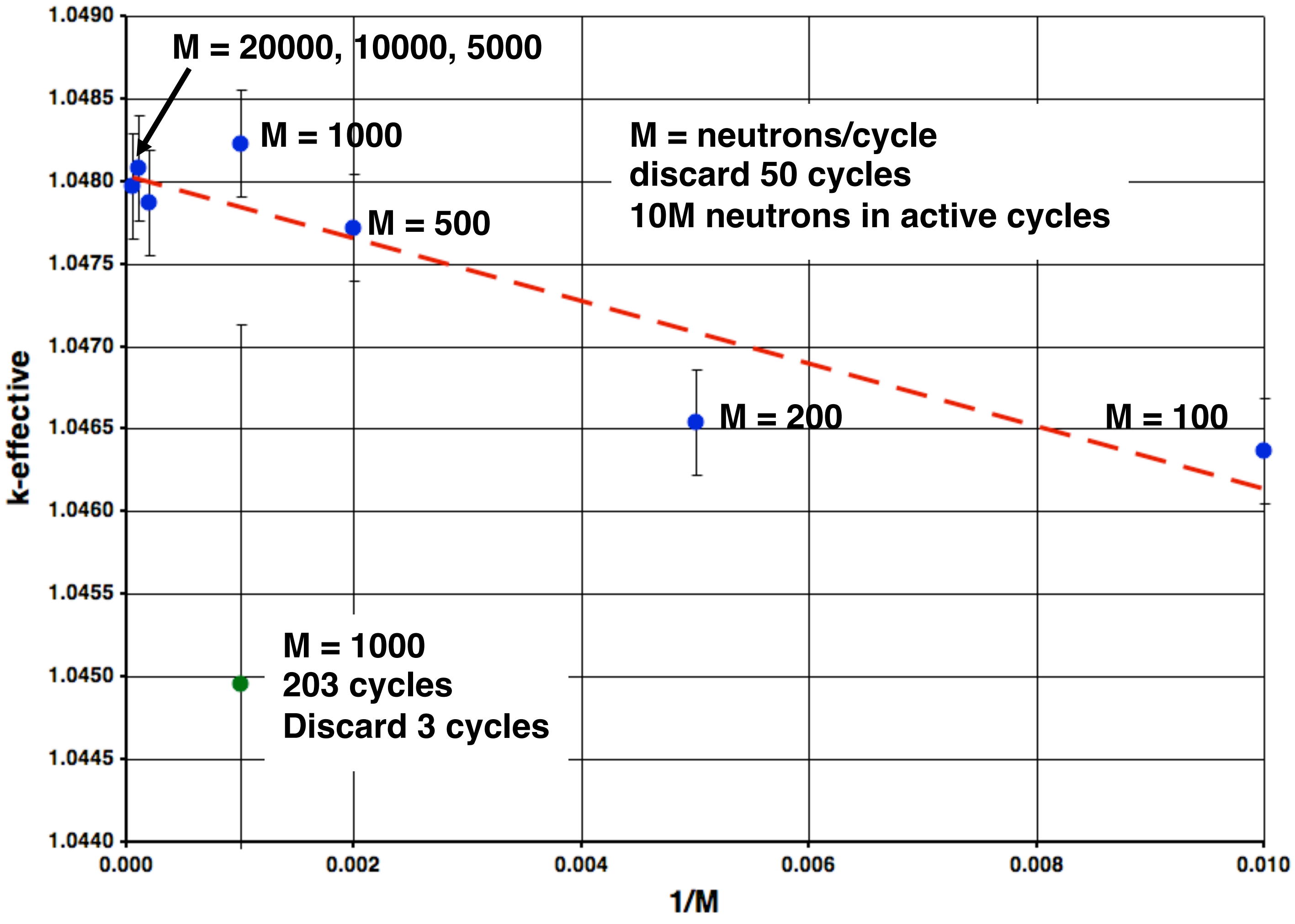
Convergence





Using ENDF/B-VI+T16 data

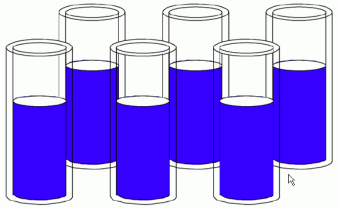
Bias in K_{eff}



M = neutrons/cycle
discard 50 cycles
10M neutrons in active cycles

M = 1000
203 cycles
Discard 3 cycles

.002 Δk



Note: **Bias in green point is a <u>convergence</u> problem due to using Keno <u>default</u> - discard 3 cycles, 203 cycles total**

Using ENDF/B-VI+T16 data

Best Practices For
MC Criticality Problems

Convergence - Guidance

- Plot K_{eff} vs cycle to check convergence of K_{eff}

- If computing any tallies (flux, fissions, dose, foils, heating, …) plot H_{src} vs cycle to check convergence of fission distribution

- Dominance ratio $\rho = k_1 / k_0$ determines the rate of convergence
  - Smaller dominance ratio ➜ fewer cycles to converge
  - To reduce the dominance ratio, use problem symmetry & reflecting boundary, to eliminate some higher modes

PWR example:	full core	1/2 core	1/4 core	1/8 core
ρ:	.98	.97	.96	.94

- Better initial source guess ➜ fewer cycles to converge
  - Reactor: good guess - uniform in core region
  - Criticality Safety: good guess - points in each fissionable region,
good guess - uniform in each fissionable region

- Convergence does not depend on number of neutrons/cycle (M)

Bias in K_{eff} & Tallies - Guidance

- Using too few neutrons/cycle leads to bias in K_{eff} & the fission distribution
- Bias in K_{eff} is usually small, but always negative (nonconservative)
- Bias in the fission distribution is generally larger than for K_{eff} & shows a significant tilt
- Practical solution - use large M (neutrons/cycle)
  - Using 10K neutrons/cycle or more ➜ bias negligible
    (100K or more for large models)
  - More neutrons/cycle ➜ more efficient parallel calculations

Bias in σ's - Guidance

- Uncertainties computed by MC codes exhibit a bias due to inter-cycle correlation effects that are neglected
- Primarily affects local tally statistics, not K-effective statistics
- **Computed uncertainties are always smaller than the true uncertainties for a tally**
- **Running more cycles or more neutrons/cycle does <u>not</u> reduce the biases**
- **Wielandt's method can reduce or eliminate the underprediction bias in uncertainties** (coming soon in MCNP5…)

Best Practices - Summary

- To avoid bias in K_{eff} & tally distributions:
  - Use 10K or more neutrons/cycle (maybe 100K+ for full-core)
  - Discard sufficient initial cycles
  - Always check convergence of both K_{eff} & the fission distribution
- To help with convergence:
  - Take advantage of problem symmetry, if possible
  - Use good initial source guess, cover fissionable regions
- Run at least a few 100 active cycles
  to allow codes to compute reliable statistics
- Statistics on tallies from codes are underestimated, often by 2-5x;
  possibly make multiple independent runs

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- **Previous discussion of details concerning bias, convergence, & statistics and "Best Practices" previously presented at**
  - **2008 - PHYSOR Monte Carlo workshop**
  - **2009 - M&C Monte Carlo workshop**
  - **2009 - Paper at NCSD topical meeting**
  - **2010 PHYSOR Monte Carlo Workshop**

Presentations available at http://mcnp.lanl.gov/publication/mcnp_publications.html

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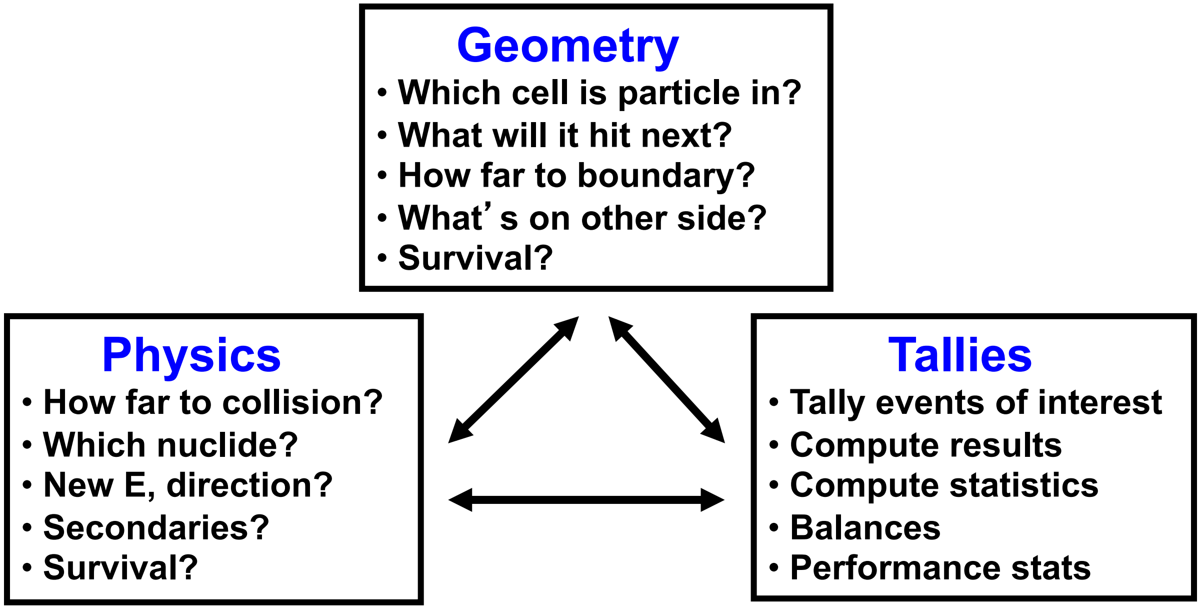
Variance Reduction

Monte Carlo Calculations



Geometry

- Which cell is particle in?
- What will it hit next?
- How far to boundary?
- What’ s on other side?
- Survival?

Physics

- How far to collision?
- Which nuclide?
- New E, direction?
- Secondaries?
- Survival?

Tallies

- Tally events of interest
- Compute results
- Compute statistics
- Balances
- Performance stats

mcnp, rcp, vim, racer, sam-ce, tart, morse, keno, tripoli, mcbend, monk, o5r, recap, andy,…..

- Variance reduction
  - Modify the PDFs for physics interactions to favor events of interest
  - Use splitting/rouletting to increase particles in certain geometric regions
  - Kill particles in uninteresting parts of problem
- May be necessary in order to sample rare events
- More samples (with less weight each) ➜ smaller variance in tallies

Monte Carlo Estimates of Integrals

Given a function R(x), where x is a random variable with PDF f(x),

- Expected value of R(x) is $\mu = \int R(x)\, f(x)\, dx$
- Variance of R(x) is

$$\sigma^2 = \int R^2(x)\, f(x)\, dx - \mu^2$$

Monte Carlo method for estimating μ = <R>

- make N random samples $\hat{x}_j$ from f(x)
- Then

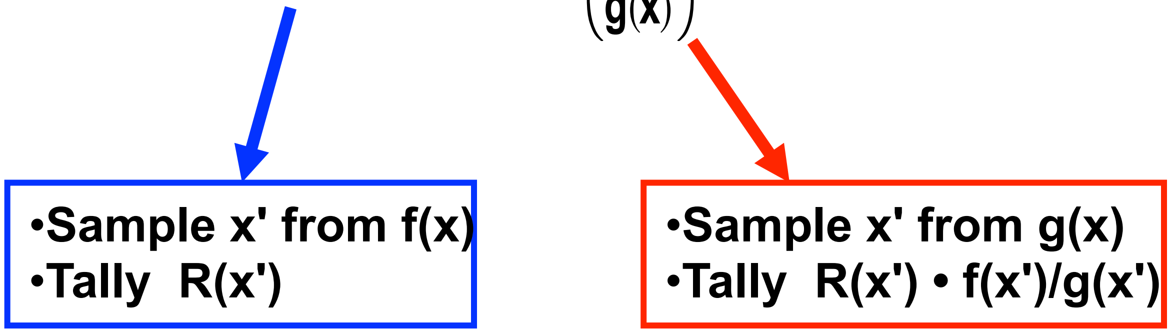
$$\bar{R} \approx \frac{1}{N}\sum_{j=1}^{N} R(\hat{x}_j)$$

$$\sigma_{\bar{R}}^2 \approx \frac{1}{N-1} \cdot \left(\frac{1}{N}\sum_{j=1}^{N} R^2(\hat{x}_j) - \bar{R}^2 \right)$$

Variance Reduction - Basic Idea

- Expected mean score is not changed by variance reduction

$$\mu = \int R(x)\, f(x)\, dx = \int R(x) \left(\frac{f(x)}{g(x)} \right) \cdot g(x) dx$$



- Sample x' from f(x)
- Tally R(x')

- Sample x' from g(x)
- Tally R(x') • f(x')/g(x')

- Variance is changed due to altered sampling scheme

$$\sigma^2 = \int [R(x)]^2 f(x)\, dx - \mu^2 \qquad \sigma^2 = \int \left[R(x) \frac{f(x)}{g(x)} \right]^2 g(x)\, dx - \mu^2$$

Goal: Choose g(x) such that variance is reduced

Review

- Given a set of random samples, $x_1, x_2, \ldots, x_N,$
  - Mean

$$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j$$

  - Variance of the mean

$$\sigma_{\bar{x}}^2 = \frac{1}{N-1} \cdot \left(\frac{1}{N}\sum_{j=1}^{N} x_j^2 - \bar{x}^2 \right)$$

  - Relative Error

$$RE = \frac{\sigma_{\bar{x}}}{\bar{x}}$$

  - Figure of Merit

$$\mathrm{FOM} = \frac{1}{RE^2 \cdot T}$$

- Variance reduction: Reduce RE or T, to increase FOM

Analog vs. Weighted Monte Carlo

- **Analog Monte Carlo**
  - Faithful simulation of particle histories
  - No alteration of PDFs (i.e., no biasing or variance reduction)
  - Particle is born with weight = 1.0
  - Weight unchanged throughout history until particle is killed
  - Scores are weighted by 1.0 when tallying events of interest

- **Weighted Monte Carlo (non-analog)**
  - Alter the PDFs to favor events of interest
  - Particle is born with weight = 1.0
  - Weight, wgt, is altered if biased PDF is used
  - Weight can also be changed by Russian roulette/splitting & other variance reduction techniques
  - Scores are weighted by wgt when tallying events of interest

Variance Reduction - General Approaches

- Truncation
  - Remove particles from parts of phase space that do not contribute significantly to the tallies
- Population control
  - Use particle splitting and Russian rouletting to control the number of samples taken in various regions of phase space
- Modified sampling
  - Modify the PDFs representing problem physics, to favor tallies of interest
- Deterministic methods
  - Replace portions of a particle random walk by the expected results obtained from a deterministic calculation

Typical Variance Reduction Techniques

- **MCNP has 14 variance reduction techniques**
  1. Time and energy cutoffs
  2. Geometry splitting & roulette
  3. Weight windows
  4. Exponential transform
  5. Forced collisions
  6. Energy splitting & roulette
  7. Time splitting & roulette
  8. Point and ring detectors
  9. DXTRAN
  10. Implicit capture
  11. Weight cutoff
  12. General source biasing
  13. Secondary particle biasing
  14. Bremsstrahlung energy biasing

Survival Biasing

- Also called implicit absorption or non-absorption weighting
- Modify collision process according to expected outcome
- Particle always survives collision
  - Tally expected absorption, $wgt \bullet (\Sigma_A/\Sigma_T)$
  - Reduce weight of surviving particle, $wgt' = wgt \bullet (1 - \Sigma_A/\Sigma_T)$
- Extends particle history so that more particles reach events which occur after many collisions
- Most effective for thermal reactor problems, but doesn't hurt in other types of problems
- Must also use some form of low-weight cutoff to eliminate particles with very low weight

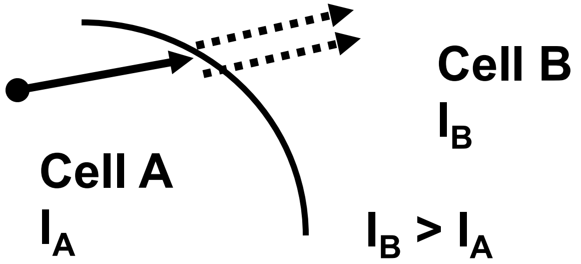
Geometry Splitting & Russian Roulette

- Increase the number of particles in "important" regions, decrease the number of particles in "unimportant" regions

- Assign each cell an importance, I_{cell}
  - Arbitrary, use best guess or adjoint fluxes from deterministic calculation
  - Could use one value for all energies or separate values for different energy ranges
  - Higher value --> more important
  - $I_{cell} > 0$
  - $I_{cell}=0$ is a way to declare regions as not in physical problem
  - Values of I_{cell} must not change during Monte Carlo calculation

- Modify random walk simulation at surface crossings:
  - If $(I_{enter}/I_{leave}) > 1$, perform splitting
  - If $(I_{enter}/I_{leave}) < 1$, perform Russian roulette

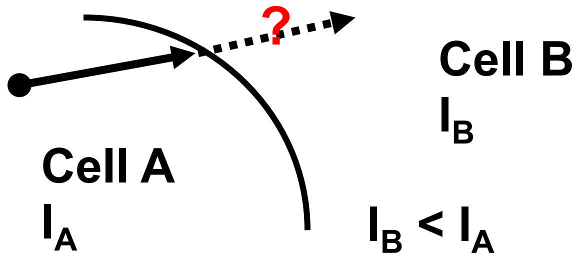
Geometry Splitting & Russian Roulette



- Let $r = I_B / I_A$
  $n = \text{floor}(r)$
- If n > 1, split into n particles with weight (wgt/n)
  - All of the n particles emerging from splitting have identical attributes (e.g., x,y,z, u,v,w, E) including wgt' = wgt/n
  - All of the n particles from a splitting are part of the same history, and their tallies must be combined
  - Typically, (n-1) particles are banked, 1 particle is followed until its death, then a particle is removed from the bank & followed, etc.
- Avoid over-splitting
  - Splitting into a large number of particles can increase CPU-time & lead to (apparent) bias in results
  - Typically, choose cell importances to split 2-for-1 or 3-for-1
  - Typically, can limit the splitting to n-for-1 or less
- Total particle weight is exactly conserved in splitting

Geometry Splitting & Russian Roulette

- **Let $r = I_B / I_A$**



- **If $r < 1$, play** Russian roulette
  - **With probability r, keep the particle & alter its weight to (wgt/r)**
  - **With probability (1-r), kill the particle (set its weight to 0)**

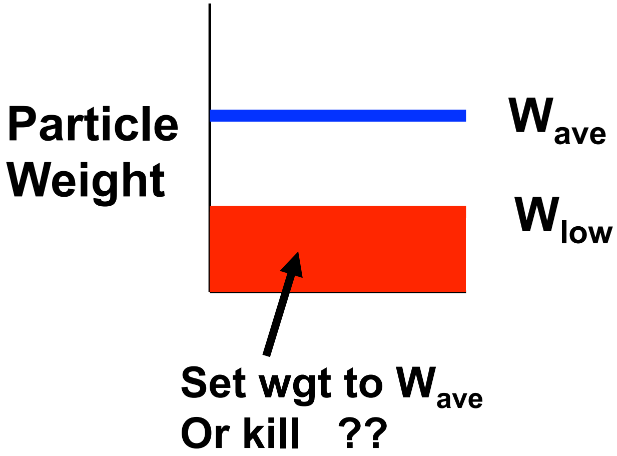
```
if  ξ < r,
    wgt' = wgt/r
else
    wgt' = 0
```

- **Russian roulette effectively merges a number of low-weight particles into one with higher weight**

- **Total particle weight is only conserved statistically (expected value)**

Weight Cutoff

- Specify a cutoff weight, W_{low}, and a survival weight, W_{ave}
- If particle weight drops below W_{low}, play Russian roulette with weight of W_{ave} for survivors
  - Probability of surviving RR = wgt/W_{ave}
  - Probability of being killed = $1 - wgt/W_{ave}$



Particle Weight

W_{ave}

W_{low}

Set wgt to W_{ave}
Or kill ??

```
If   $wgt < W_{low}$,
          if   $\xi < wgt/W_{ave}$,
                 $wgt' = W_{ave}$
          else
                 $wgt' = 0$
```

- Expected value of surviving weight is conserved, $(wgt/W_{ave})\cdot W_{ave}$

Weight Cutoff

- In some codes (e.g., MCNP), the weight cutoff parameters are functions of cell importance

  – Let R_j = (importance of source cell) / (importance of cell j)

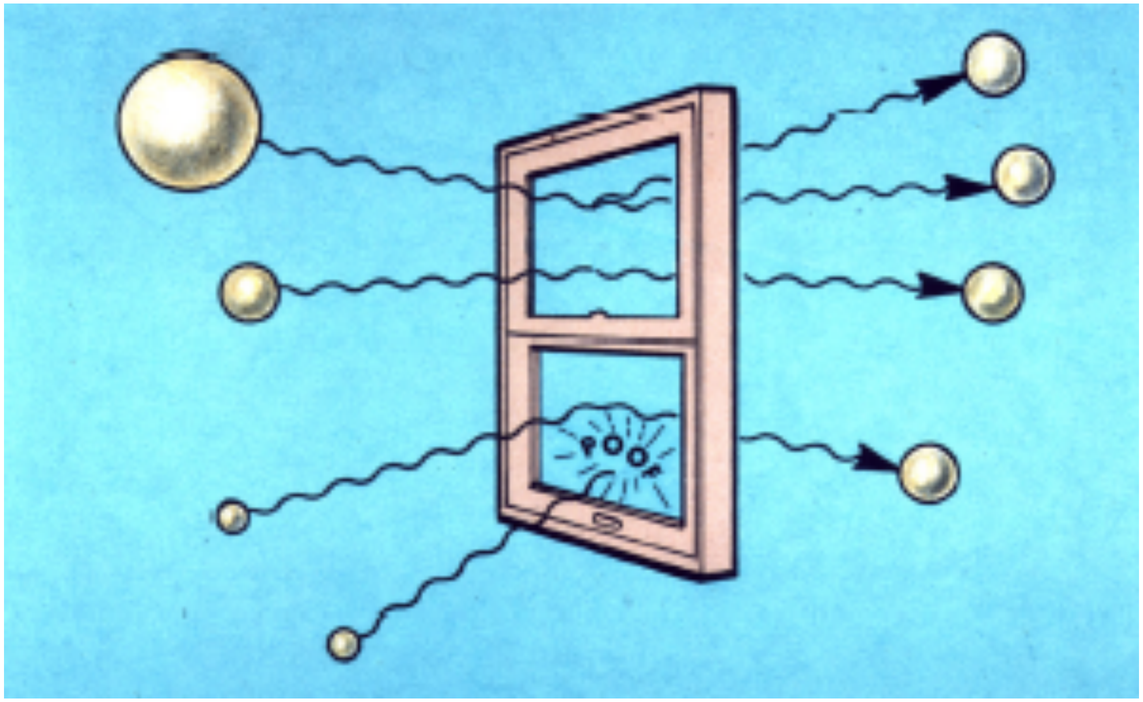
  – Then,

$$W_{ave}(j) = W_{ave} \bullet R_j$$
$$W_{low}(j) = W_{low} \bullet R_j$$

- Weight cutoffs reduce computing time, not variance

- Weight cutoffs can be applied anytime the particle weight changes - after collisions, after boundary crossings, …

Weight Windows



- Prevent particle weights from getting too large or too small
  - Weight too large ➜ splitting
  - Weight too small ➜ Russian Roulette

Weight Windows

- Large fluctuations in particle weights contributing to a tally lead to larger variance
- Weight windows eliminate large or small weights (outside the window) by creating or destroying particles
- Weight windows can be applied any time - after collisions, after surface crossings, …

```
If     $wgt > W_{hi}$
    splitting
Elseif    $wgt < W_{low}$
    roulette
```

Weight Windows

- MCNP weight window scheme

Input: W_{low} for each cell (can be energy or time dependent),
$[W_{ave}/W_{low}]$, $[W_{hi}/W_{low}]$, mxspln

```
If   $wgt > W_{hi}$
        $n = \min(\text{mxspln}, 1 + wgt/W_{hi})$   <-- max splitting is mxspln-to-1
        $wgt = wgt/n$
        bank n-1 copies of particle          <-- n-to-1 splitting

Elseif   $wgt < W_{low}$
        $P = \max(1/\text{mxspln}, wgt/W_{ave})$   <-- limits survivor to mxspln*wgt
        if  $\xi < P$
            $wgt = wgt/P$                      <-- particle survives
        else
            $wgt = 0$                          <-- particle killed
```

Source Biasing

- Bias the PDFs used to select the angle, energy, or position or source particles
  - Produce more source particles (with lower weights) in desired parts of phase space

True source: $f(R,E,\Omega)$

Sample (R',E',Ω') from $g(R,E,\Omega)$

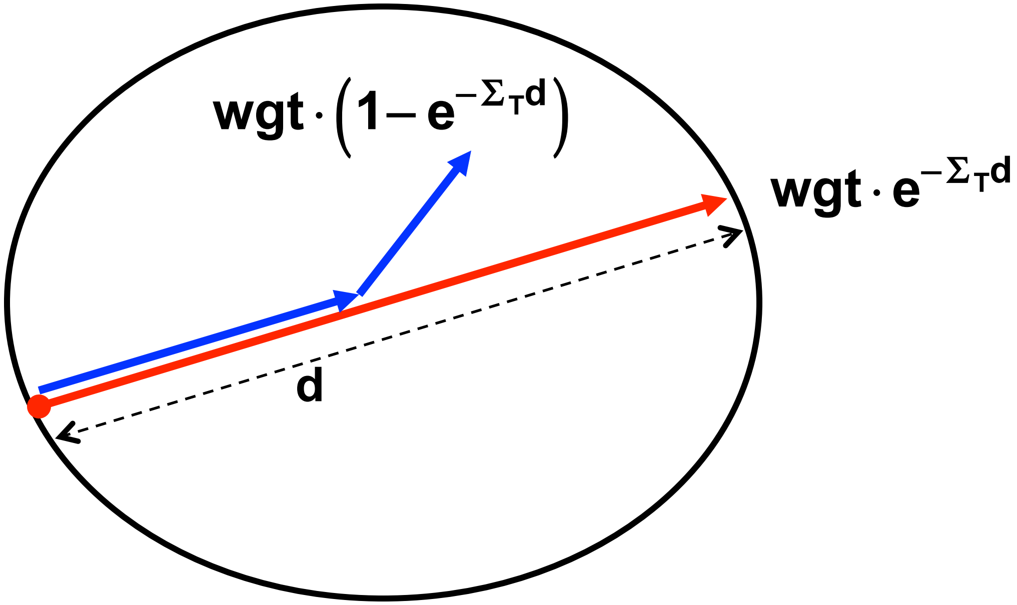
& assign weight $f(R',E',\Omega')/g(R',E',\Omega')$ to source particle

Choose $g(R,E,\Omega)$ to favor directions more important to tallies

Forced Collisions

- **Particles entering specified cells are split into collided & uncollided parts**
  - For distance-to-boundary d

$$\text{Prob(no collision)} = \exp(-\Sigma_T d)$$
$$\text{Prob(collision)} \quad = 1 - \exp(-\Sigma_T d)$$


$\text{wgt} \cdot \left(1 - e^{-\Sigma_T d}\right)$
$\text{wgt} \cdot e^{-\Sigma_T d}$
d

Forced Collisions

- **Sampling the flight distance s for a forced collision with max flight distance d**

Sampling from a truncated exponential PDF:

$$f(s) = \Sigma_T \cdot \frac{e^{-\Sigma_T s}}{1 - e^{-\Sigma_T d}}, \qquad 0 \le s \le d$$

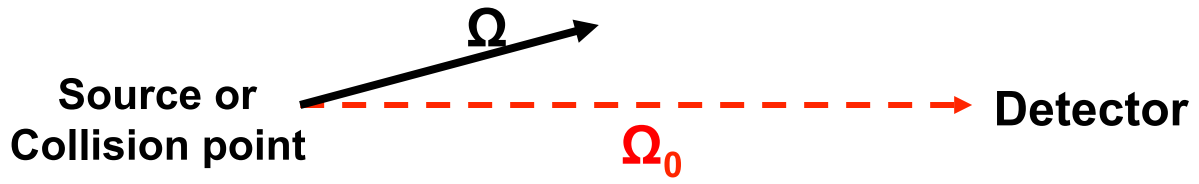
$$F(s) = \frac{1 - e^{-\Sigma_T s}}{1 - e^{-\Sigma_T d}}$$

$$\text{Solve for } s: \quad \xi = F(s)$$

$$s = \frac{-\ln\left[1 - (1 - e^{-\Sigma_T d})\xi\right]}{\Sigma_T}$$

Exponential Transform

- **Encourage particles to head in a certain preferred direction, $\boxed{?}_0$**



– **Replace Σ_T by $\Sigma^* = \Sigma_T [1 - p\ \Omega \bullet \Omega_0]$**

p = a parameter, $0<p<1$

Ω_0 = unit vector from particle position to detector

Ω = actual particle direction

– **Sample flight distance s' from $g(s) = \Sigma^* \exp(-\Sigma^* s)$**

– **Adjust weight by factor:**

$$f(s')/g(s') = \exp(-p\ \Omega \bullet \Omega_0\ \Sigma_T s')/[1 - p\ \Omega \bullet \Omega_0]$$

- Paths toward detector are stretched $(\Sigma^* < \Sigma_T)$
- Paths away from detector are shortened $(\Sigma^* > \Sigma_T)$

Variance Reduction Goals & Cautions

- Maximize FOM - either reduce RE or T
- Keep the number of particles per cell roughly constant from source to detector
- Reduce the number of particles in unimportant regions
- Achieve adequate sampling of all portions of phase space
- Avoid over-biasing (e.g., over-splitting)
- Ensure that tallies pass statistical checks

References

– T.E. Booth, "A Sample Problem for Variance Reduction in MCNP",
LA-10363-MS, LANL Report (Oct 1985)

– X-5 Monte Carlo Team, "MCNP - A General Monte Carlo N-Particle Transport Code, Version 5", LA-UR-03-1987 (April 2003)

– L.L. Carter & E.D. Cashwell, "Particle Transport Simulation with the Monte
Carlo Method", TID-26607, National Technical Information Service (1975)

Parallel Monte Carlo

Perspective

- Fast desktop computers

1980s super:	200 MHz	16 MB	10 GB	$ 20 M
Today, Mac Pro:	8 x 3000 MHz	8000 MB	250 GB	$ 5 K

- Linux clusters + MPI + multi-core
  - Cheap parallel computing
  - Everyone can do parallel computing, not just national labs

- Mature Monte Carlo codes
  - MCNP, VIM, KENO, MCBEND, MONK, COG, TART, RACER, RCP, …

- New generation of engineers/scientists
  - Less patience for esoteric theory & tedious computing procedures
  - Computers are tools, not to be worshipped
  - What's a slide rule ???

➜ More calculations with Monte Carlo codes

Trends in Computing Technology

- **Commodity chips**

  Through early-2000s (little change since then):

  - **Microprocessor speed → ~2x gain / 18 months**
  - **Memory size → ~2x gain / 18 months**
  - **Memory latency → ~ no change (getting worse)**

- **High-end scientific computing**
  - **Key driver (or limit) → economics: mass production of desktop PCs & commercial servers**
  - **Architecture → clusters: with moderate number of commodity microprocessors on each node**

    multicore: multiple CPUs per processor

    permits threading within each node

- **Operating systems**
  - **Desktop & server → Windows, Linux**
  - **Supercomputers → Unix, Linux**

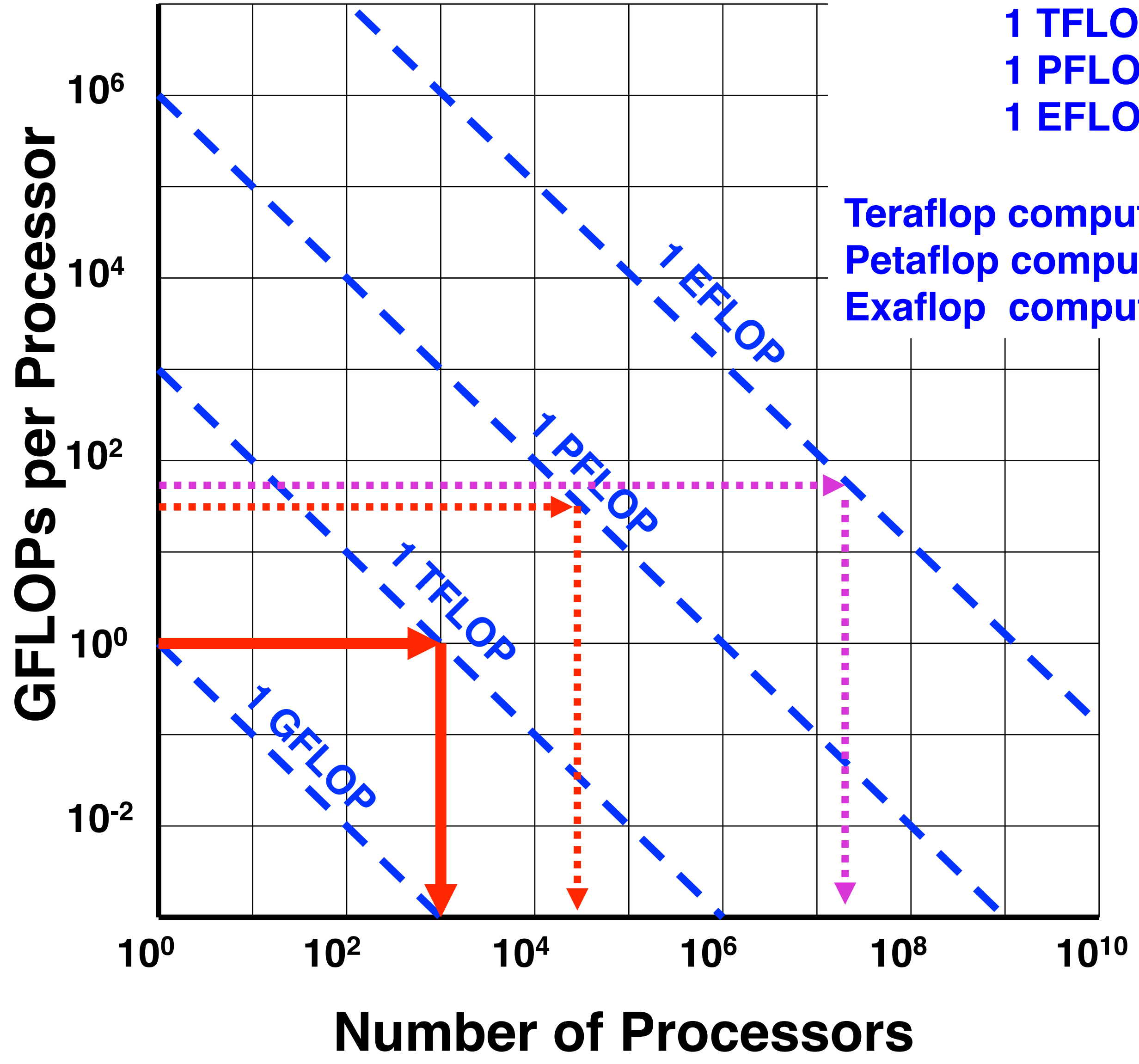
CPU performance on supercomputer ➜ same as desktop PC

High-performance scientific computing ➜ parallel computing

Parallel Computers

1 GFLOP = 10^9 FLOP
1 TFLOP = 10^{12} FLOP
1 PFLOP = 10^{15} FLOP
1 EFLOP = 10^{18} FLOP

Teraflop computers → ~ 10^3 processors
Petaflop computers → ~ 10^5 processors
Exaflop computers → ~ 10^7 processors (?)

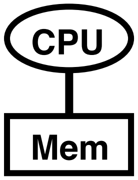


Parallel Computers

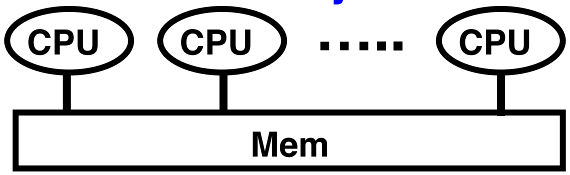
- **Characterize computers by:**
  - CPU: scalar, vector, superscalar, RISC, …..
  - Memory: shared, distributed, cache, banks, bandwidth, …..
  - Interconnects: bus, switch, ring, grid, …..

- **Basic types:**

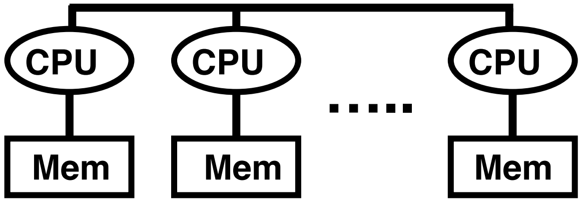
Traditional



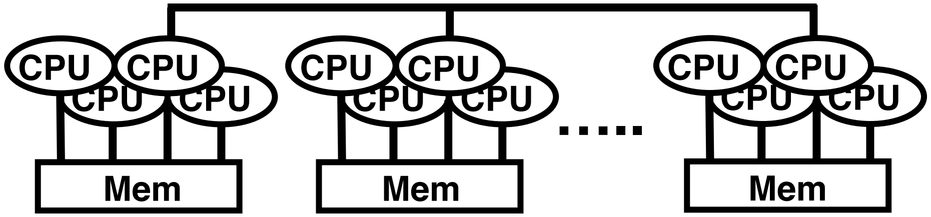
Shared Memory Parallel



Distributed Memory Parallel



Clustered Shared Memory



Approaches to Parallel Processing

High-level

- Independent programs + message-passing
- Distribute work among processors
- Loosely-coupled
- Programmer must modify high-level algorithms

Mid-level

- Threads (task-level)
- Independent tasks (subprograms) + shared memory
- For shared memory access, use locks on critical regions
- Compiler directives by programmers

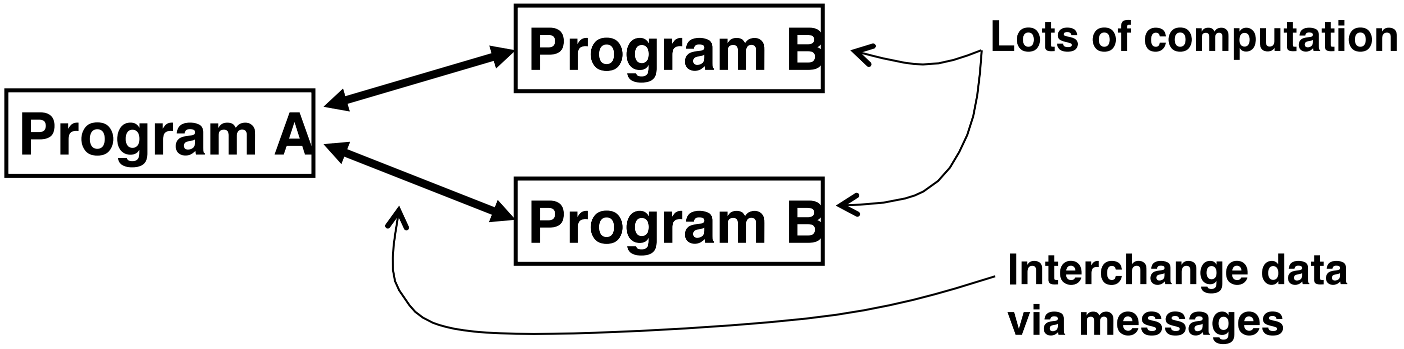
Low-level

- Threads (loop-level)
- Split DO-loop into pieces, compute, synchronize
- Compiler directives by programmers

Low-level

- Pipelining or vectorization
- Pipelined execution of DO-loops
- Automatic vectorization by compilers &/or hardware, or compiler directives by programmers

Message-passing



Program A

Program B

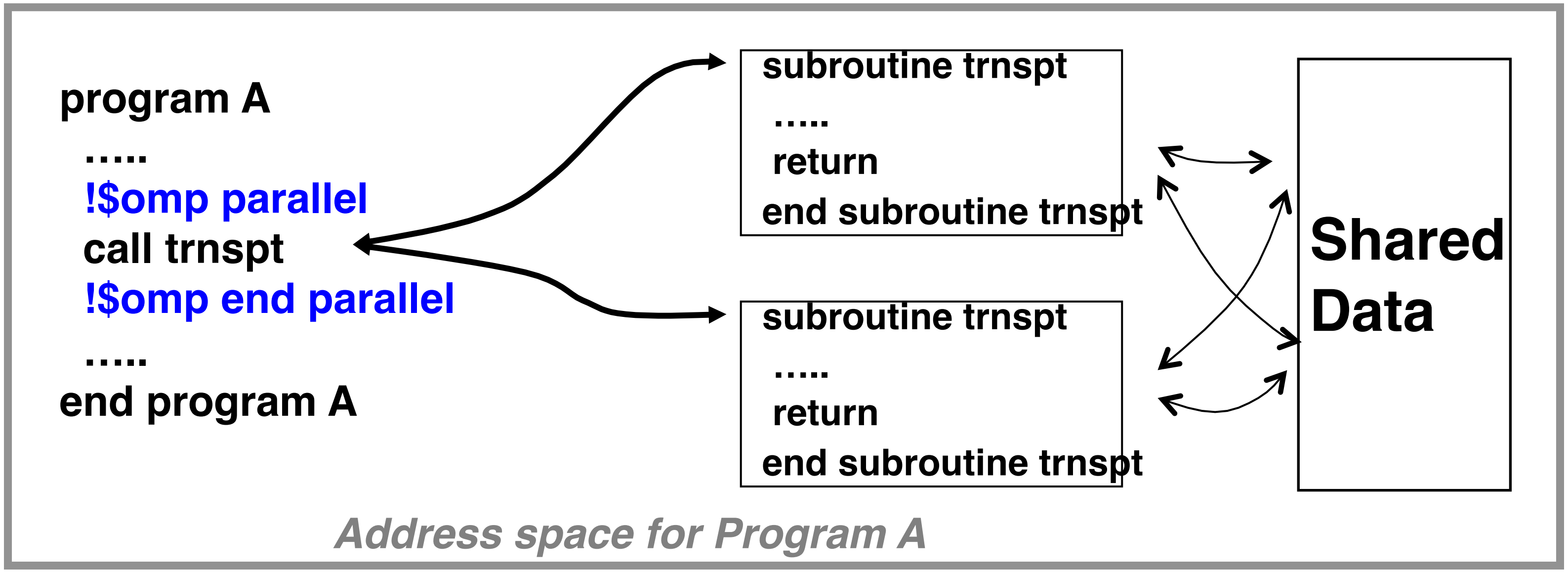
Program B

Lots of computation

Interchange data via messages

- – Independent programs
- – Separate memory address space for each program (private memory)
- – All control information & data must be passed between programs by explicit messages (SENDs & RECEIVEs)
- – Can run on distributed or shared memory systems
- – Efficient only when $T_{computation} >> T_{messages}$
- – Standard message-passing:
  - MPI

Threading (task-level)



```
program A
  …..
  !$omp parallel
  call trnspt
  !$omp end parallel
  …..
end program A
```

```
subroutine trnspt
 …..
 return
end subroutine trnspt
```

```
subroutine trnspt
 …..
 return
end subroutine trnspt
```

Shared Data

Address space for Program A

- Single program, independent sections or subprograms
- Each thread executes a portion of the program
- Common address space, must distinguish private & shared data
- Critical sections must be "locked"
- Can run only on shared memory systems, not distributed memory
- Thread control by means of compiler directives
- Standard threading:
  - OpenMP

Amdahl's Law

If a computation has fast (parallel) and slow (scalar) components, the overall calculation time will be dominated by the slower component

$$\text{Overall System Performance} = \text{Single CPU Performance} * \frac{1}{1\text{-}F + F/N}$$

where F = fraction of work performed in parallel

N = number of parallel processors

Speedup = 1 / (1-F + F/N)

For N=10

F	S	F	S
20%	1.2	90%	5.3
40%	1.6	95%	6.9
60%	2.2	99%	9.2
80%	3.6	99.5%	9.6

For N=infinity

F	S	F	S
20%	1.3	90%	10
40%	1.7	95%	20
60%	2.5	99%	100
80%	5	99.5%	200

Amdahl's Law

My favorite example …..

Which system is faster?

System A:	(16 processors)•(1 GFLOP each)	=	16 GFLOP total
System B:	(10,000 procs)•(100 MFLOP each)	=	1,000 GFLOP total

Apply Amdahl's law, solve for F:

$$1 / (1-F + F/16) = .1 / (1-F + F/10000)$$

➔ System A is faster, unless >99.3% of work is parallel

- In general, a smaller number of fatter nodes is better
- For effective parallel speedups, must parallelize everything

Parallel
Monte Carlo

Parallel Algorithms

- **Possible parallel schemes:**

– **Jobs**	**run many sequential MC calculations, combine results**
– **Functional**	**sources, tallies, geometry, collisions, …..**
– **Phase space**	**space, angle, energy**
– **Histories**	**Divide total number of histories among processors**

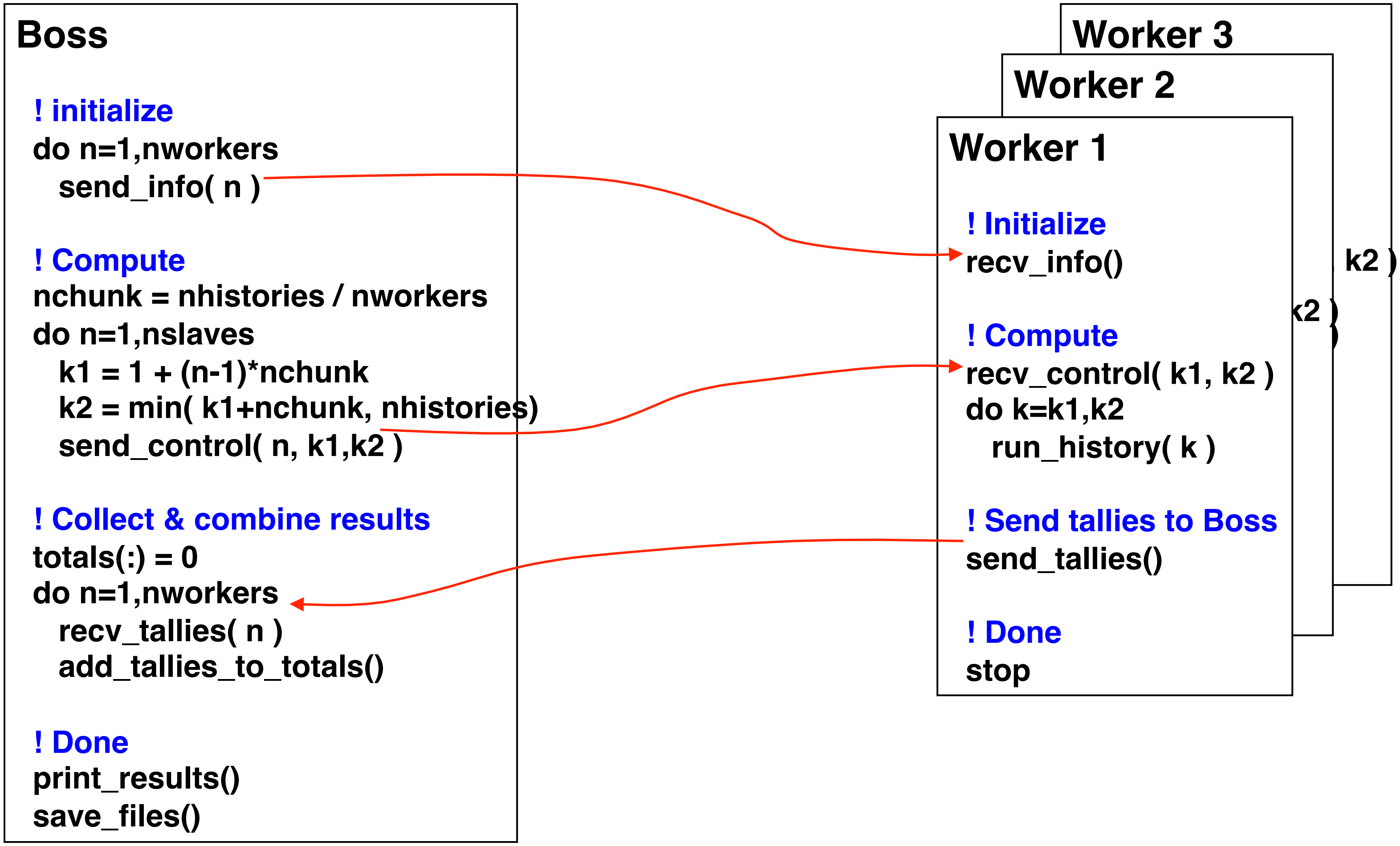
- **All successful parallel Monte Carlo algorithms to date have been history-based.**
  - **Parallel jobs always works, variation on parallel histories**
  - **Some limited success with spatial domain decomposition**

Boss / Worker Algorithm (Simple)

- Boss task: **control + combine tallies from each Worker**
- Worker tasks: **Run histories, tallies in private memory**
  - **Initialize:**
    Boss sends problem description to each Worker
    (geometry, tally specs, material definitions, …)
  - **Compute, on each of N Workers:**
    Each Worker task runs 1/N of total histories.
    Tallies in private memory.
    Send tally results back to Boss.
  - **Combine tallies:**
    Boss receives tallies from each Worker &
    combines them into overall results.
- **Concerns:**
  - **Random number usage**
  - **Load-balancing**
  - **Fault tolerance (rendezvous for checkpoint)**
  - **Scaling**

Boss / Worker Algorithm (Simple)

Control + Bookkeeping **Computation**



Boss

```
! initialize
do n=1,nworkers
  send_info( n )

! Compute
nchunk = nhistories / nworkers
do n=1,nslaves
  k1 = 1 + (n-1)*nchunk
  k2 = min( k1+nchunk, nhistories)
  send_control( n, k1,k2 )

! Collect & combine results
totals(:) = 0
do n=1,nworkers
  recv_tallies( n )
  add_tallies_to_totals()

! Done
print_results()
save_files()
```

Worker 3

Worker 2

Worker 1

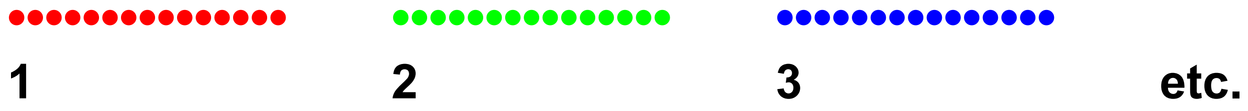
```
! Initialize
recv_info()

! Compute
recv_control( k1, k2 )
do k=k1,k2
  run_history( k )

! Send tallies to Boss
send_tallies()

! Done
stop
```

Random Number Usage

- **Linear Congruential RN Generator**

  $S_{k+1} = g\, S_k + C \quad \text{mod } 2^M$

- **RN Sequence & Particle Histories**



MCNP stride for new history: 152,917

- **To skip ahead k steps in the RN sequence:**

  $S_k = g\, S_{k-1} + C \quad \text{mod } 2^M \quad = g^k\, S_0 + C\,(g^k-1)/(g-1) \quad \text{mod } 2^M$

- **Initial seed for n-th history**

  $S_0^{(n)} = g^{n*152917}\, S_0 + C\,(g^{n*152917}-1)/(g-1) \quad \text{mod } 2^M$

  This is easy to compute quickly using exact integer arithmetic

- **Each history has a unique number**
  - Initial problem seed → initial seed for nth particle on mth processor
  - If Worker knows initial problem seed & unique history number, can initialize RN generator for that history

Fault Tolerance

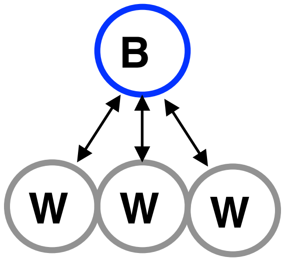
- On parallel systems with complex system software & many CPUs, interconnects, disks, memory, MTBF for system is a major concern.

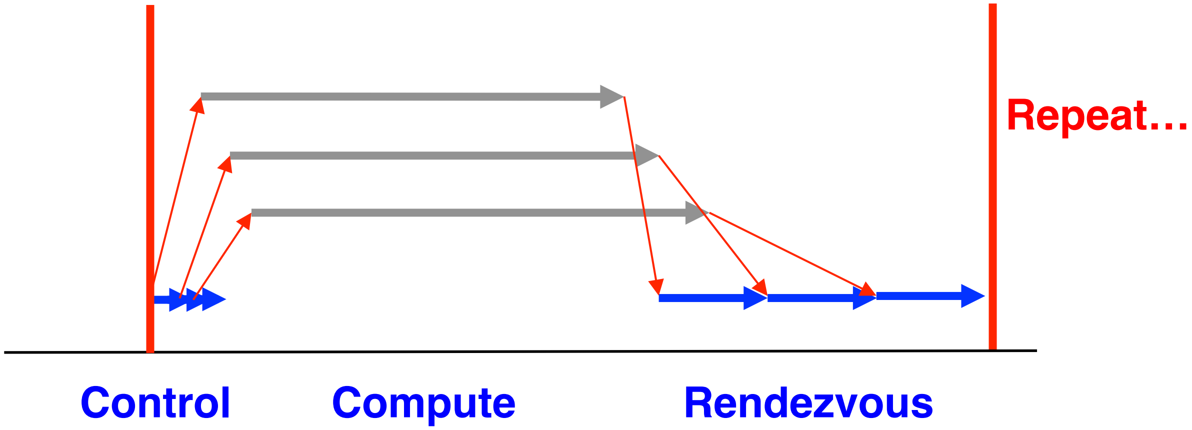
- Simplest approach to fault tolerance:
  - Dump checkpoint files every M histories (or XX minutes)
  - If system crashes, restart problem from last checkpoint

- Algorithm considerations
  - Rendezvous every M histories.
  - Workers send current state to Boss, Boss saves checkpoint files

  - Parallel efficiency affected by M.

Fault Tolerance





- **For efficiency, want (compute time) >> (rendezvous time)**
  - **Compute time:** Proportional to #histories/task
  - **Rendezvous time:** Depends on amount of tally data & latency+bandwidth for message-passing

Boss / Worker Algorithm, with Rendezvous

– **Initialize:**

  Boss sends problem description to each Worker
  (geometry, tally specs, material definitions, …)

– **For rendezvous = 1, L**

- **Compute**, on each of N Workers:

  Each Worker task runs 1/N of (total histories)/L.
  Tallies in private memory.
  Send tally results back to Boss.

- **Combine tallies:**

  Boss receives tallies from each Worker &
  combines them into overall results.

- **Checkpoint:**

  Boss saves current tallies & restart info in file(s)

Load Balancing

- **Time per history may vary significantly**
  - **For problems using variance reduction:**
    - Particles headed in "wrong" direction may be killed quickly, leading to a short history.
    - Particles headed in "right" direction may be split repeatedly. Since the split particles created are part of the same history, may give a very long history.
  - **For problems run on a workstation cluster:**
    - Workstation nodes in the cluster may have different CPU speeds
    - Workstations in the cluster may be simultaneously used for interactive work, with highly variable CPU usage on that node.
    - Node performance effectively varies continuously over time.
- **Naïve solution**
  - **Monitor performance per node (e.g., histories/minute)**
  - **Periodically adjust number of histories assigned to each node, according to node performance**

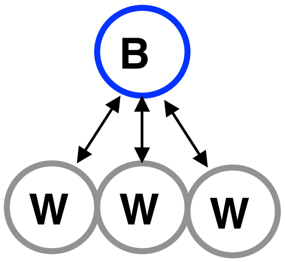
# histories assigned to node n ~ measured speed of node n

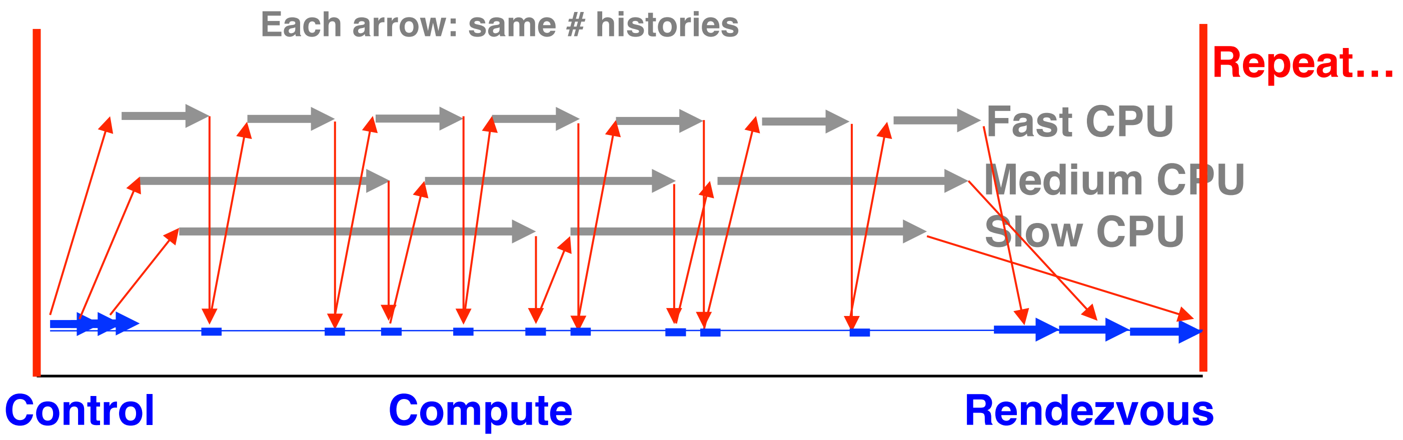
- **Better solution:** **self-scheduling**

Load Balancing – Self-Scheduling

- For a problem with N Worker processors, divide histories into more than N chunks.
  - Let L = number of chunks, $L > N$
  - Typically, $L \sim 20\ N$ or $L \sim 30\ N$
  - Histories/chunk = (total histories) / L
  - Worker: If idle, ask Boss for work. Repeat until no more work.
  - Boss: Send chunk of work to idle Worker. Repeat until no more work.
  - On average, imbalance in workload should be $< 1/L$
- Additional gains:
  - Naïve Boss/Worker algorithm is synchronous
  - Self-scheduling Boss/Worker algorithm is asynchronous. More overlap of communication & computation ➔ reduced wait times & better performance

Load Balancing – Self-Scheduling

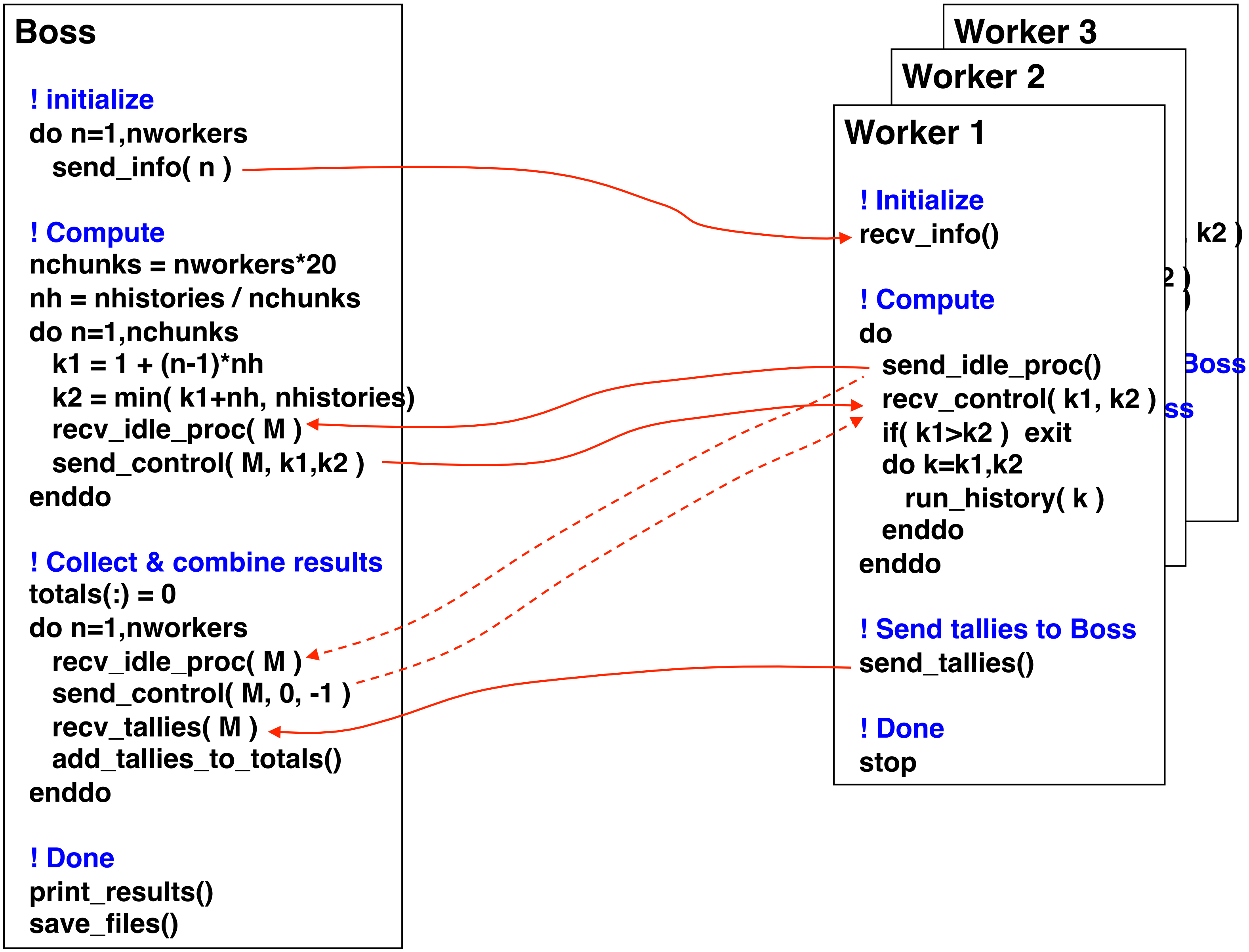




- **Much more communication with Boss, but only minimal amount of control info needed (1st & last history in chunk)**

- **Need to handle stopping condition carefully – avoid "dangling" messages**

Load Balancing – Self-Scheduling

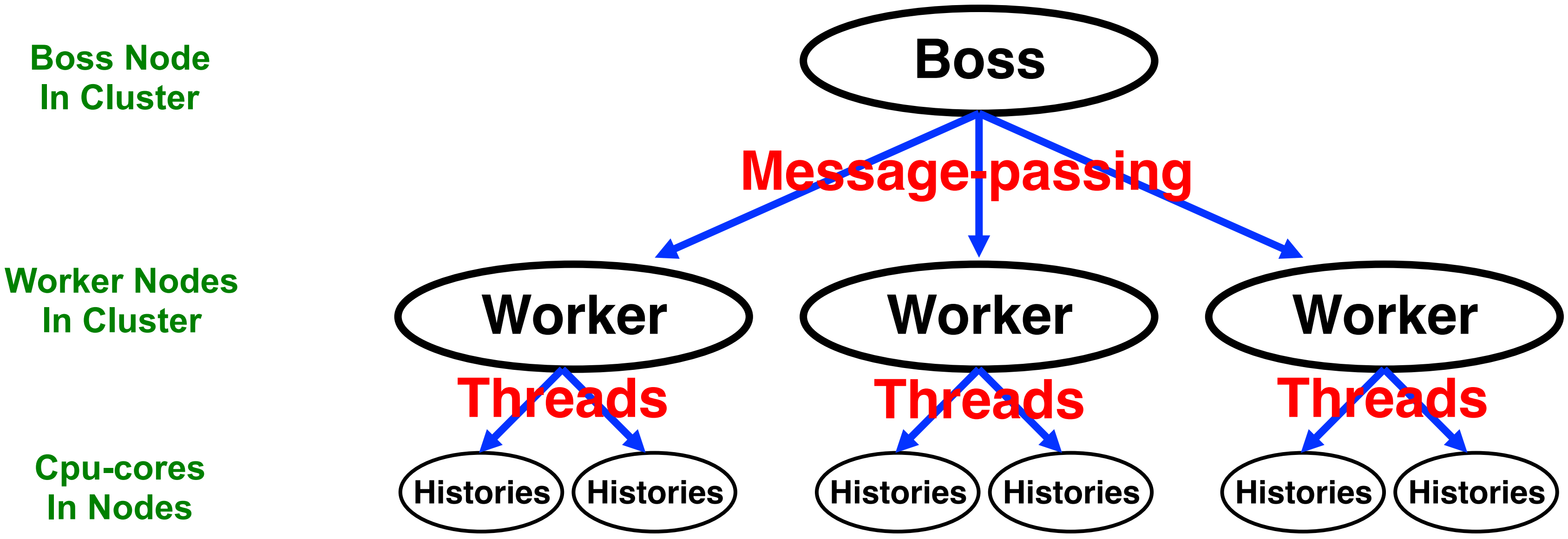


```
Boss

 ! initialize
 do n=1,nworkers
   send_info( n )

 ! Compute
 nchunks = nworkers*20
 nh = nhistories / nchunks
 do n=1,nchunks
   k1 = 1 + (n-1)*nh
   k2 = min( k1+nh, nhistories)
   recv_idle_proc( M )
   send_control( M, k1,k2 )
 enddo

 ! Collect & combine results
 totals(:) = 0
 do n=1,nworkers
   recv_idle_proc( M )
   send_control( M, 0, -1 )
   recv_tallies( M )
   add_tallies_to_totals()
 enddo

 ! Done
 print_results()
 save_files()
```

```
Worker 1

 ! Initialize
 recv_info()

 ! Compute
 do
   send_idle_proc()
   recv_control( k1, k2 )
   if( k1>k2 )  exit
   do k=k1,k2
     run_history( k )
   enddo
 enddo

 ! Send tallies to Boss
 send_tallies()

 ! Done
 stop
```

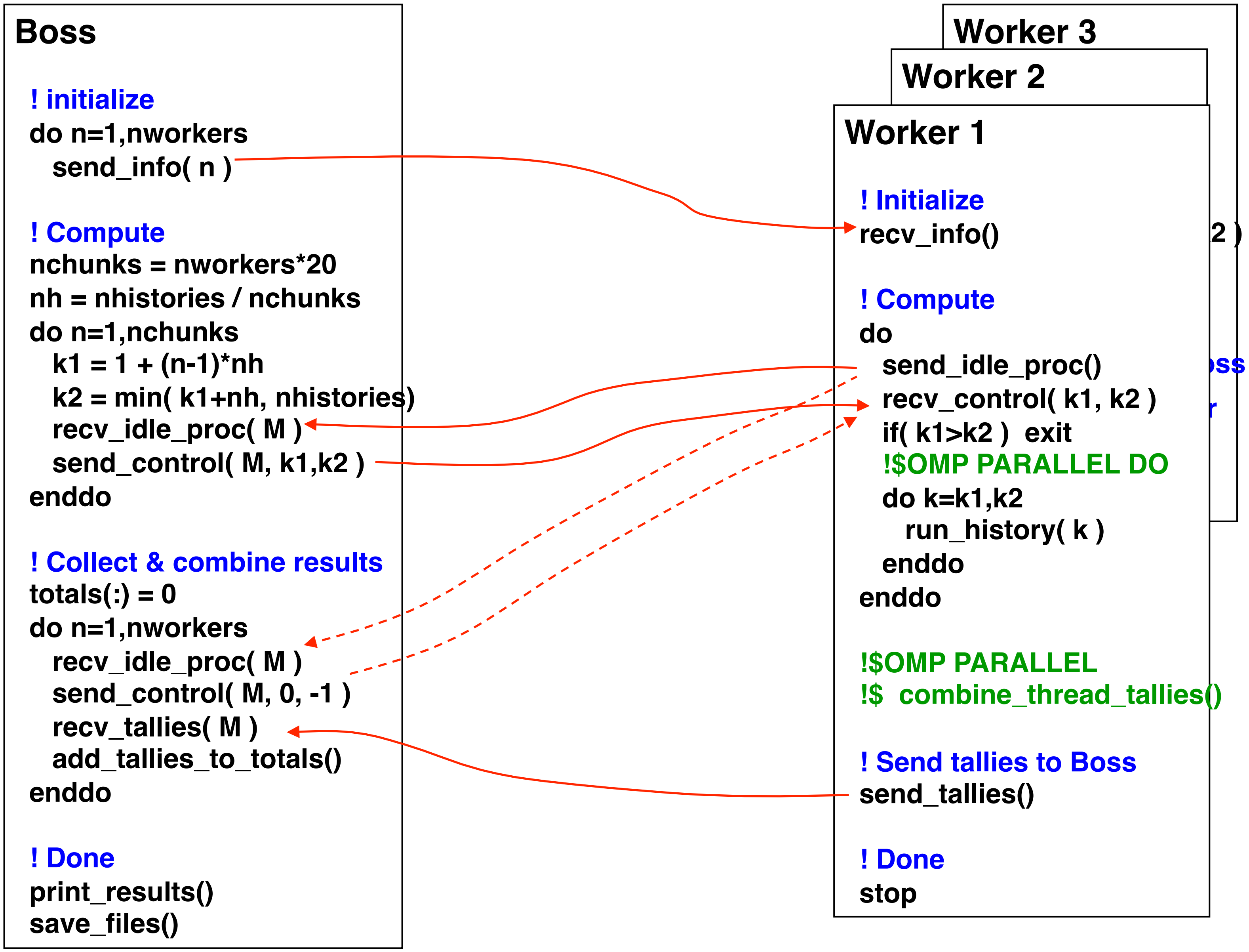
Hierarchical Parallelism

- For clustered SMPs,
  - Use message-passing to distribute work among Workers ("boxes")
  - Use threading to distribute histories among individual processors on box



- Only the Master thread (thread 0) on each Worker uses MPI send/recv's

Boss / Worker Algorithm, threaded & self-scheduling



Boss

```
! initialize
do n=1,nworkers
  send_info( n )

! Compute
nchunks = nworkers*20
nh = nhistories / nchunks
do n=1,nchunks
  k1 = 1 + (n-1)*nh
  k2 = min( k1+nh, nhistories)
  recv_idle_proc( M )
  send_control( M, k1,k2 )
enddo

! Collect & combine results
totals(:) = 0
do n=1,nworkers
  recv_idle_proc( M )
  send_control( M, 0, -1 )
  recv_tallies( M )
  add_tallies_to_totals()
enddo

! Done
print_results()
save_files()
```

Worker 1

```
! Initialize
recv_info()

! Compute
do
  send_idle_proc()
  recv_control( k1, k2 )
  if( k1>k2 )  exit
  !$OMP PARALLEL DO
  do k=k1,k2
    run_history( k )
  enddo
enddo

!$OMP PARALLEL
!$  combine_thread_tallies()

! Send tallies to Boss
send_tallies()

! Done
stop
```

Parallel Monte Carlo Performance

Parallel MC Computational Characteristics

- **For Boss/Worker algorithms (with self-scheduling, fault tolerance, & threads):**
  - **No communication among Worker tasks**
  - **Occasional communication between Boss & Workers (rendezvous)**
  - **Worker tasks are compute-intensive**
    - Few DO-loops
    - 40% of ops are test+branch (IF… GOTO…)
    - Irregular memory access, no repetitive patterns
  - **For fixed-source problems:**
    - Only 1 rendezvous is strictly necessary, at end of calculation
    - More rendezvous used in practice, for fault tolerance
  - **For eigenvalue problems (K-effective):**
    - Must have a rendezvous every cycle (cycle = batch = generation)
    - Boss controls iteration & source sampling
- **Common-sense approach to performance:**

  Fewer rendezvous ➔ better parallel performance

Parallel MC Performance Measures

- Metrics
  - Speedup $S_N = T_1 / T_N$ N = # Worker processors
  - Efficiency $E_N = S_N / N$
- Fixed overall work (fixed problem size)
  - Efficiency decreases with N
  - Speedup (eventually) drops as N increases
  - Why?

    As N increases, same communication/processor, but less work/processor (fewer histories/processor) ➔ (computation/communication) decreases
- Fixed work per processor (scaled problem size)
  - Efficiency approx. constant with N
  - Speedup approx. linear with N
  - Why?

    As N increases, same communication/processor, same work/processor (# histories ~ N) ➔ (computation/communication) stays approx. same
  - Called scaled speedup

Parallel MC Performance Limits

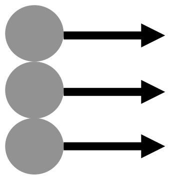
- Another way to determine efficiency

$$\text{Parallel Efficiency} = T_C / (T_C + T_M)$$

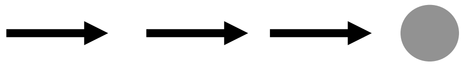
T_C = computing time

T_M = time for messages, not overlapped with computing

- Workers can send messages in parallel

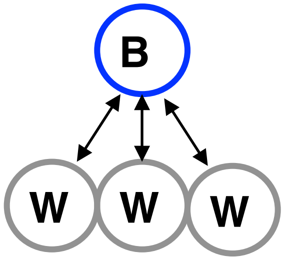


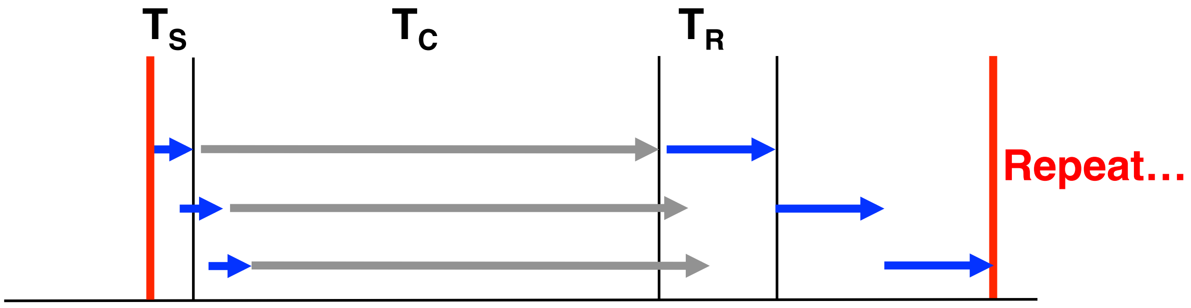
- Boss receives & processes messages serially



If enough messages are sent to Boss, extra wait time will limit performance

Parallel MC Performance Scaling




T_S T_C T_R

Repeat…

Control Compute Rendezvous

N = # processors

T_1 = CPU time for M histories using 1 processor

(Depends on physics, geometry, compiler, CPU speed, memory, etc.)

L = amount of data sent from 1 Worker each rendezvous

$T_S = 0$ negligible, time to distribute control info

$T_R = s + L/r$ s = latency for message, r = streaming rate

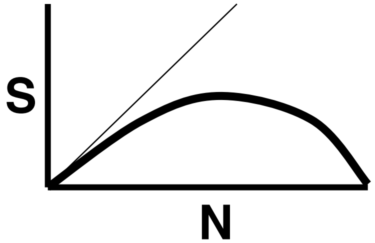
$T_C^{fix} = T_1 / N$ fixed problem size, M histories/rendezvous

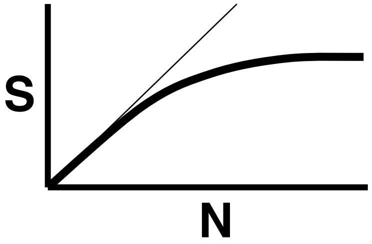
$T_C^{scale} = T_1$ scaled problem size, NM histories/rendezvous

Parallel MC Performance Scaling

- **Scaling models, for Boss/Worker with serial rendezvous**
  - "fixed" = constant number of histories/rendezvous, M (constant work)
  - "scaled" = M histories/Worker per rendezvous, NM total (constant time)

Histories/rendezvous	Speedup
fixed	$S = N / (1 + cN^2)$
scaled	$S = N / (1 + cN)$





N = number of Workers

$c = (s + L/r) / T_1$

$T_1 \sim M$, more histories/rendezvous ➔ larger T_1 , smaller c

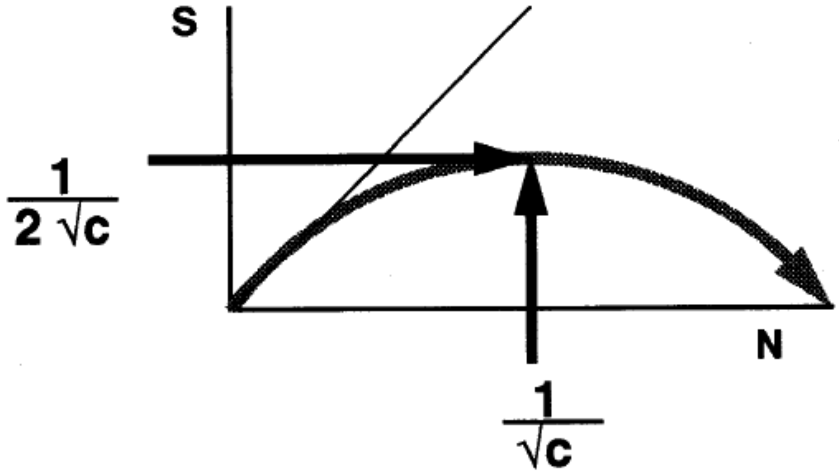
S+L/r, fixed, determined by number of tallies, ….

As M→infinity, c→0, S→N (limit for 1 rendezvous)

Parallel MC Performance Scaling

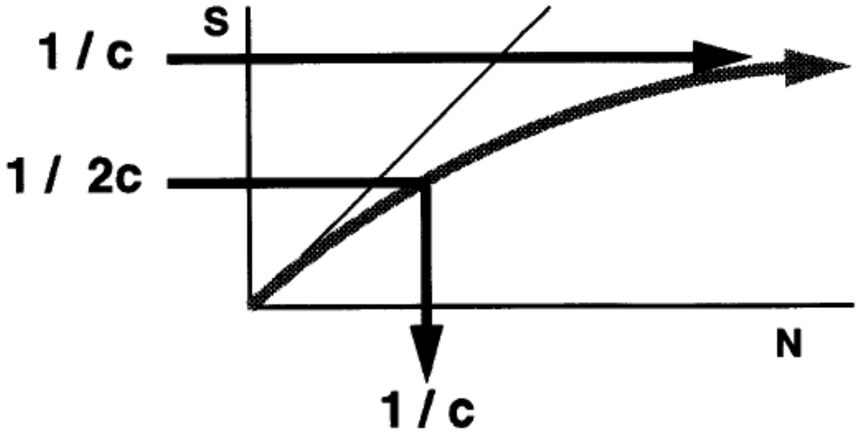
Fixed size, serial messages

$$S \quad = \quad N / (1 + cN^2)$$



Scaled size, serial messages

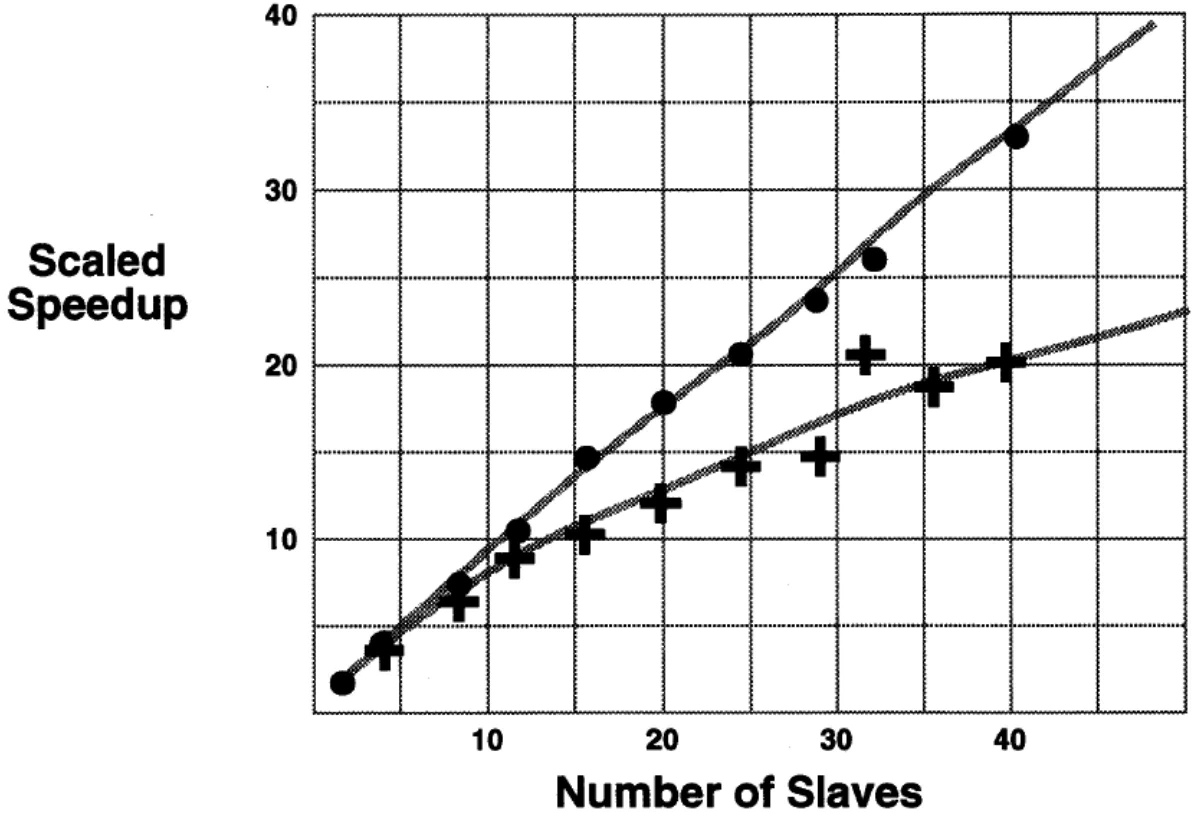
$$S \quad = \quad N / (1 + cN)$$



N = number of Workers
c = (s + L/r) / ($M_1 t_h$)

Parallel MC Performance Scaling

VIM Monte Carlo — Measured Performance on SP1 — TREAT reactor



● SP1 — P4 + EUIH S = N / (1 + .0056 N)

✚ SP1 — P4 + ethernet S = N / (1 + .028 N)

Measured message passing on SP1 is 2-3 times slower than specs (busy machine; experimental software; flaky hardware)

Parallel MC Summary

- **Boss/Worker algorithms work well**
  - Load-balancing: Self-scheduling
  - Fault-tolerance: Periodic rendezvous
  - Random numbers: Easy, with LCG & fast skip-ahead algorithm
  - Tallies: Use OpenMP "critical sections"
  - Scaling: Simple model, more histories/Worker + fewer rendezvous
  - Hierarchical: Boss/Worker MPI, OpenMP threaded Workers
  - Portability: MPI/OpenMP, clusters of anything

- **Remaining difficulties**
  - Memory size: Entire problem must fit on each Worker
    - Domain-decomposition has had limited success
      - Should be OK for reactor problems
      - May not scale well for shielding or time-dependent problems
      - For general 3D geometry, effective domain-decomposition is unsolved problem
    - Random access to memory distributed across nodes gives huge slowdown
      - May need functional parallelism with "data servers"

MCNP
Parallel
Calculations

DOE Advanced Simulation & Computing – ASC

Blue Mountain – 3 TeraOps

(R.I.P.)

Q – 20 TeraOps

(R.I.P.)

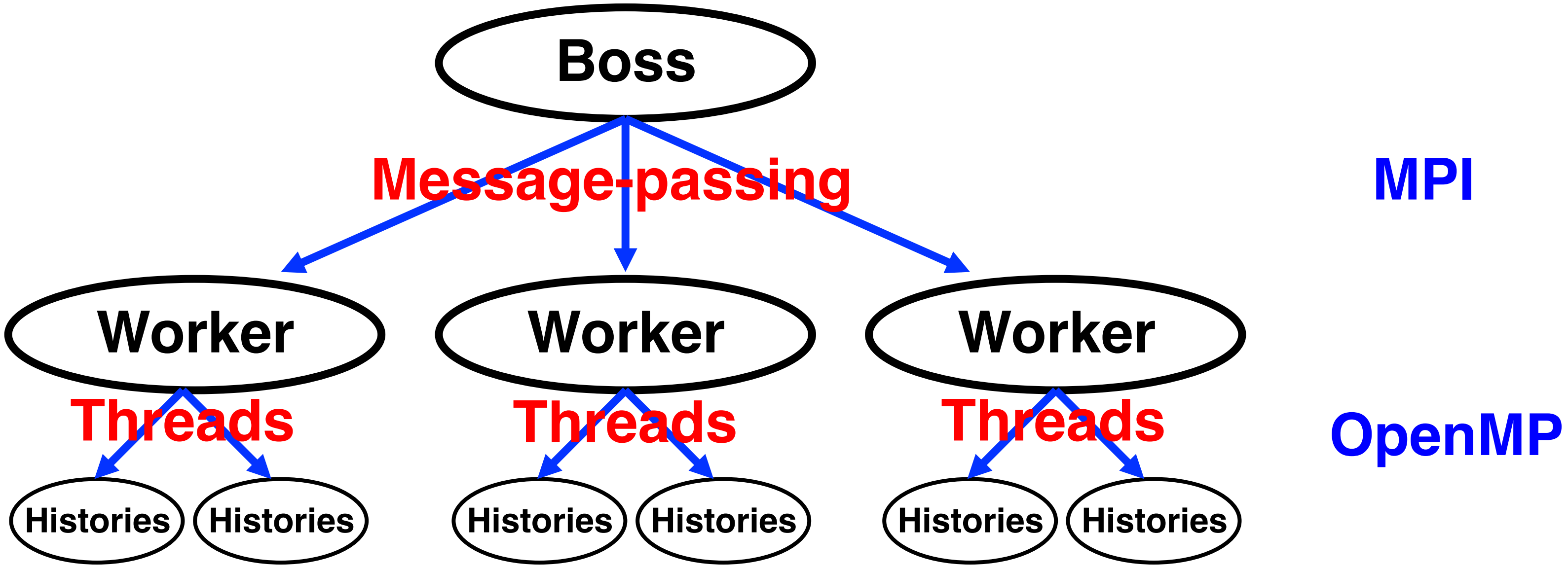
Red Storm
Blue Gene/L
Hurricane
Moonlight
Cielo

Lightning – 30 TeraOps
(R.I.P.)

Roadrunner – 1.3 PetaOps

Hierarchical Parallelism

- Use **message-passing** to distribute work among Workers ("boxes")
- Use **threading** to distribute histories among individual cpus on box



- **1,000 processor jobs are "routine"**

MCNP Parallel Calculations

N = total number of MPI tasks, Boss + (N-1) Workers

M = number of OpenMP threads/Worker

- **Running on parallel systems with MPI only**

```
mpirun   -np  N  -bynode   mcnp6.mpi     i=inp01  …..
```

- **Running with threads only**

```
mcnp6   tasks  M   i=inp01  …..
```

- **Running on parallel systems with MPI & threads**

```
mpirun   -np  N  -bynode  mcnp6.mpi   tasks  M   i=inp01
…..
```

If submitting jobs through a batch system (e.g., LSF, Moab, ...),
N & M must be consistent with LSF requested resources

MCNP Parallel Calculations

- **How many threads ?**
  - **Max number of threads = # CPU-cores per node**
    - ASCI Bluemountain: 128 cpus / node
    - ASCI Q: 4 cpus /node
    - Laptop PC cluster: 1 cpu / node
  - **Experience on many systems has shown that a moderate number of threads per Worker is efficient; using too many degrades performance**
    - ASCI Bluemountain: 4-12 threads/Worker usually effective
>16 threads/Worker usually has bad performance
    - ASCI Q: 4 threads/Worker is effective
  - **Rules-of-thumb vary for each system**
    - Thread efficiency is strongly affected by operating system design
    - Scheduling algorithm for threads used by operating system is generally designed to be efficient for small number of threads (<16)
    - For large number of threads, context-switching & cache management may take excessive time, giving poor performance
    - Other jobs on system (& their priority) affect thread performance
    - No definite rules – need to experiment with different numbers of threads

MCNP Parallel Calculations

- **Parallel performance is sensitive to number of rendezvous**
  - **Can't control number of rendezvous directly**
  - **The following things cause a rendezvous:**
    - Printing tallies
    - Dumping to the RUNTPE file
    - Tally Fluctuation Chart (TFC) entries
    - Each cycle of eigenvalue problem

- **Use PRDMP card to minimize print/dump/TFC**

PRDMP ndp ndm mct ndmp dmmp

ndp = increment for printing tallies 🡐 **use large number**
ndm = increment for dump to RUNTPE 🡐 **use large number**
mct = flag to suppress time/date info in MCTAL
ndmp = max number of dumps in RUNTPE
dmmp = increment for TFC & rendezvous 🡐 **use large number**

For fixed-source problems, increments are in particles
For eigenvalue problems, increments are in cycles

MCNP Parallel Calculations

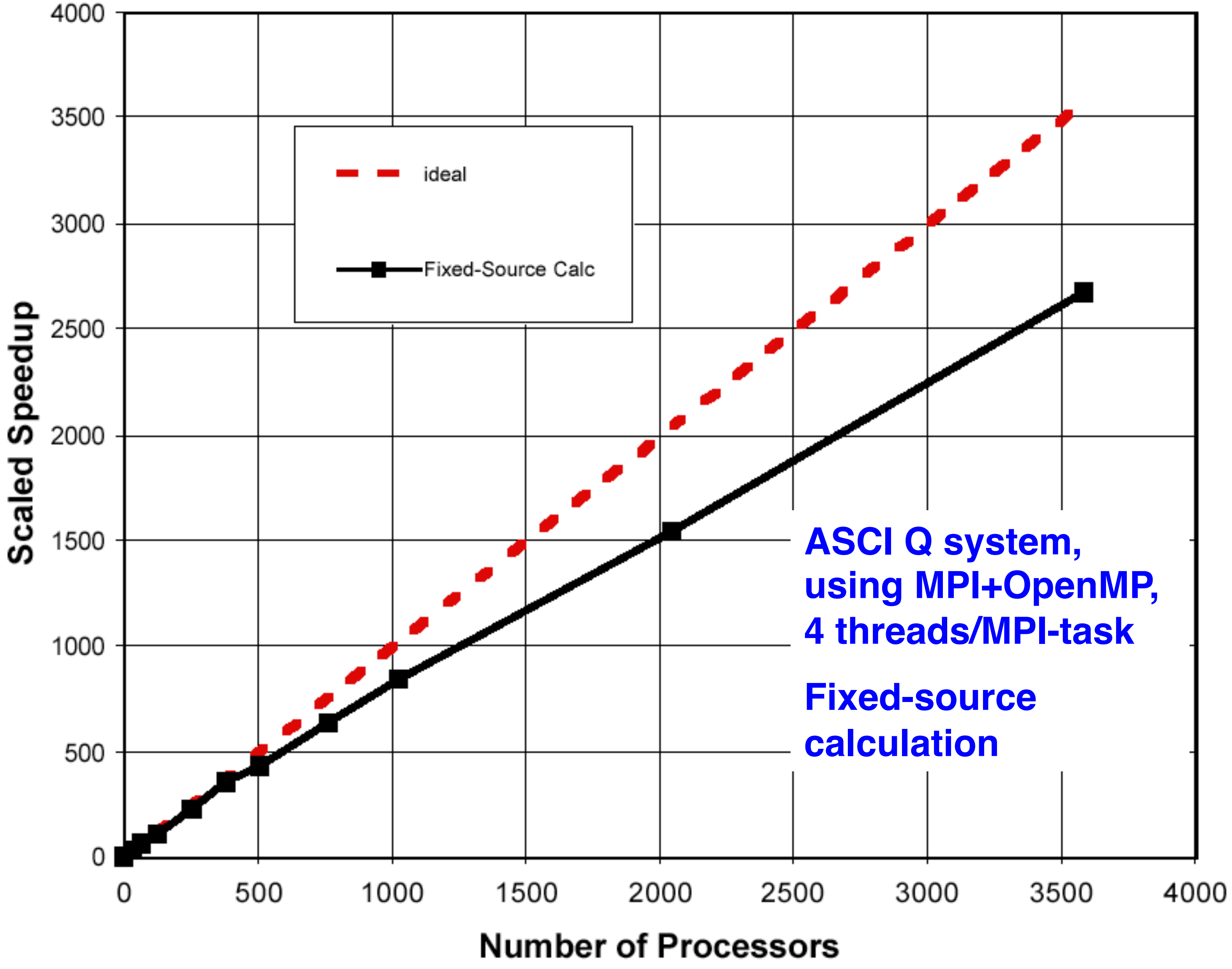
- **Keff calculations: Use KCODE card for hist/cycle**
  - Want to reduce the number of cycles
  - More histories in each cycle
  - Should run hundreds of cycles or more for good results

KCODE nsrck rkk ikz kct …..

nsrck = histories / cycle ← use a large number
rkk = initial guess for Keff
ikz = number of initial cycles to discard
kct = total number of cycles to run

Suggested: nsrck ~ (thousands) x (number of processors)

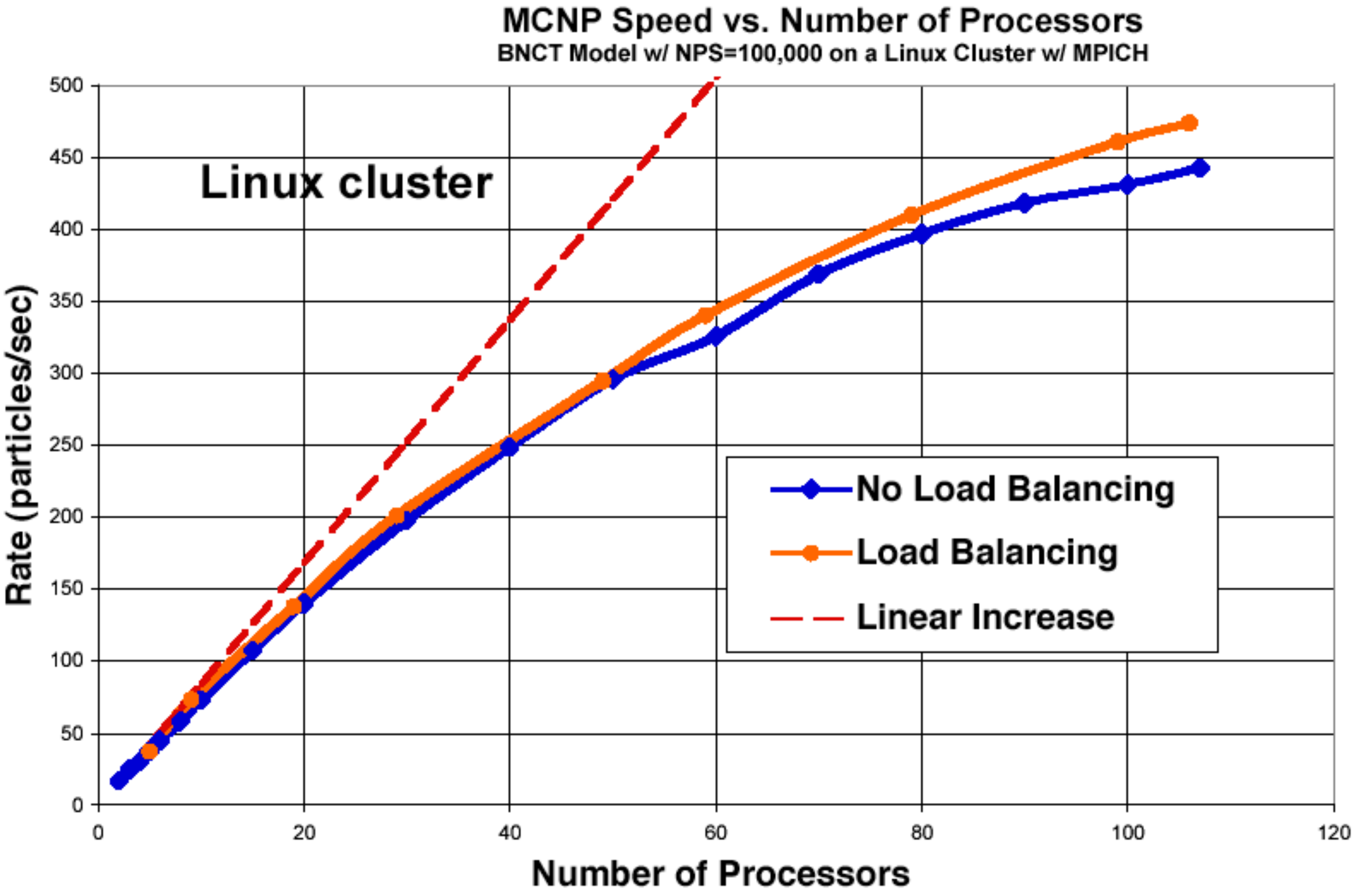
MCNP5 Parallel Scaled Speedup



ASCI Q system, using MPI+OpenMP, 4 threads/MPI-task

Fixed-source calculation

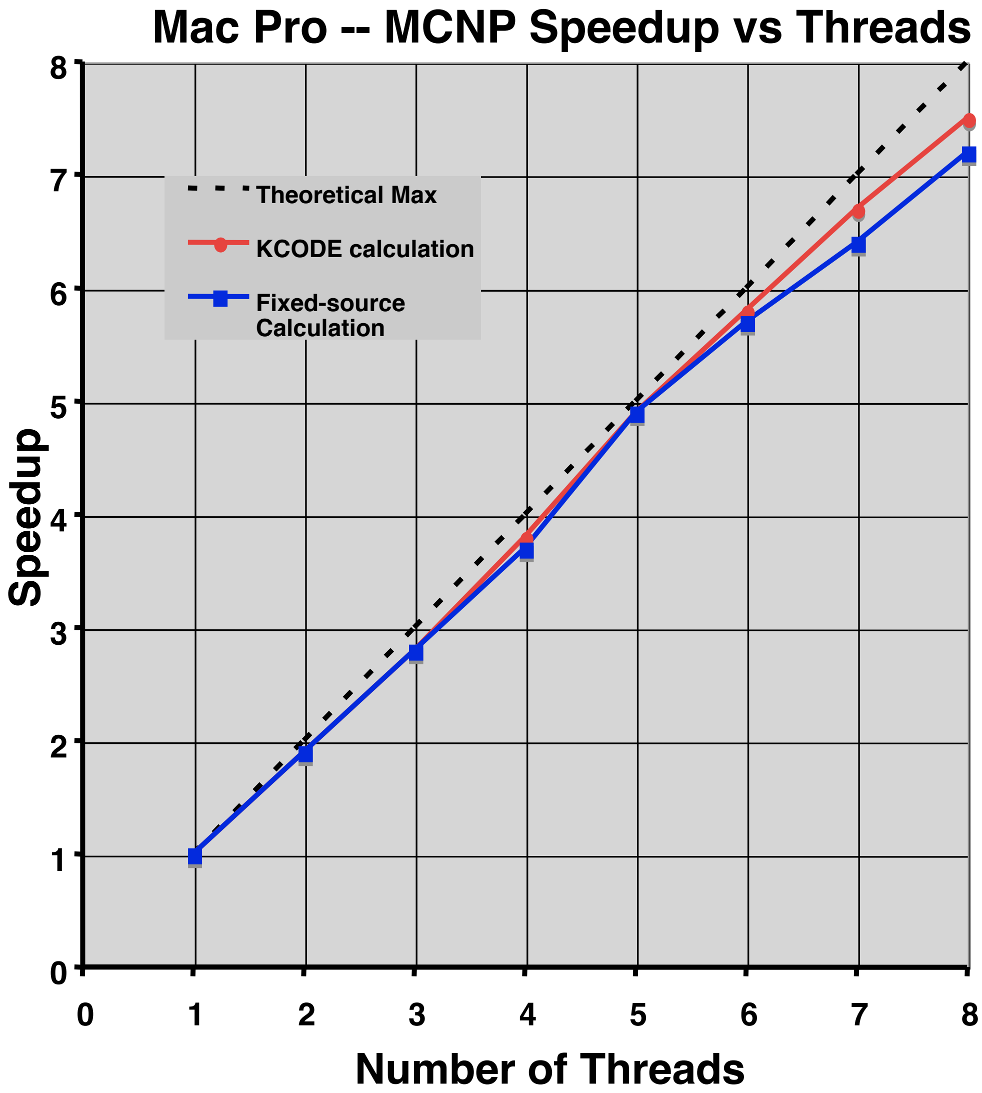
MCNP5 Parallel Calculations



MCNP - Threading with OpenMP

- MCNP performance - both serial & parallel - depends strongly on the Fortran-90 compiler & options used
  - Runtime factors of 2-4x with different compilers on same hardware
  - Runtime factors of 2-4x with different options on same hardware & compiler
- Parallel performance
  - MCNP5 & MCNP6 have always supported parallel calculations with message-passing (MPI) & threading (OpenMP)
  - Prior to mid-2006, Fortran compilers for Windows/Linux/Mac did a terrible job at threading. We recommended using only MPI.
  - Recently, using OpenMP threading with Intel compilers on Windows/Linux/Mac shows excellent speedups -- nearly 2x on dual-core, 3-4x on quad-core

MCNP - Threading on the Mac Pro



Hardware

- Mac Pro
- 2 x Quad-core Xeon
- 3GHz
- 8 GB memory

Software

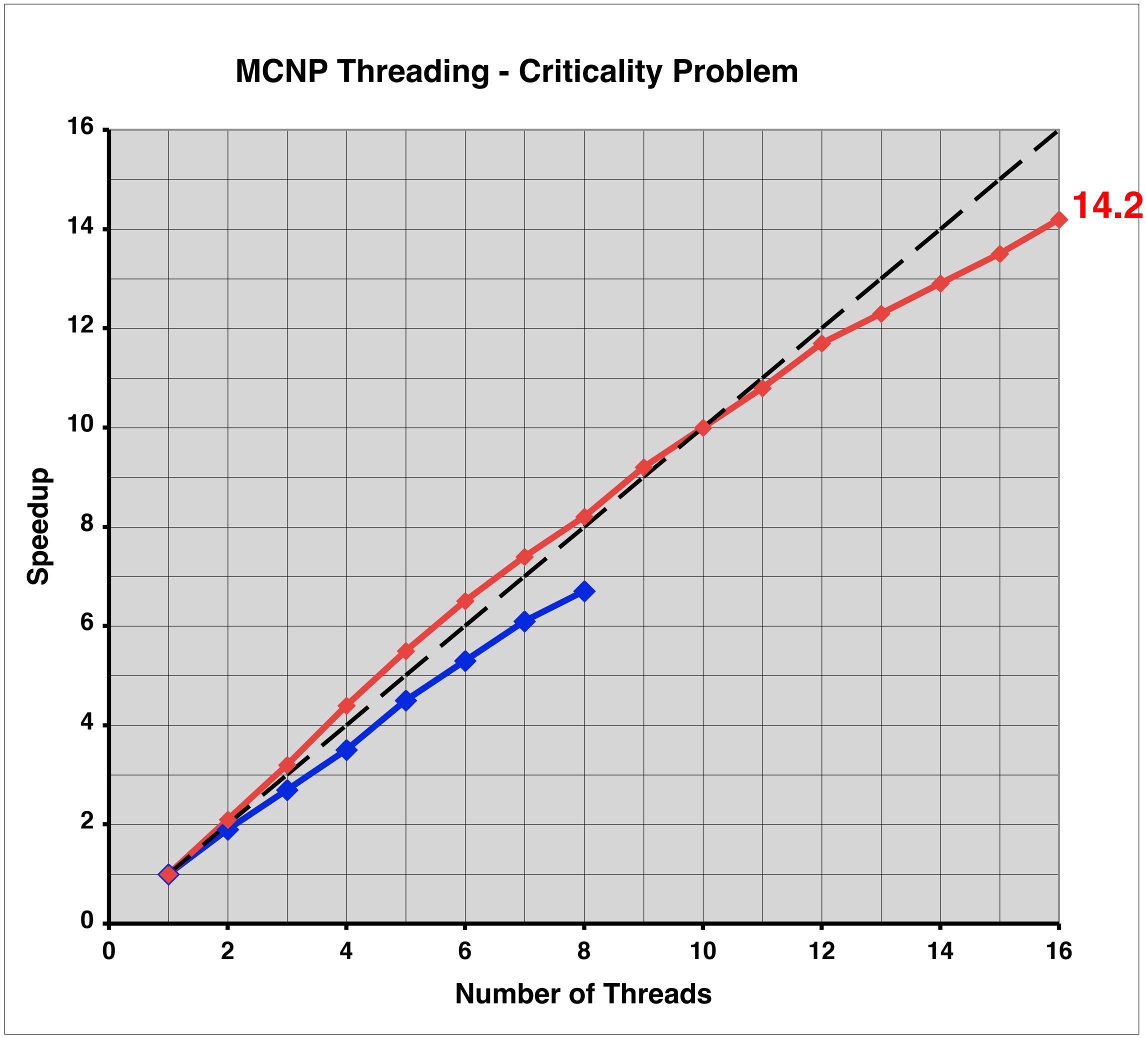
- Mac OS X 10.4.11
- Intel F90, 10.0.017
  -O1 -openmp
- MCNP5 / 1.50

MCNP Calculations

- KCODE
  - BAWXI2 benchmark
  - kcode 5000 1 10 204
- Fixed-source
  - oil-well log, mode n
  - nps 500000

MCNP - Threading

2009-03-03



Hardware

- Lobo
  - 4 x Quad-core AMD Opteron
  - 2.2 GHz, 32 GB memory
- Mac Pro
  - 2 x Quad-core Intel Xeon
  - 3GHz, 8 GB memory

Software

- MCNP5-1.51
- Intel-10 F90, "-O1 -openmp"

MCNP Calculations

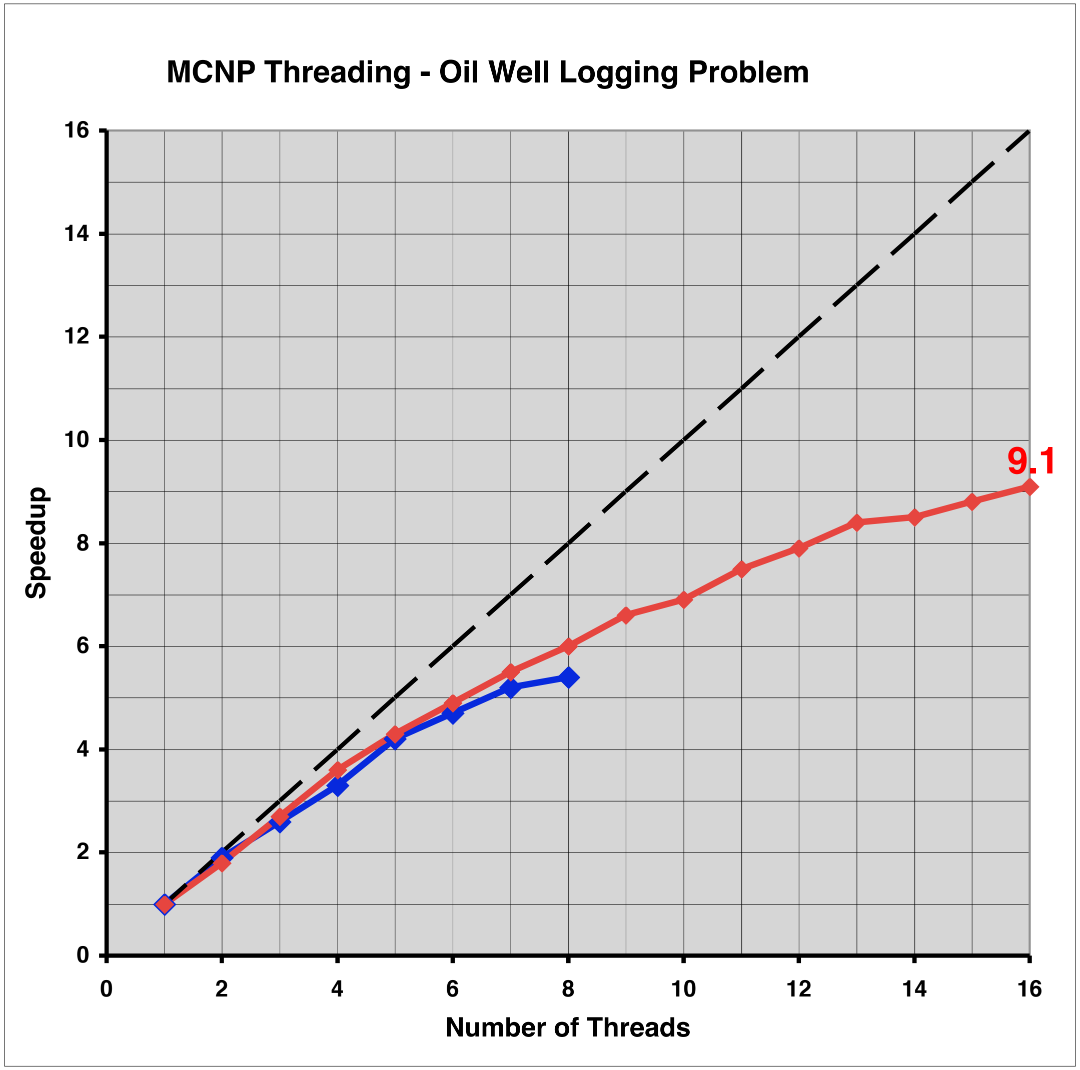
Criticality Calculation

BAWXI2 benchmark

kcode 25000 1 10 204

MCNP - Threading

2009-03-03



Hardware

- Lobo
  - 4 x Quad-core AMD Opteron
  - 2.2 GHz, 32 GB memory
- Mac Pro
  - 2 x Quad-core Intel Xeon
  - 3GHz, 8 GB memory

Software

- MCNP5-1.51
- Intel-10 F90, "-O1 -openmp"

MCNP Calculations

Oil Well Logging Calculation

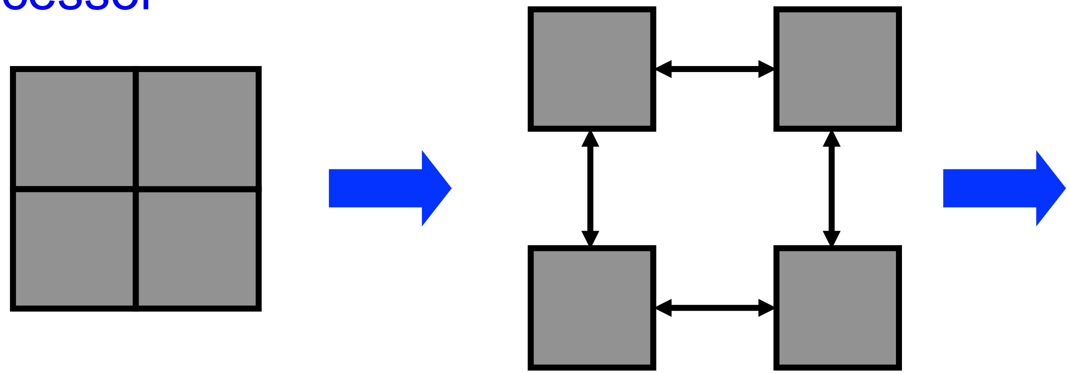
inp12 benchmark

Nps 500000

Parallel Processing For Large Monte Carlo Calculations

Domain Decomposition

If a Monte Carlo problem is too large to fit into memory of a single processor



Decompose problem into spatial domains

Follow histories in each domain in parallel, move particles to new domains as needed

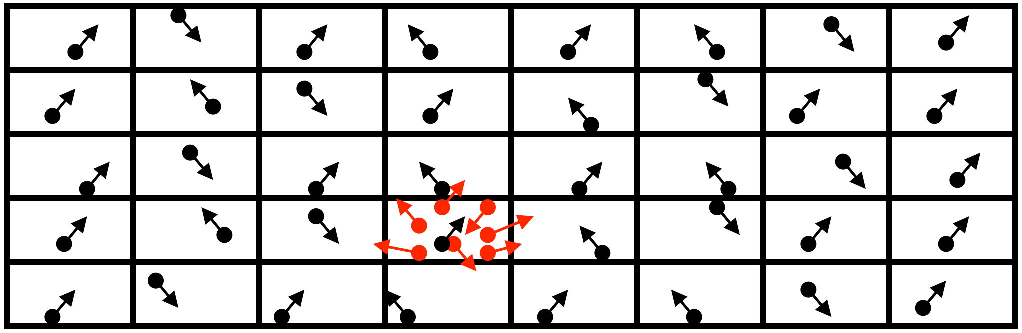
Collect Problem Results

- **Need periodic synchronization to interchange particles among nodes**
- **Use message-passing (MPI) to interchange particles**

➜ **Domain decomposition is often used when the entire problem will not fit in the memory of a single SMP node**

Parallel Monte Carlo

- Inherent parallelism is on <u>particles</u>
  - Scales well for all problems
- Domain decomposition
  - Spatial domains on different processors
  - Scales OK for Keff or α calculations,
    where particle distribution among domains is roughly uniform
  - Does not scale for time-dependent problems
    due to severe load imbalances among domains
- Domain decomposition - scaling with N processors
  - Best: performance ~ N (uniform distribution of particles)
  - Worst: performance ~ 1 (localized distribution of particles)



Parallel Monte Carlo

- Data is distributed by domain decomposition, but parallelism is on particles

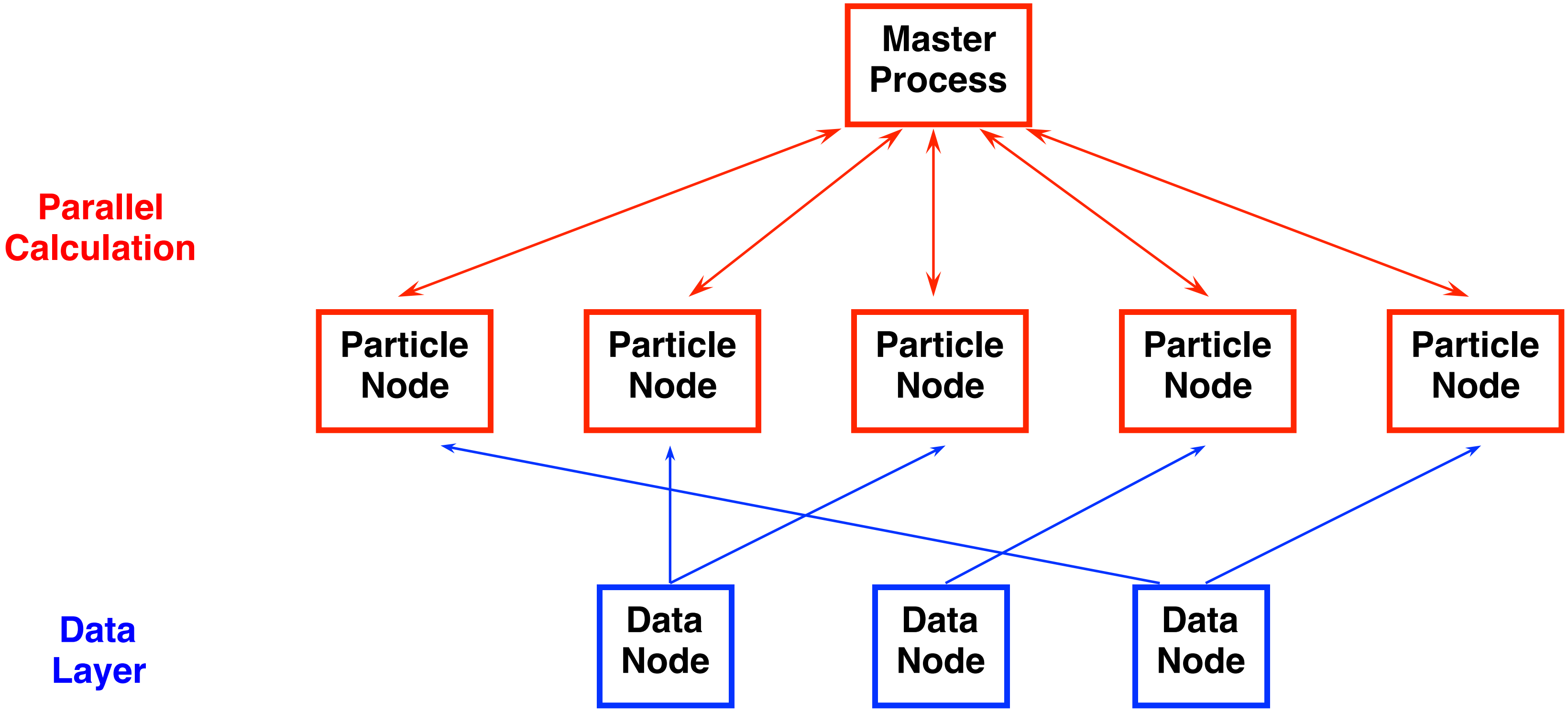
- Solution ?

Parallel on particles + distributed data

- **Particle parallelism + Data Decomposition**
  - **Existing parallel algorithm for particles**
  - **Distribute data among processor nodes**
  - **Fetch the data to the particles as needed (dynamic)**
  - **Essentially same approach as used many years ago for CDC (LCM) or CRAY (SSD) machines**
  - **Scales well for all problems (but slower)**

Parallel Monte Carlo

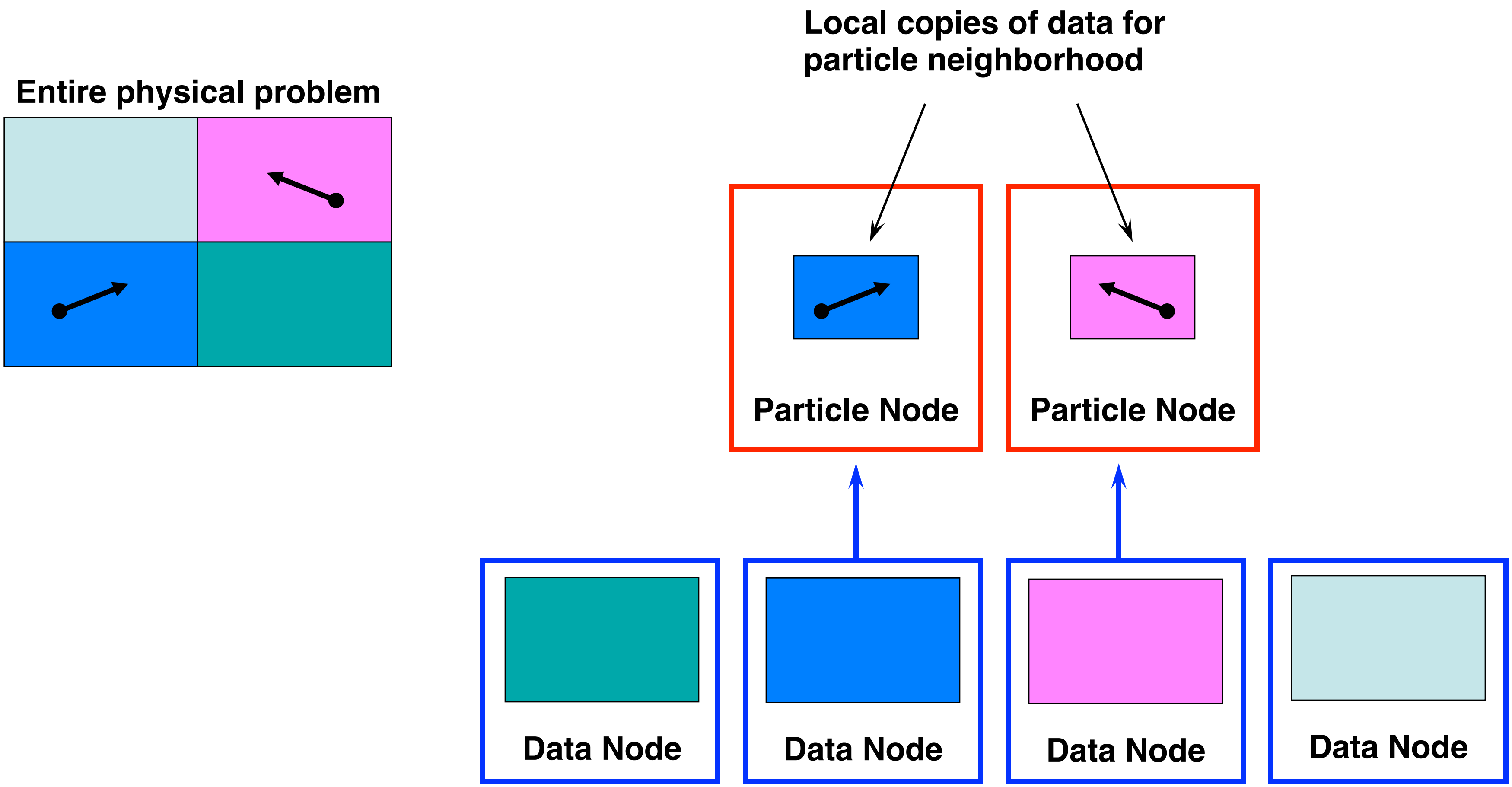
- Particle parallelism + data decomposition -- logical view:



- Mapping of logical processes onto compute nodes is flexible:
  - Could map particle & data processes to different compute nodes
  - Could map particle & data processes to same compute nodes
- Can replicate data nodes if contention arises

Parallel Monte Carlo

- Particle parallelism + data decomposition



Parallel Monte Carlo

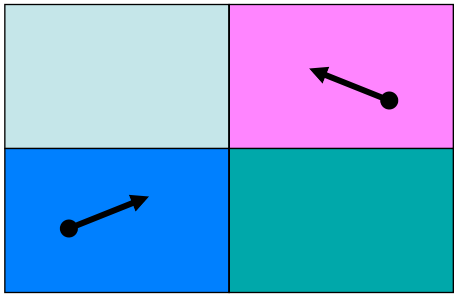
- History modifications for data decomposition

```
source

while   wgt > cutoff

.           compute distances & keep minimum:
.                       dist-to-boundary
.                       dist-to-time-cutoff
.                       dist-to-collision
.                       dist-to-data-domain-boundary

.           move particle
.           pathlength tallies

.           if    distance == dist-to-data-domain-boundary
.                      fetch new data

.           collision physics
.           roulette & split
. . .
```

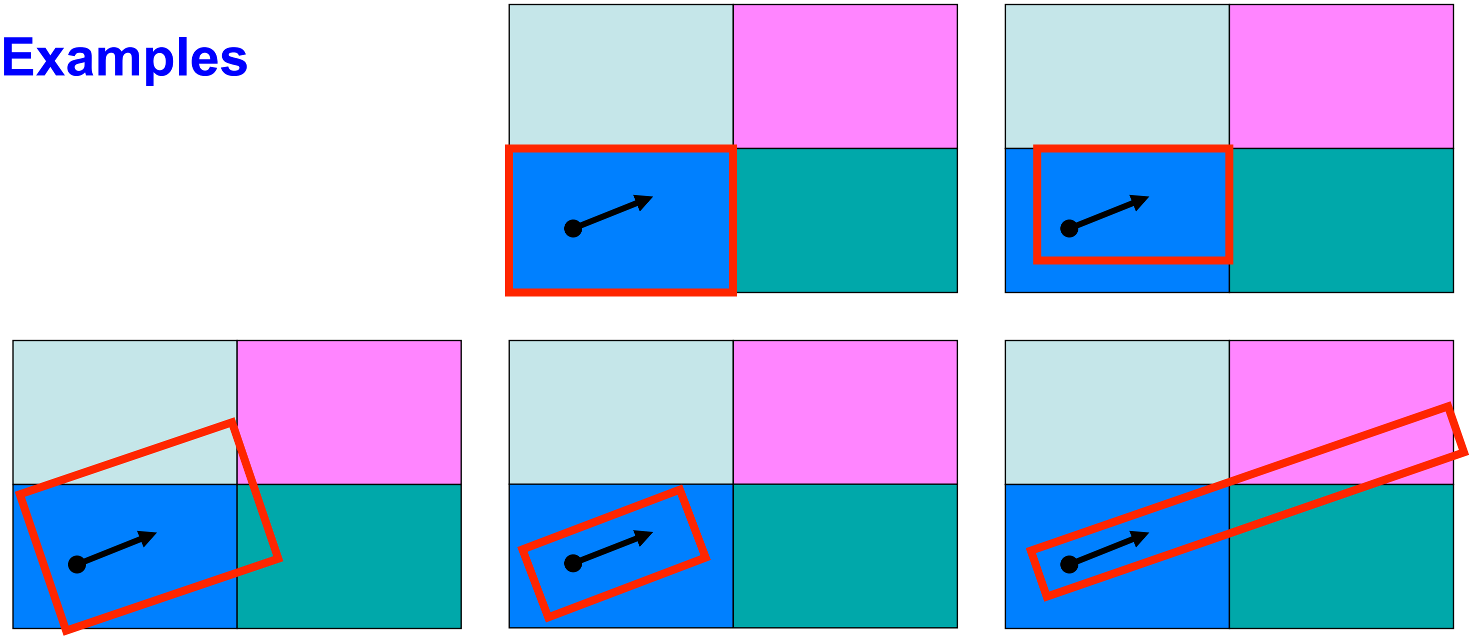
Parallel Monte Carlo

- **Data windows & algorithm tuning**
  - **Defining the "particle neighborhood" is an art**
  - **Anticipating the flight path can guide the pre-fetching of blocks of data**
  - **Tuning parameters:**
    - How much data to fetch ?
    - Data extent vs. particle direction ?

Entire physical problem



- **Examples**



Conclusions

For Monte Carlo problems which can fit in memory:

- Concurrent scalar jobs - ideal for Linux clusters
- Boss/Worker parallel algorithm (replication) works well
  - **Load-balancing: Self-scheduling**
  - **Fault-tolerance: Periodic rendezvous**
  - **Random numbers: Easy, with LCG & fast skip-ahead algorithm**
  - **Tallies: Use OpenMP "critical sections"**
  - **Scaling: Simple model, more histories/Worker + fewer rendezvous**
  - **Hierarchical: Boss/Worker MPI, OpenMP threaded Workers**
  - **Portability: MPI/OpenMP, clusters of anything**

For Monte Carlo problems too large to fit in memory:

- Spatial domain decomposition (with some replication) can work for some problems
- Particle parallelism + data decomposition is a promising approach which should scale for all problems

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9. "MPI: A Message Passing Interface", http://www-unix.mcs.anl.gov/mpi/index.html
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11. "OpenMP Fortran Application Program Interface", http://www.openmp.org

From LA-UR-16-23533

Monte Carlo Parameter Studies & Uncertainty Analyses With MCNP6

Los Alamos NATIONAL LABORATORY EST. 1943

NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

Outline

- Introduction
- mcnp_pstudy
- Examples
- Usage
  - Parameter definition
  - Parameter expansion
  - Constraints
  - Case setup & execution
  - Collecting & combining results
- Statistics
- Practical Examples from Criticality Safety
- Advanced Topics

Frequent Questions

How are calculated results affected by:

- Nominal dimensions
  - With minimum & maximum values ?
  - With as-built tolerances ?
  - With uncertainties ?
- Material densities
  - With uncertainties ?
- Data issues
  - Different cross-section sets ?
- Stochastic materials
  - Distribution of materials ?

Monte Carlo perturbation theory can handle the case of independent variations in material density, but does not apply to other cases.

Brute force approach:

Run many independent Monte Carlo calculations,
varying the input parameters.

mcnp_pstudy

- To simplify & streamline the setup, running, & analysis of Monte Carlo parameter studies & total uncertainty analyses, a new tool has been developed: mcnp_pstudy

- Control directives are inserted into a standard MCNP input file
  - Define lists of parameters to be substituted into the input file
  - Define parameters to be sampled from distributions & then substituted
  - Define arbitrary relations between parameters
  - Specify constraints on parameters, even in terms of other parameters
  - Specify repetitions of calculations
  - Combine parameters as outer-product for parameter studies
  - Combine parameters as inner-product for total uncertainty analysis
- Sets up separate calculations
- Submits or runs all jobs
- Collects results

mcnp_pstudy

- Completely automates the setup/running/collection for parameter studies & total uncertainty analyses
  - Painless for users
  - 1 input file & run command can spawn 100s or 1000s of jobs
  - Fast & easy way to become the #1 user on a system
    (Added bonus: make lots of new friends in computer ops &
    program management.)
- Ideal for Linux clusters & parallel ASC computers:
  - Can run many independent concurrent jobs, serial or parallel
  - Faster turnaround: Easier to get many single-cpu jobs through the queues, rather than wait for scheduling a big parallel job
  - Clusters always have some idle nodes

mcnp_pstudy

- mcnp_pstudy is written in *perl*
  - 640 lines of *perl* (plus 210 lines of comments)
  - Would have taken many thousands of lines of Fortran or C
- Portable to any computer system
  - Tested on Unix, Linux, Mac OS X, Windows
  - For Windows PCs, need to have *perl* installed

    (ActivePerl is free at `activestate.com/activeperl`, easy to install)
- Can be modified easily if needed
  - To add extra features
  - To accommodate local computer configuration
    - Node naming conventions for parallel cluster
    - Batch queueing system for cluster
    - Names & configuration of disk file systems (ie, local or shared)
    - Location of MCNP6 and MCNP6.mpi

Examples

MCNP input for simple Godiva calculation

```
gdv
c
1  100 -18.74  -1   imp:n=1
2  0             1   imp:n=0

1     so 8.741

kcode 10000  1.0  15  115
ksrc  0 0 0
m100  92235 -94.73   92238 -5.27
prdmp 0 0 1 1 0
```

MCNP input using *mcnp_pstudy*, Run 3 different cases - Each with a different radius

```
gdv-A
C @@@  RADIUS = 8.500  8.741  8.750
1  100 -18.74  -1   imp:n=1
2  0             1   imp:n=0

1     so  RADIUS

kcode 10000  1.0  15  115
ksrc  0 0 0
m100  92235 -94.73   92238 -5.27
prdmp 0 0 1 1 0
```

Basics

- Within an MCNP input file, all directives to mcnp_pstudy must begin with

```
C   @@@
```

- To continue a line, use "\" as the last character

```
c   @@@   XXX = 1    2    3    4    5   6   \
c   @@@         7    8    9   10
```

- Parameter definitions have the form

```
c   @@@    P =     value or list
c   @@@    P = (  arithmetic-expression  )
```

- Constraints have the form

```
c   @@@    CONSTRAINT = (   expression    )
```

- Control directives have the form

```
c   @@@    OPTIONS =   list-of-options
```

Parameter Definition

- **Parameters**
  - Like C or Fortran variables
  - Start with a letter, contain only letters, integers, underscore
  - Case sensitive
  - Parameters are assigned values, either number(s) or string(s)
  - Examples: `R1, r1, U_density, U_den`
- **Single value**

```
C   @@@       P1   =   value
```

- **List of values**

```
C   @@@       P2   =   value1   value2   …   valueN
```

- **List of N random samples from Probability Densities:**
  - Uniform

```
      C   @@@   P3   =   uniform   N    min    max
```

  - Normal

```
      C   @@@   P4   =   normal   N    ave    dev
```

  - Lognormal

```
      C   @@@   P5   =   lognormal   N    ave    dev
```

  - Beta

```
      C   @@@   P6   =   beta  N   a   b      [a,b are integers]
```

Parameter Definition

- Arithmetic expression

```
C   @@@       P5   = (   arithmetic-statement   )
```

  - Can use numbers & previously defined parameters
  - Can use arithmetic operators +, -, *, /, % (mod), ** (exponentiation)
  - Can use parentheses ( )
  - Can use functions: sin(), cos(), log(), exp(), int(), abs(), sqrt()
  - Can generate random number in (0,N): rand(N)
  - Can use rn_seed() to get odd seed for mcnp RN generator in [1,2^{48}-1]
  - Must evaluate to a single value
  - Examples:

```
c   @@@    SEED = (   rn_seed()   )
c   @@@   FACT   = normal 1   1.0 .05
c   @@@   UDEN   = ( 18.74 * FACT )
c   @@@   URAD   = ( 8.741 * (18.74/UDEN)**.333333 )
```

- Repetition (list of integers, 1..N)

```
C   @@@       P6   =   repeat   N
```

Parameter Definition

- Examples

```
C  rod height in inches, for search
C  @@@  HROD = 5  10  15  20  25  30  35  40  45  50

C  nominal dimension, with uncertainty
C  @@@  X1 = normal  25   1.234  .002

C  dimension, with min & max
C  @@@  X2 = uniform 25   1.232  1.236

C  try different cross-sections
C  @@@  U235 = 92235.42c  92235.49c  92235.52c  \
C  @@@         92235.60c  92235.66c

C  different random number seeds (odd)
C  @@@  SEED = (  rn_seed()  )
```

Parameter Expansion

- After all parameters are defined, mcnp_pstudy expands them into sets to be used for each separate MCNP calculation
  - Outer product expansion: All possible combinations. Parameters specified first vary fastest.
  - Inner product expansion: Corresponding parameters in sequence. If not enough entries, last is repeated.

Example:

```
c @@@  A  =  1  2
c @@@  B  =  3  4
c @@@  C  =  5
```

```
Outer:     Case 1:     A=1,   B=3,   C=5
           Case 2:     A=2,   B=3,   C=5
           Case 3:     A=1,   B=4,   C=5
           Case 4:     A=2,   B=4,   C=5

Inner:     Case 1:     A=1,   B=3,   C=5
           Case 2:     A=2,   B=4,   C=5
```

Constraint Conditions

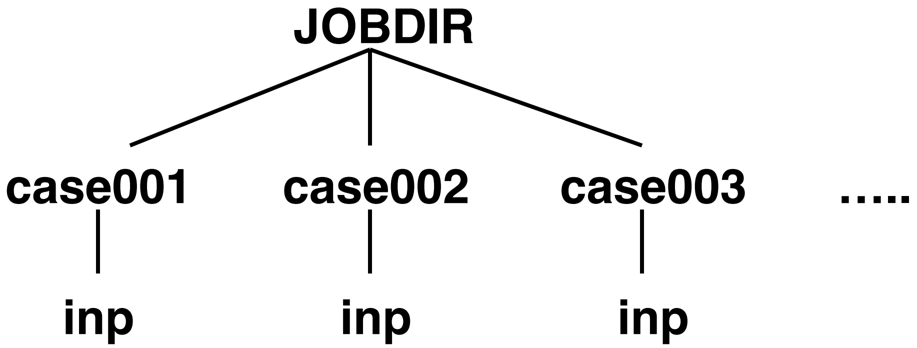
- After all parameters are defined & expanded, constraint conditions are evaluated
- Constraints involve comparison operators (>, <, >=, <=, ==, !=) or logical operators (&& (and), || (or), ! (not)), and may involve arithmetic or functions
- Constraints must evaluate to True or False
- If a any constraint is not met, the parameters for that case are discarded & re-evaluated until all of the constraints are satisfied

Example

```
C pick dimensions between min & max
C
C @@@  X1  =  uniform 1  3.9  4.1
C @@@  X2  =  uniform 1  5.9  6.1
C
C keep x1 & x2 if  x1+x2 <= 10.0,  otherwise reject & try again
C
C @@@  CONSTRAINT = ( X1 + X2  <=  10.0 )
```

Creating INP Files & Job Directories

- Directory structure for MCNP5 jobs



JOBDIR

case001 case002 case003 …..

inp inp inp

  – Unix filesystem conventions followed

```
JOBDIR/case001/inp,  JOBDIR/case002/inp, etc.
```

- Values of parameters are substitued into the original MCNP5 input file to create the input files for each case
  - Parameters substituted only when exact matches are found
  - Example: `UDEN` matches `UDEN`, and not `UDEN1, UDENS, uden`

Job Options

- **Specifying options for running jobs**
  - Can be specified on the mcnp_pstudy command-line

```
mcnp_pstudy  -inner    -setup -i inp01
```

  - Within the INP file

```
c @@@ OPTIONS = -inner
```

- **Common options**

`-i  str`	The INP filename is `str`, default = inp
`-jobdir  str`	Use `str` as the name of the job directory
`-case    str`	Use `str` as the name for case directories
`-mcnp_opts str`	Append `str` to the MCNP5 run command, may be a string such as `'o=outx tasks 4'`
`-bsub_opts str`	`str` is appended to the LSF bsub command
`-inner`	Inner product approach to case parameter substitution
`-outer`	Outer product approach to case parameter substitution
`-setup`	Create the cases & INP files for each
`-run`	Run the MCNP5 jobs on this computer
`-submit`	Submit the MCNP5 jobs using LSF bsub command
`-collect`	Collect results from the MCNP5 jobs

Running or Submitting Jobs

- Jobs can be run on the current system, or can be submitted to a batch queueing system (e.g., LSF)
- Tally results & K-effective can be collected when jobs finish

Examples:

```
bash:  mcnp_pstudy -inner -i inp01 -setup
bash:  mcnp_pstudy -inner -i inp01 -run
bash:  mcnp_pstudy -inner -i inp01 -collect
```

```
bash:  mcnp_pstudy -inner -i inp01 -setup -run -collect
```

```
bash:  mcnp_pstudy -inner -i inp01 -setup -submit
```

… wait till all jobs complete…

```
bash:  mcnp_pstudy -inner -i inp01   -collect
```

Creating Input Files ONLY

- To bypass the creation of job directories, and running/submitting problems:

  – A special command line option is available: -inponly

  – Invoking this option performs the parsing & setup of the input files for each case, but the resulting mcnp input files are placed in the current directory with default names of the form

  ```
  inp_case001,   inp_case002, etc.
  ```

  – Using `-case study01a -inponly` would result in files with names

  ```
  inp_study01a001,  inp_study01a002,  etc.
  ```

  – Other options `-run, -submit` cannot be used if `-inponly` is present

  – The option `-whisper` can be used, and is equivalent to `-inponly`

Combining Results

- Tally results & K-effective from separate cases can be combined using batch statistics:

$$\overline{X} = \frac{1}{M} \cdot \sum_{k=1}^{M} X_k \qquad \sigma_{\overline{X}} = \sqrt{\frac{1}{M-1} \cdot \left[\frac{1}{M} \sum_{k=1}^{M} X_k^2 - \overline{X}^2 \right]}$$

where M is the number of cases & X_k is some tally or Keff for case k

- Variance due to randomness in histories decreases as 1/M, but variance due to randomness in input parameters is constant

$$\sigma_{\overline{X}}^2 \approx \sigma_{\overline{X},\ \text{Monte Carlo}}^2 + \sigma_{\overline{X},\ \text{Initial Conditions}}^2$$

Varies as 1/M ~ Constant

Examples

Vary the fuel density randomly & adjust radius for constant mass, for 50 cases

```
gdv-E
c vary fuel density - normal, 5%sd,
c adjust the radius to keep constant mass
c
c @@@ FACT= normal 50  1.0 .05
c @@@ UDEN= ( 18.74*FACT )
c @@@ URAD= ( 8.741*(18.74/UDEN)**.333333 )
c
1     100  -UDEN   -1   imp:n=1
2     0             1   imp:n=0

1     so  URAD

kcode 10000  1.0  15  115
ksrc  0. 0. 0.
m100  92235 -94.73   92238 -5.27
prdmp 0 0 1 1 0
```

Vary fuel density & mass independently, for 50 cases

```
gdv-F
c vary fuel radius - normal, 5%sd
c vary fuel density- normal, 5%sd
c
c @@@ OPTIONS = -inner
c
c @@@ DFACT = normal 50  1.0 .05
c @@@ UDEN = ( DFACT * 18.74 )
c
c @@@ UFACT = normal 50  1.0 .05
c @@@ URAD  = ( UFACT * 8.741 )
c
1     100  -UDEN   -1   imp:n=1
2     0             1   imp:n=0

1     so  URAD

kcode 10000  1.0  15  115
ksrc  0. 0. 0.
m100  92235 -94.73   92238 -5.27
prdmp 0 0 1 1 0
```

Examples

Table 1. Results from varying parameters in the Godiva problem

Problem	Description	K-effective	$\sigma_{K\text{-eff}}$
base	**Base case**, discard 15 initial cycles, retain 100 cycles with 10K histories/cycle, **1M total histories**	0.9970	**0.0005**
A	Repeat the base problem 50 times, **50M total histories**	0.9972	**0.0001**
B	**Vary the fuel density only**: sample from a normal distribution with 5% std.dev, **50M total histories**	0.9961	**0.0061**
C	**Vary the fuel radius only**: sample from a normal distribution with 5% std.dev, **50M total histories**	1.0057	**0.0051**
D	**Vary the enrichment only**, sample from a normal distribution with 5% std.dev, **50M total histories**	0.9890	**0.0027**
E	**Sample the fuel density from a normal distribution with 5% std.dev, and adjust the fuel radius to keep constant fuel mass, 50M total histories**	0.9966	**0.0042**
F	**Sample the fuel density from a normal distribution with 5% std.dev, and independently sample the radius from a normal distribution with 5% std.dev, 50M total histories**	1.0073	**0.0076**

Applications

- Parameter studies
  - Run a series of cases with different control rod positions
  - Run a series of cases with different soluble boron concentrations
  - Run a series of cases sampling certain dimensions from a Uniform or Normal probability density
  - Run a series of cases substituting different versions of a cross-section
- Total uncertainty analysis
  - Run a series of cases varying all input parameters according to their uncertainties
- Parallel processing using a "parallel jobs" approach
  - Running N separate jobs with 1 cpu each will be more efficient than running 1 job with N cpus
  - Eliminates queue waiting times while cpus are reserved
  - Take advantage of cheap Linux clusters
- Simulation of stochastic geometry
  - Run a series of cases with portions of geometry sampled randomly, with a different realization in each case

Conclusions

- **mcnp_pstudy works**
  - **In use regularly at LANL for a variety of real applications**
  - **Developed on Mac & PC, runs anywhere**
  - **Easy to customize, if you have special needs**

- **To get it:**
  - **Included with MCNP6 distribution**

FB Brown, JE Sweezy, RB Hayes, "Monte Carlo Parameter Studies and Uncertainty Analyses with MCNP5", PHYSOR-2004, Chicago, IL (April, 2004)

Practical Examples from Criticality Safety

Examples

- **wval4:** 4.5 kg Pu Sphere, Ta-reflected with varying reflector thickness
- **wval1:** 4.5 kg Pu Ingot, solid cylinder with varying H/D
- **wval2:** 4.5 kg Pu Ring, hollow cylinder with varying H & R_{in}

Example

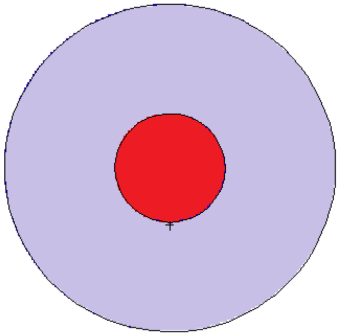
wval4,

4.5 kg Pu Sphere,

Ta-reflected

Example wval4: 4.5 kg Pu Sphere, Ta-reflected (1)

- 4.5 kg Pu-239 sphere
- Pu density = 19.8 g/cm^3
- Reflected radially with Ta



- Vary the Ta-reflector thickness over the range 0.$^+$ – 30. cm
  - Start with wval4.txt, input for thickness=7.62

    mcnp6 i=wval4.txt

  - Copy wval4.txt to wval4p.txt, then insert directives for mcnp_pstudy
    - Define list for thickness:

      ```
      c @@@ THICK =  0.01  5.  10.  15.  20.  25.  30.
      ```

    - For a given THICK, compute reflector Rin & Rout
    - Use parameters for dimensions & location of KSRC point
    - Run:

      ```
      mcnp_pstudy -i wval4.txt  -mcnp_opts ‘tasks 4’  -setup
      ```

      …… examine files case*/inp

      ```
      mcnp_pstudy -i wval4.txt  -mcnp_opts ‘tasks 4’  -run
      ```

Example wval4: 4.5 kg Pu Sphere, Ta-reflected (2)

```
wval4:  Study of Pu reflected with Ta
c
c  Pu mass     = 4500 g
c  Pu density = 19.8 g/cc
c  Pu volume  = 227.272727
c
c  reflector definition:
c    reflector thickness    = 7.62
c    reflector inner radius = 3.7857584
c    reflector outer radius = 11.405758
c
  1   4 -19.80  -1         imp:n=1
  2   1 -16.69  +1 -2      imp:n=1
 20   0         +2         imp:n=0

  1 so  3.7857584
  2 so  11.405758

 kcode 10000 1.0 50 250
 sdef pos=0 0 0  rad=d1
  si1  0 3.78
  sp1  -21 2
c
 m1  73180.80c 0.00012   73181.80c 0.99988
 m4  94239.80c 1
 prdmp 9e9 9e9 1 9e9
```

```
wval4p:  Study of Pu reflected with Ta
c
c  Pu mass     = 4500 g
c  Pu density = 19.8 g/cc
c  Pu volume  = 227.272727
c
c  vary reflector thickness from 0+ to 30 cm
c
c  @@@  THICK   = .01  5. 10. 15. 20. 25. 30.
c  @@@  R_INNER = 3.7857584
c  @@@  R_OUTER = ( R_INNER + THICK )
c
c  reflector definition:
c    reflector thickness    = THICK cm
c    reflector inner radius = R_INNER cm
c    reflector outer radius = R_OUTER cm
c
  1   4 -19.80  -1         imp:n=1
  2   1 -16.69  +1 -2      imp:n=1
 20   0         +2         imp:n=0

  1 so    R_INNER
  2 so    R_OUTER

 kcode 10000 1.0 50 250
 sdef pos=0 0 0 rad=d1
  si1  0  R_INNER
  sp1  -21 2
c
 m1  73180.80c 0.00012   73181.80c 0.99988
 m4  94239.80c 1
 prdmp 9e9 9e9 1 9e9
```

Example wval4: 4.5 kg Pu Sphere, Ta-reflected (3)

wval4, thick=7.62

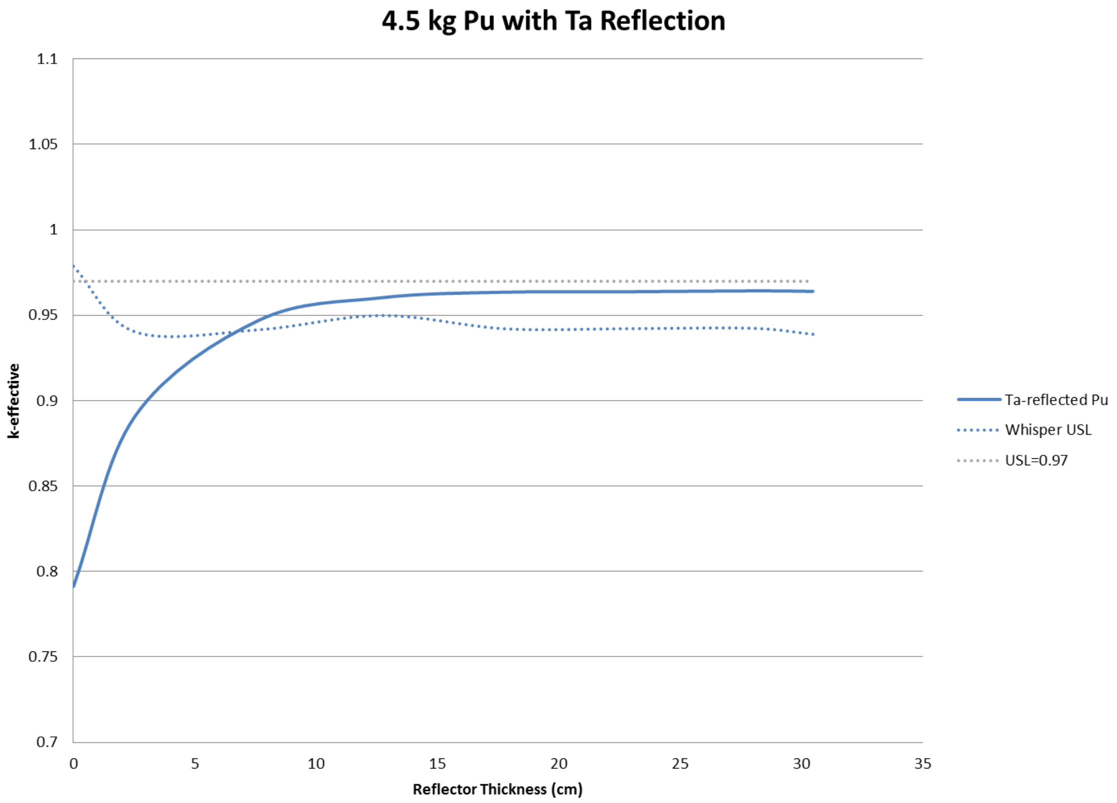
```
mcnp6  i=wval4.txt
```

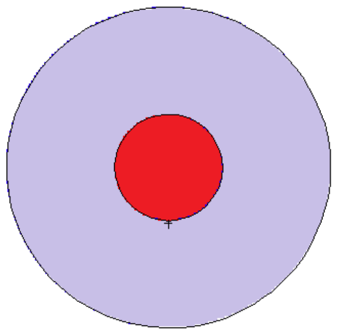
k = 0.94638 (41)

wval4p, varying thick

```
mcnp_pstudy  -i wval4p.txt  -setup  -run
```

```
T=.01   case001 KEFF   7.91693E-01   KSIG   3.14948E-04
T=5.0   case002 KEFF   9.27157E-01   KSIG   4.47334E-04
T=10.   case003 KEFF   9.54775E-01   KSIG   4.11031E-04
T=15.   case004 KEFF   9.61644E-01   KSIG   4.34033E-04
T=20.   case005 KEFF   9.62867E-01   KSIG   4.37235E-04
T=25.   case006 KEFF   9.63899E-01   KSIG   4.04508E-04
T=30.   case007 KEFF   9.63160E-01   KSIG   4.27633E-04
```



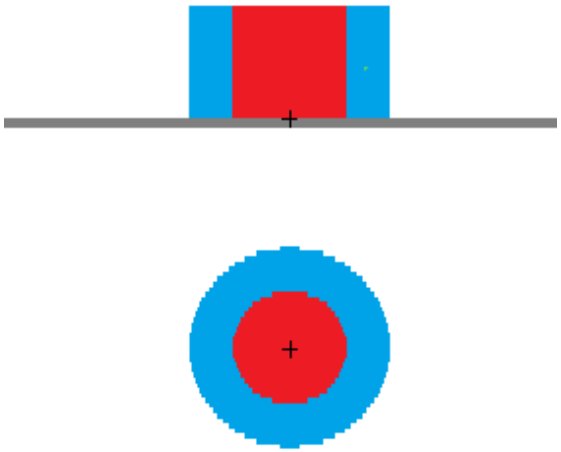


Example

wval1,
4.5 kg Pu Ingot,
varying H/D

Example wval1: 4.5 kg Pu Ingot, varying H/D (1)

- **4.5 kg Pu-239 right-circular cylinder**
- **Pu density = 19.86 g/cm^3**
- **Reflected radially with 1 inch of water**
- **Reflected on the bottom with ¼ inch steel**



- **Vary the height-to-diameter (H/D) over the range 0.5 – 3.0**
  - **Start with wval1.txt, input for H/D = 1**

    mcnp6 i=wval1.txt

  - **Copy wval1.txt to wval1p.txt, then insert directives for mcnp_pstudy**
    - Define list for HD:

```
c @@@ HD =  0.5  1.0  1.5  2.0  2.5  3.0
```

    - For a given H/D, compute Pu radius, then other dimensions

$$V = (\text{Pu mass})/(\text{Pu density})$$

$$V = H\pi R^2 = (\text{H/D}) \cdot 2\pi R^3$$

$$R = \left[V/2\pi(\text{H/D})\right]^{1/3}$$

    - Use parameters for dimensions & location of KSRC point

Example wval1: 4.5 kg Pu Ingot, varying H/D (2)

```
wval1:  4500 g Pu metal,  H/D = 1
c reflected 1 inch water radially,
c 0.25 in steel bottom
c
 1 1 -19.860000  -1            imp:n=1
11 3 -1.0        +1 -11        imp:n=1
14 6 -7.92       -30           imp:n=1
15 0             +11 +30 -20   imp:n=1
20 0 +20                       imp:n=0

 1  rcc  0 0 0       0 0 6.607662 3.303831
11  rcc  0 0 0       0 0 6.607662 5.843831
20  rcc  0 0 -2.54   0 0 91.44     91.44
30  rcc  0 0 -0.635  0 0 0.635     76.20

 kcode  10000 1.0 50 250
 ksrc  0 0 3.303831
 m1  94239.80c 1
 m3   1001.80c 0.66667    8016.80c 0.33333
 mt3  lwtr.20t
 m6  24050.80c 0.000757334
     24052.80c 0.014604423
     24053.80c 0.001656024
     24054.80c 0.000412220
     26054.80c 0.003469592
     26056.80c 0.054465174
     26057.80c 0.001257838
     26058.80c 0.000167395
     25055.80c 0.00174
     28058.80c 0.005255537
     28060.80c 0.002024423
     28061.80c 0.000088000
     28062.80c 0.000280583
     28064.80c 0.000071456
 prdmp 9e9 9e9 1 9e9
```

```
wval1p:  4500 g Pu metal, various H/D
c reflected 1 inch water radially,
c 0.25 in steel bottom
c
c   V = H pi R**2 = (H/D) 2pi R**3
c   R = (V/(2pi H/D)**1/3
c
c @@@  PI     = 3.141592654
c @@@  VOL_PU = ( 4500. / 19.86 )
c @@@  HD     = 0.5  1.0  1.5  2.0  2.5  3.0
c @@@  R_PU   = ( (VOL_PU/(2*PI*HD))**(1/3) )
c @@@  H_PU   = ( 2*R_PU*HD )
c @@@  R_H2O  = ( R_PU + 2.54 )
c @@@  KSRC_Z = ( H_PU * 0.5 )
c
c Pu cylinder:
c      mass        = 4500 g
c      density     = 19.86 g/cc
c      volume      = VOL_PU
c      radius Pu   = R_PU
c      height Pu   = H_PU
c      H/D         = HD
c
c H2O  outer radius = R_H2O
c
  1   1 -19.860000   -1            imp:n=1
 11   3 -1.0         +1 -11        imp:n=1
 14   6 -7.92        -30           imp:n=1
 15   0              +11 +30 -20   imp:n=1
 20   0              +20           imp:n=0

  1  rcc  0 0 0          0 0 H_PU   R_PU
 11  rcc  0 0 0          0 0 H_PU   R_H2O
 20  rcc  0 0 -2.540000  0 0 91.44  91.44
 30  rcc  0 0 -0.635000  0 0 0.635  76.20

 kcode  10000 1.0 50 250
 ksrc   0. 0. KSRC_Z
C ………………… etc.
```

Example wval1: 4.5 kg Pu Ingot, varying H/D (3)

wval1, H/D = 1

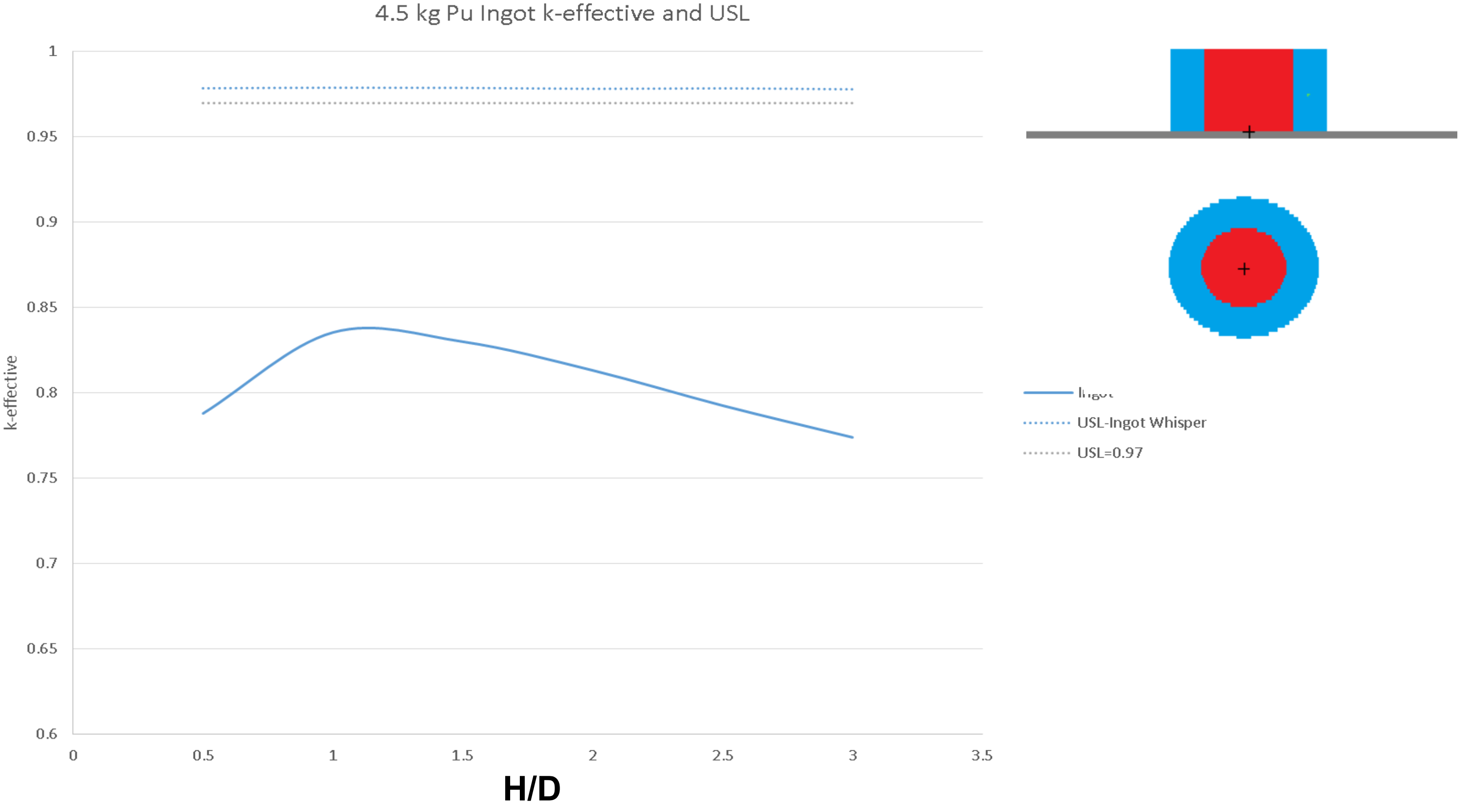
```
mcnp6  i=wval1.txt
```

k = 0.83491 (41)

wval1p, varying H/D

```
mcnp_pstudy  -i wval1p.txt  -setup  -run
```

```
HD=0.5  case001 KEFF    7.87229E-01    KSIG    4.09191E-04
HD=1.0  case002 KEFF    8.34430E-01    KSIG    4.20175E-04
HD=1.5  case003 KEFF    8.29652E-01    KSIG    4.19130E-04
HD=2.0  case004 KEFF    8.11958E-01    KSIG    4.18723E-04
HD=2.5  case005 KEFF    7.93676E-01    KSIG    4.63720E-04
HD=3.0  case006 KEFF    7.73434E-01    KSIG    4.19664E-04
```



Example

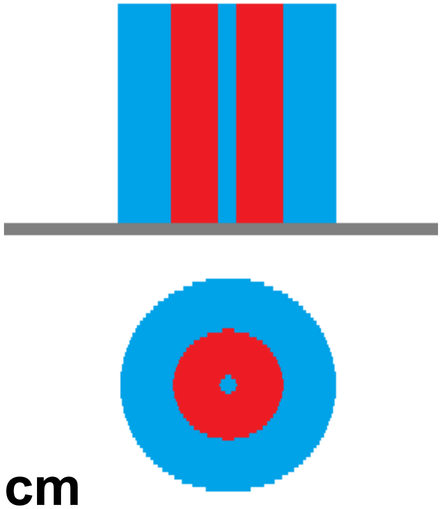
wval2,

4.5 kg Pu Annulus,

varying H & R_{in}

Example wval2: 4.5 kg Pu Annulus, varying H & R_{in} (1)

- 4.5 kg Pu-239 right-circular cylinder, hollow
- Pu density = 19.86 g/cm^3
- Reflected radially with 1 inch of water
- Reflected on the bottom with ¼ inch steel



- Set the height to be same as solid cylinder with height-to-diameter (H/D) = 1.0, 2.0, 3.0
- For given height, vary inner radius over 0$^+$ - 2 cm
  - Start with wval2.txt input

    ```
    mcnp6   i=wval2.txt
    ```

  - Copy wval2.txt to wval2p.txt, then insert directives for mcnp_pstudy
    - Define list for solid HD:

      ```
      c @@@ HD =  1.0  2.0  3.0
      ```

    - For a given H/D, compute Pu height
    - Define list for inner radius RIN_PU

      ```
      c @@@ RIN_PU =  0.001  0.5  1.0  2.0
      ```

    - Then other dimensions & source

Solid cylinder

$$V = (\text{Pu mass})/(\text{Pu density})$$

$$V = H\pi R^2 = (\text{H/D})\cdot 2\pi R^3$$

$$H = \left[4V(\text{H/D})^2/\pi\right]^{1/3}$$

Hollow cylinder

$$V = H\pi(R_{out}^2 - R_{in}^2)$$

$$R_{out} = \left[R_{in}^2 + V/\pi H\right]^{1/2}$$

Example wval2: 4.5 kg Pu Annulus, varying H & R_{in} (2)

```
wval2: 4500 g Pu metal ring, fixed Rin
  1   3 -1.0         -1             imp:n=1
  2   1 -19.860000   +1 -2          imp:n=1
 11   3 -1.0         +2 -11         imp:n=1
 14   6 -7.92        -30            imp:n=1
 15   0              +11 +30 -20    imp:n=1
 20   0              +20            imp:n=0

  1 rcc  0 0 0       0 0  6.608   0.100000
  2 rcc  0 0 0       0 0  6.608   3.305259
 11 rcc  0 0 0       0 0  6.608   5.845259
 20 rcc  0 0 -2.540  0 0 91.44   91.44
 30 rcc  0 0 -0.635  0 0 0.635   76.20

kcode  10000 1.0 50 250
sdef pos=0 0 0  rad=d1 axs=0 0 1  ext=d2
 si1  0.100  3.305259
 sp1  -21 1
 si2  0.0   6.60800
 sp2  0   1
m1   94239.80c 1
m3   1001.80c 0.66667    8016.80c 0.33333
mt3  lwtr.20t
m6   24050.80c 0.000757334
     24052.80c 0.014604423
     24053.80c 0.001656024
     24054.80c 0.000412220
     26054.80c 0.003469592
     26056.80c 0.054465174
     26057.80c 0.001257838
     26058.80c 0.000167395
     25055.80c 0.00174
     28058.80c 0.005255537
     28060.80c 0.002024423
     28061.80c 0.000088000
     28062.80c 0.000280583
     28064.80c 0.000071456
prdmp 9e9 9e9 1 9e9
```

```
wval2p: 4500 g Pu metal ring, various H & Rin
c
c @@@  PI     = 3.141592654
c @@@  VOL_PU = ( 4500. / 19.86 )
c      Pu mass    = 4500 g
c      Pu density = 19.86 g/cc
c      Pu volume  = VOL_PU
c
c set height to match ingot with various H/D
c @@@  HD     =  1.0  2.0  3.0
c @@@  HEIGHT = ( (4*VOL_PU*(HD**2)/PI)**(1/3) )
c
c for hollow cylinder:
c   use same height as for solid ingot
c   set various inner radii
c   set Rout for given height, mass, Rin
c @@@  RIN_PU = .001  0.5  1.0  2.0
c @@@  ROUT_PU=(sqrt(RIN_PU**2+VOL_PU/(PI*HEIGHT)))
c @@@  ROUT_H2O = ( OUTER_PU + 2.54 )
c
  1   3 -1.0         -1             imp:n=1
  2   1 -19.860000   +1 -2          imp:n=1
 11   3 -1.0         +2 -11         imp:n=1
 14   6 -7.92        -30            imp:n=1
 15   0              +11 +30 -20    imp:n=1
 20   0              +20            imp:n=0

  1  rcc   0 0 0         0 0  HEIGHT  RIN_PU
  2  rcc   0 0 0         0 0  HEIGHT  ROUT_PU
 11  rcc   0 0 0         0 0  HEIGHT  ROUT_H2O
 20  rcc   0 0 -2.540    0 0 91.44    91.44
 30  rcc   0 0 -0.635    0 0 0.635    76.20

kcode  10000 1.0 50 250
sdef  pos= 0. 0. 0.   rad=d1  axs=0 0 1  ext=d2
 si1  RIN_PU  ROUT_PU
 sp1  -21 1
 si2  0 HEIGHT
 sp2  0  1
…………… etc.
```

Example wval2: 4.5 kg Pu Annulus, varying H & R_{in} (3)

wval2

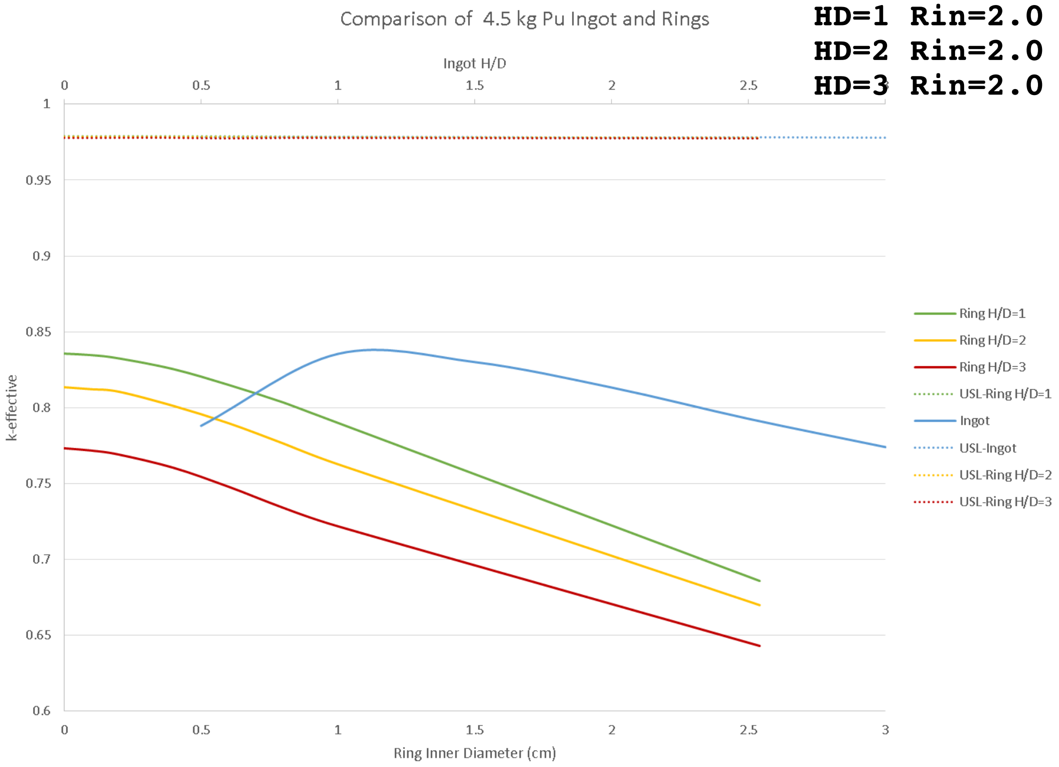
```
mcnp6  i=wval2.txt
```

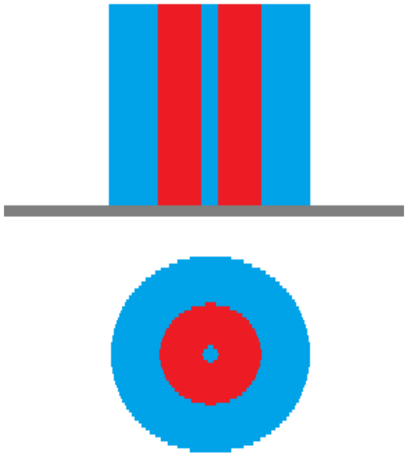
k = 0.83413 (42)

wval2p, varying H & R_{in}

```
mcnp_pstudy  -i wval2p.txt  -setup  -run
```

```
HD=1 Rin=.001 case001 KEFF    8.34752E-01   4.35668E-04
HD=2 Rin=.001 case002 KEFF    8.12612E-01   4.09516E-04
HD=3 Rin=.001 case003 KEFF    7.72725E-01   3.82627E-04
HD=1 Rin=0.5  case004 KEFF    8.20432E-01   4.01135E-04
HD=2 Rin=0.5  case005 KEFF    7.95375E-01   4.60388E-04
HD=3 Rin=0.5  case006 KEFF    7.54174E-01   3.96580E-04
HD=1 Rin=1.0  case007 KEFF    7.88497E-01   3.95026E-04
HD=2 Rin=1.0  case008 KEFF    7.62394E-01   3.90299E-04
HD=3 Rin=1.0  case009 KEFF    7.20810E-01   4.27354E-04
HD=1 Rin=2.0  case010 KEFF    7.21523E-01   4.02775E-04
HD=2 Rin=2.0  case011 KEFF    6.97954E-01   4.88269E-04
HD=3 Rin=2.0  case012 KEFF    6.64037E-01   4.88326E-04
```





Advanced Topics

Tied parameters

Concurrent jobs

Parameter Expansion (1)

- Standard inner & outer schemes for determining job parameters

Example:

```
c @@@  A  =   1   2
c @@@  B  =   3   4
c @@@  C  =   5   6
c @@@  D  =   7   8
c @@@  E  =   9
```

```
Outer:       all combinations, 16 cases
             {1,3,5,7,9}, {2,3,5,7,9}, {1,4,5,7,9}, {2,4,5,7,9},
             {1,3,6,7,9}, {2,3,6,7,9}, {1,4,6,7,9}, {2,4,6,7,9},
             {1,3,5,8,9}, {2,3,5,8,9}, {1,4,5,8,9}, {2,4,5,8,9},
             {1,3,6,8,9}, {2,3,6,8,9}, {1,4,6,8,9}, {2,4,6,8,9},

Inner:       2 cases
             {1,3,5,7, 9},  {2,4,6,8, 9}
```

- The inner & outer schemes for determining job parameters can be modified
  - Often desirable to deal with groups of parameters that are varied
  - 2 or more parameters can be “tied” together, to vary in an inner manner
  - Tied parameter lists must have the same lengths

Parameter Expansion (2)

These examples assume that the -outer option is in effect for all parameter combinations

Example:

```
c @@@  tied = A B
c @@@  A  =   1   2
c @@@  B  =   3   4
c @@@  C  =   5   6
c @@@  D  =   7   8
c @@@  E  =   9

Cases, {A,B,C,D,E}:
{1,3, 5, 7, 9},  {1,3, 6, 7, 9},
{1,3, 5, 8, 9},  {1,3, 6, 8, 9},
{2,4, 5, 7, 9},  {2,4, 6, 7, 9},
{2,4, 5, 8, 9},  {2,4, 6, 8, 9}
```

Example:

```
c @@@  tied = A B C
c @@@  A  =   1   2
c @@@  B  =   3   4
c @@@  C  =   5   6
c @@@  D  =   7   8
c @@@  E  =   9

Cases, {A,B,C,D,E}:
{1,3,5, 7,9},  {1,3,5, 8,9},
{2,4,6, 7,9},  {2,4,6, 8,9}
```

Example:

```
c @@@  tied = A B
c @@@  A  =   1   2
c @@@  B  =   3   4
c @@@  tied = C D
c @@@  C  =   5   6
c @@@  D  =   7   8
c @@@  E  =   9

Cases, {A,B,C,D,E}:
{1,3, 5,7, 9},  {1,3, 6,8, 9},
{2,4, 5,7, 9},  {2,4, 6,8, 9}
```

Example:

```
c @@@  tied = A B C D
c @@@  A  =   1   2
c @@@  B  =   3   4
c @@@  C  =   5   6
c @@@  D  =   7   8
c @@@  E  =   9

Cases, {A,B,C,D,E}:
{1,3,5,7, 9},  {2,4,6,8, 9}
```

Parameter Expansion (3)

The -inner & -outer options can be varied for different parameters, and mixed with tied parameters

Example:

```
c @@@  options = -inner
c @@@  A   =   1   2
c @@@  B   =   3   4
c @@@  C   =   5   6
c @@@  D   =   7   8
c @@@  E   =   9

Cases:
{1,3,5,7, 9},  {2,4,6,8, 9},
```

Example:

```
c @@@ options = -inner
c @@@  A   =   1   2
c @@@  B   =   3   4
c @@@ options = -outer
c @@@  C   =   5   6
c @@@  D   =   7   8
c @@@  E   =   9

Cases:
{1,3, 5, 7, 9},  {1,3, 6, 7, 9},
{1,3, 5, 8, 9},  {1,3, 6, 8, 9},
{2,4, 5, 7, 9},  {2,4, 6, 7, 9},
{2,4, 5, 8, 9},  {2,4, 6, 8, 9}
```

Example:

```
c @@@ options = -outer
c @@@  tied = A B
c @@@  A   =   1   2
c @@@  B   =   3   4
c @@@  tied = C D
c @@@  C   =   5   6
c @@@  D   =   7   8
c @@@  E   =   9

Cases:
{1,3, 5,7, 9},  {1,3, 6,8, 9},
{2,4, 5,7, 9},  {2,4, 6,8, 9}
```

Example:

```
c @@@  tied = A B C D
c @@@  A   =   1   2
c @@@  B   =   3   4
c @@@  C   =   5   6
c @@@  D   =   7   8
c @@@  E   =   9

Cases:
{1,3,5,7, 9},  {2,4,6,8, 9}
```

Concurrent Jobs (1)

- **By default, jobs for the different cases are run sequentially**
  - For –run: jobs for each case are run on the current computer, sequentially (one-at-a-time)
  - For –submit: separate batch jobs are submitted for each case,
  - For either –run or -submit, multiple threads can be used for the mcnp6 runs in each case, by using the option `–mcnp_opts 'tasks 8'`
- **For Linux & Mac systems, not Windows:**
  - Multiple concurrent cases can be run, even when threads are used
  - The `–ppn n` option specifies the number of processes per node (ie, cases to be run concurrently)
- **Examples:**
  - On a system with 24 hyperthreads, could run 6 cases at a time with 4 threads each:

```
mcnp_pstudy –i inp.txt -mcnp_opts 'tasks 4' -ppn 6 -setup –run
```

  - For a cluster with 16 cores/node, can submit jobs with 16 cases each:

```
mcnp_pstudy –i inp.txt -ppn 16  -setup –submit
```

From LA-UR-12-25156

Fission Matrix & Higher Eigenmodes

Forrest Brown

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National Lab Professor, University of New Mexico

Los Alamos NATIONAL LABORATORY EST. 1943

Advanced Simulation & Computing™

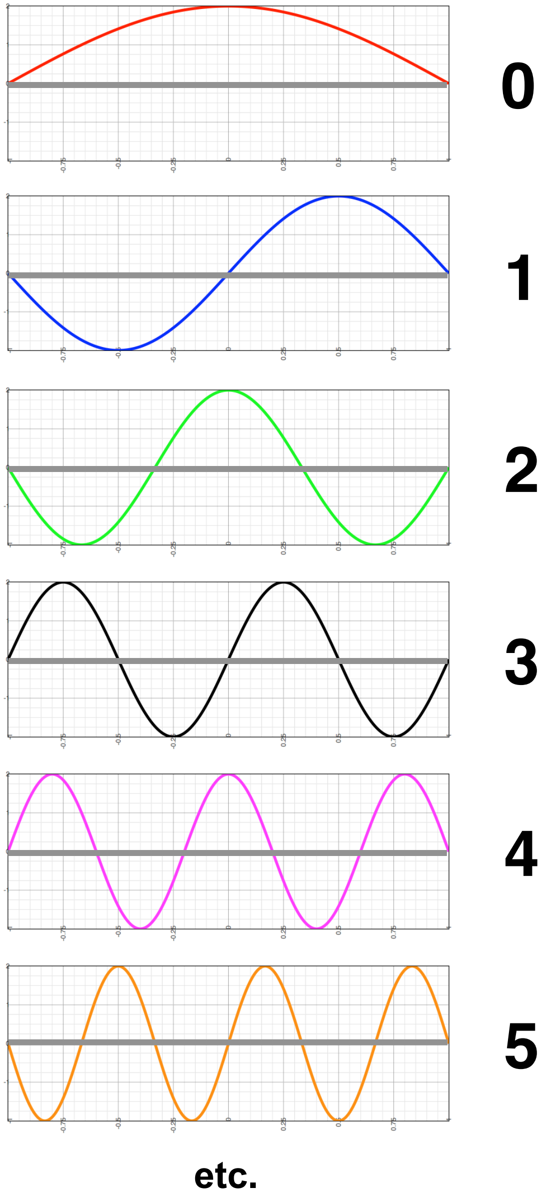
NNSA Nuclear Criticality Safety Program

Fission Matrix Capability for MCNP Monte Carlo

- Introduction
  - MCNP
  - Higher Eigenmodes
  - Green's Functions & Transport
- Fission Matrix
  - Theory
  - Sparse Storage
  - Transport Theory
- Examples
  - Homogeneous 2D Reactor
  - Whole-core PWR, 2D
  - Whole-core PWR, 3D (Kord Smith)
  - Advanced Test Reactor
  - Spent Fuel Storage Vault
- Conclusions

Carney, Brown, Kiedrowski, Martin,
“Fission Matrix Capability for MCNP Monte Carlo”,
Trans ANS 107, San Diego, 2012

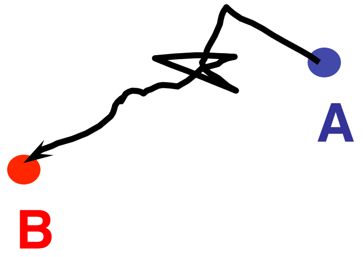
Introduction - Higher Eigenmodes



Vibrating strings:

- Higher modes add "tone", but die away quickly
- Fundamental mode persists
- Feedback, instability, nonlinear effects, …, may excite higher modes

Introduction - Green's Functions & Transport Theory



$$S_B = S_A \cdot F(A \rightarrow B)$$

- F(A→B)
  - Green's function, "here-to-there" function
  - Probability that source at point A produces source at point B

- Transport theory - Peierl's equation for multiplying system

$$S(\vec{r}) = \frac{1}{k_{eff}} \cdot \int_{\text{all } \vec{r}'} d\vec{r}' \cdot S(\vec{r}') \cdot F(\vec{r}' \rightarrow \vec{r})$$

  - Discretize space into blocks, or mesh regions
  - Compute F(r'→r) with Monte Carlo
  - Solve matrix eigenvalue problem for sources:

$$\vec{S} = \frac{1}{k_{eff}} \cdot \bar{F} \cdot \vec{S}$$

  - Can also solve for higher modes

Fission Matrix
In
MCNP Monte Carlo

Fission Matrix - Theory

- **Transport equation, k-eigenvalue form**

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

$$\begin{aligned} M\cdot\Psi(\vec{r},E,\hat{\Omega}) &= \hat{\Omega}\cdot\nabla\Psi(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}) \\ &\quad - \iint dE'\,d\hat{\Omega}'\Sigma_S(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\Psi(\vec{r},E',\hat{\Omega}'), \end{aligned}$$

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

- **Define Green's function & integral transport equation**

$$M\cdot G(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0)\cdot\delta(E-E_0)\cdot\delta(\hat{\Omega}-\hat{\Omega}_0),$$

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

- **Multiply by $\nu\Sigma_F$, integrate over E, Ω, & initial regions (r_0) & final regions (r)**

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

$$F_{I,J} = \int_{\vec{r}\in V_I} d\vec{r}\int_{\vec{r}_0\in V_J} d\vec{r}_0\,\frac{S(\vec{r}_0)}{S_J}\cdot\int\iiint dE\,d\hat{\Omega}\,dE_0\,d\hat{\Omega}_0\cdot\nu\Sigma_F(\vec{r},E)\cdot\frac{\chi(E_0)}{4\pi}\cdot G(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega})$$

$$S_J = \int_{\vec{r}'\in V_J} S(\vec{r}')\,d\vec{r}' = \iiint_{\vec{r}'\in V_J} d\vec{r}'\,dE'\,d\hat{\Omega}'\nu\Sigma_F(\vec{r}',E')\Psi(\vec{r}',E',\hat{\Omega}'),$$

Exact equations for integral source S_I, N = # spatial regions, F is NxN matrix

Fission Matrix - Theory

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

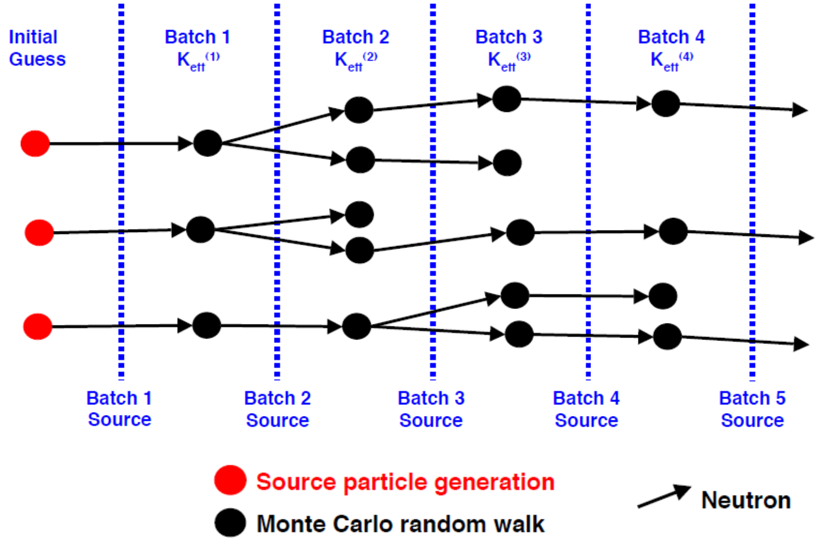
- In the equation for F,
  - $S(r_0)/S_J$ is a local weighting function within region J
  - As $V_J \rightarrow 0$:
    - $S(r_0)V_J/S_J \rightarrow 1$
    - Discretization errors → 0
    - Can accumulate tallies of $F_{I,J}$ even if not converged

- $F_{I,J}$ tallies:
  - Previous F-matrix work: tally during neutron random walks
  - Present F-matrix work: tally only point-to-point, using fission-bank in master proc (~free)
    - Eliminates excessive communications for parallel
    - Provides more consistency, $F_{I,J}$ nonzero only in elements with actual sites
    - Analog-like treatment, better for preserving overall balance

MCNP Criticality Calculations

Monte Carlo K-effective Calculation

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



For Fission Matrix calculation

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

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

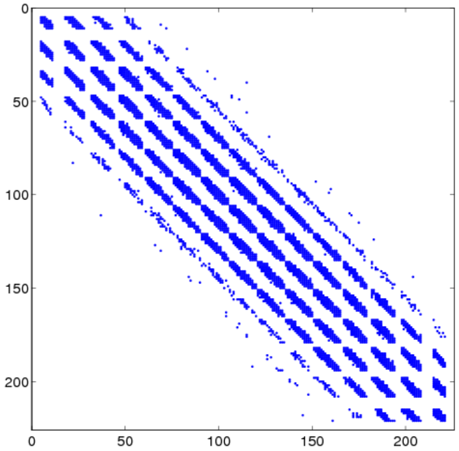
After the Monte Carlo is complete:

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

Fission Matrix – Sparse Structure

- For a spatial mesh with N regions, F matrix is N x N
  - 100 x 100 x 100 mesh → F is 10^6 x 10^6 → 8,000 GB memory
  - In the past, memory storage was the major limitation
- Sparse storage for F matrix

3D reactor with
15x15 spatial mesh,
225x225 F matrix



  - Don't store zero elements, use sparse storage scheme
  - For 100x100x100 mesh, reduces F matrix storage to a few GB

K-eigenvalue Form of Transport Equation

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

- **Structure & properties**
  - **60 years ago:**

    A single, non-negative, real, fundamental eigenfunction & eigenvalue exist
  - **50 years ago:**

    For 1-speed or 1-group: A complete set of self-adjoint, real eigenfunctions & discrete eigenvalues exists
  - **Energy-dependent transport equation is bi-orthognal,**

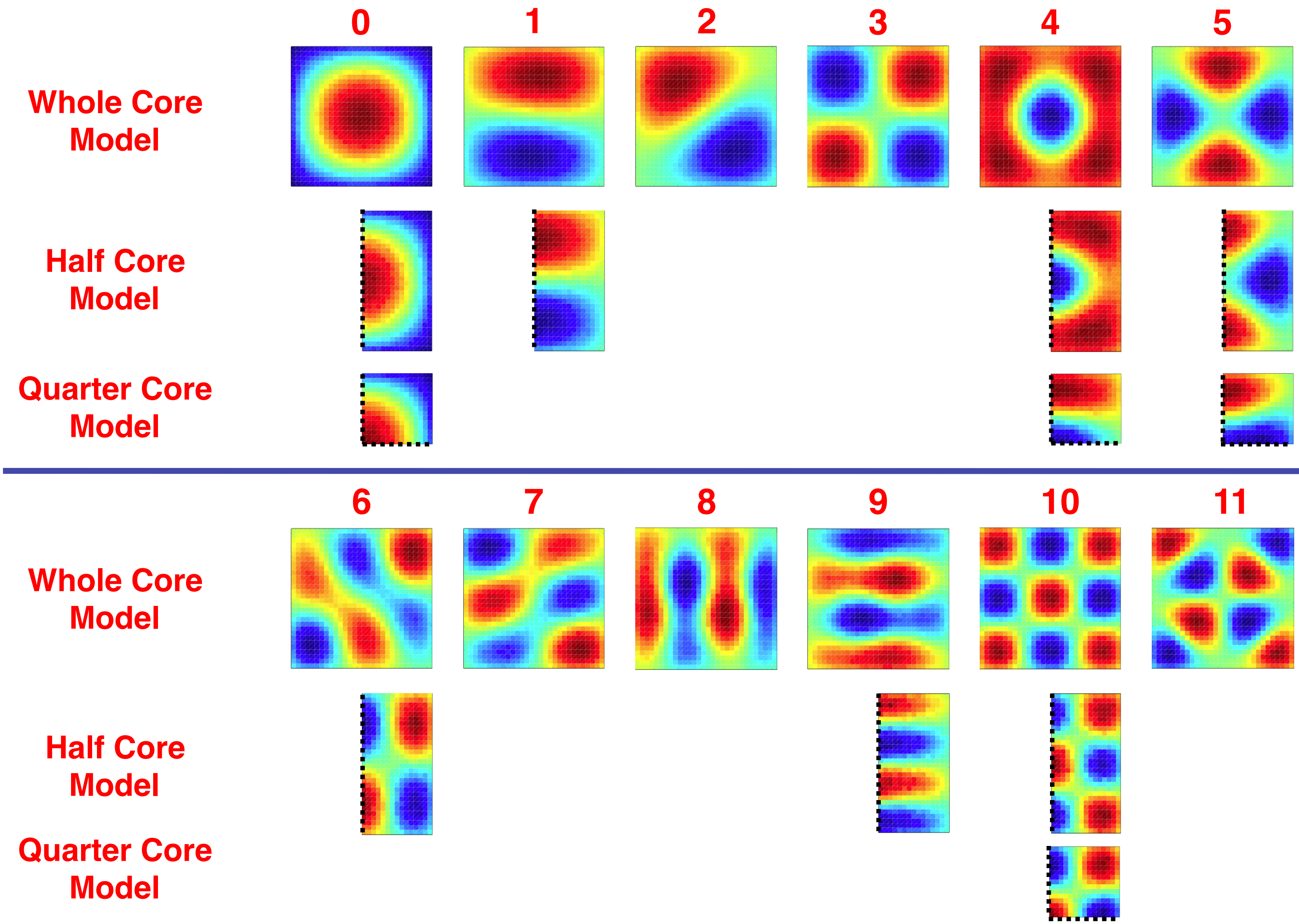
    forward & adjoint modes are orthogonal
  - **Nothing else proven, always assumed that higher-mode solutions exist**

- **In the present work based on the Fission Matrix:**
  - **We provide evidence that higher modes exist, are real, have discrete eigenvalues, and are very nearly self-adjoint** **(for reactor-like problems)**
  - **Approach is similar to Birkhoff's original proof for fundamental mode**
  - **This has never been done before using continuous-energy Monte Carlo**

Homogeneous 2D Reactor Eigenmodes for:

Whole-core Model
Half-core Model
Quarter-core Model

Eigenmodes for Homogeneous 2D Reactor



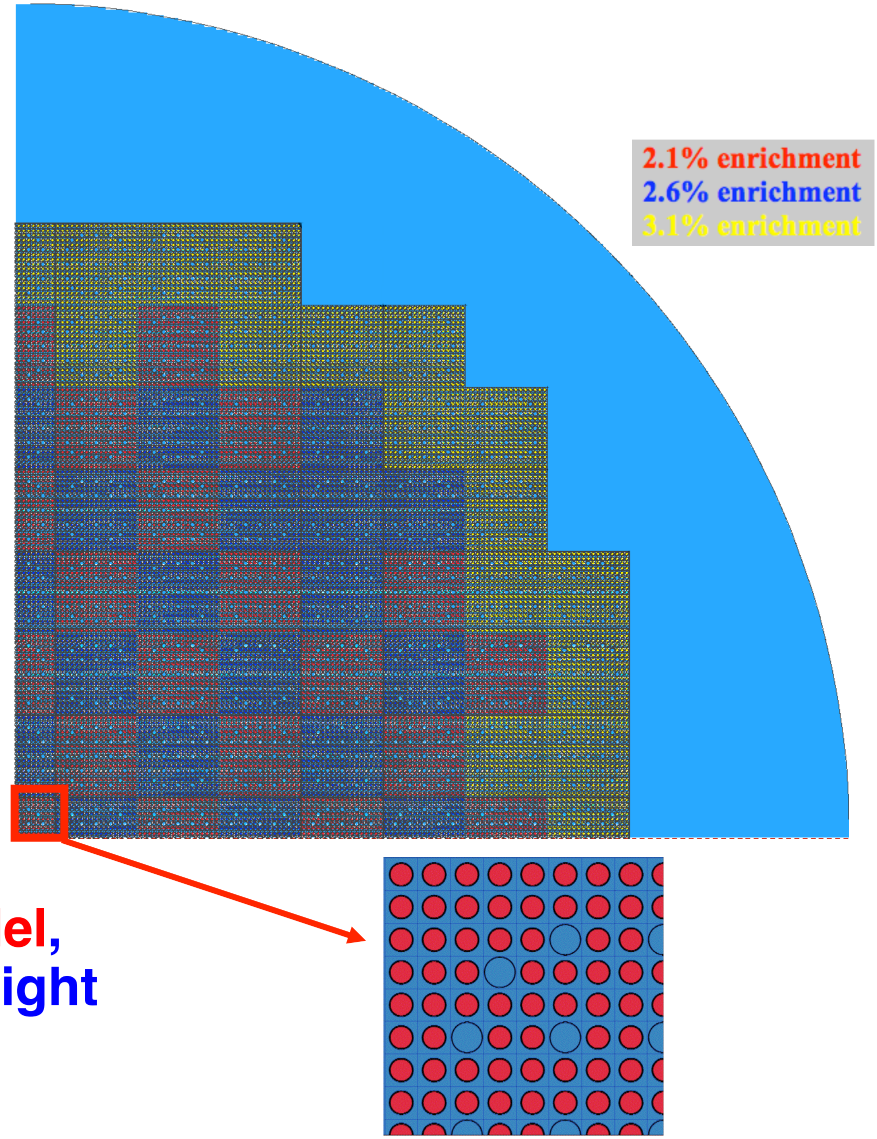
Whole-core 2D PWR

Eigenvalue spectrum
Spatial Eigenmodes

Whole-core 2D PWR Model

2D PWR (Nakagawa & Mori model)

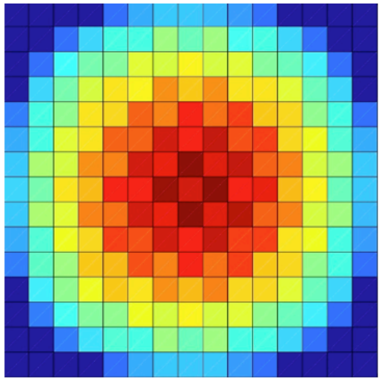
- **48 1/4 fuel assemblies:**
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes for control rods or detectors
- **Each assembly:**
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- **Dominance ratio ~ .98**



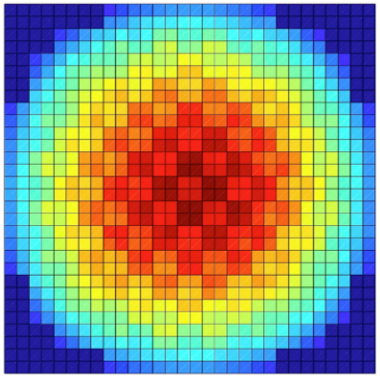
- **Calculations used whole-core model, symmetric quarter-core shown at right**
- **ENDF/B-VII data, continuous-energy**
- **Tally fission rates in each quarter-assembly**

PWR – Eigenvalue Spectrum & Fundamental Mode

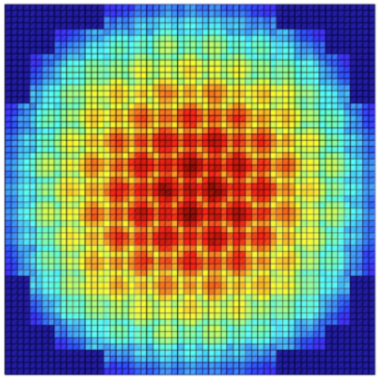
500 K neutrons / cycle
Fission matrix tallies for cycles 4-55



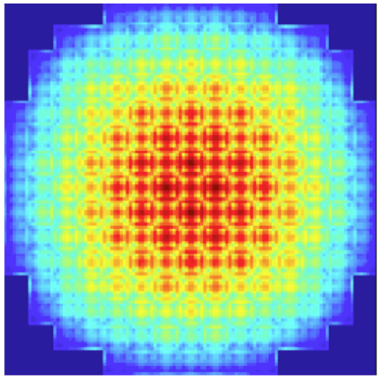
15 x 15 mesh



30 x 30 mesh



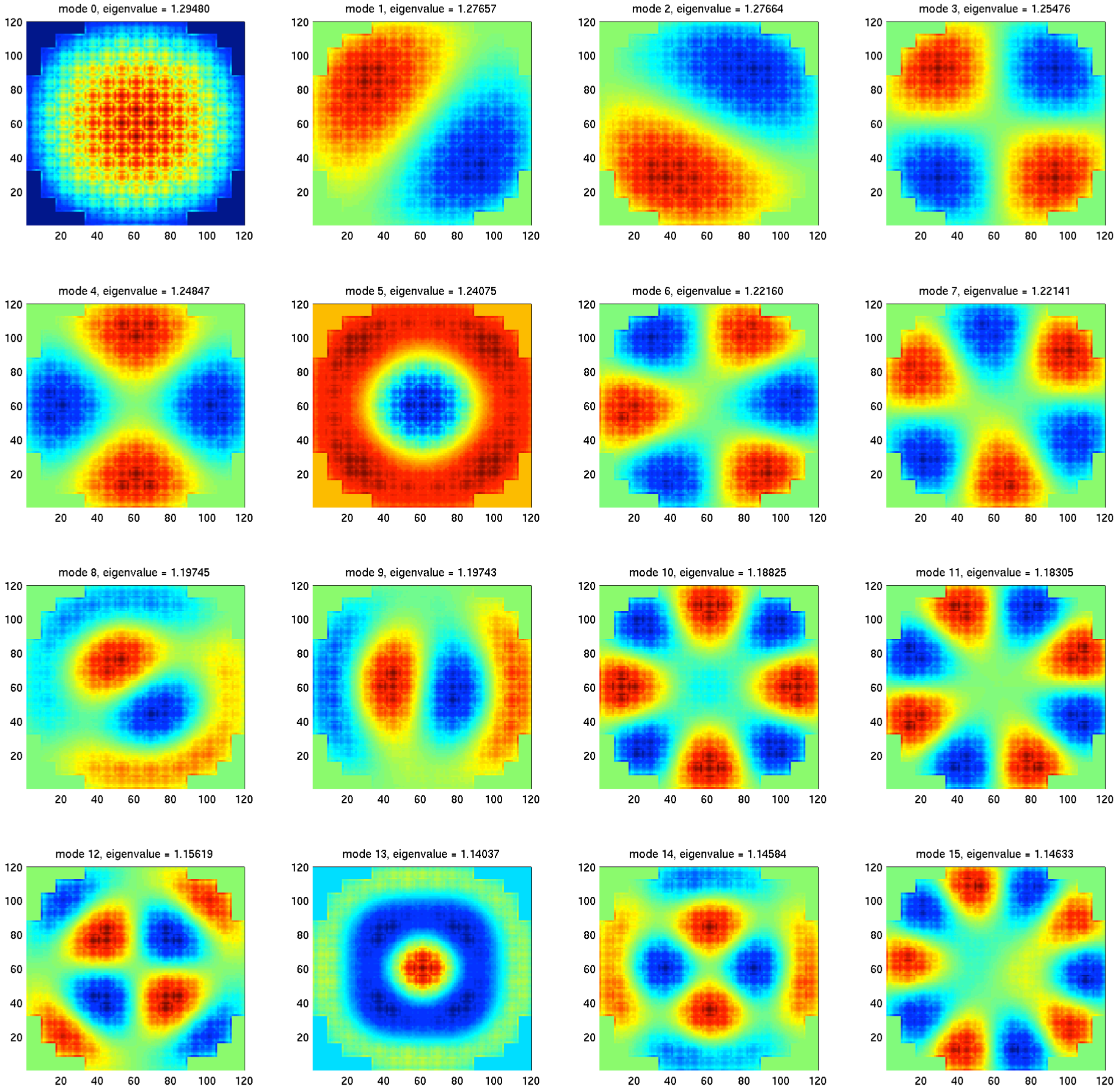
60 x 60 mesh



120 x 120 mesh

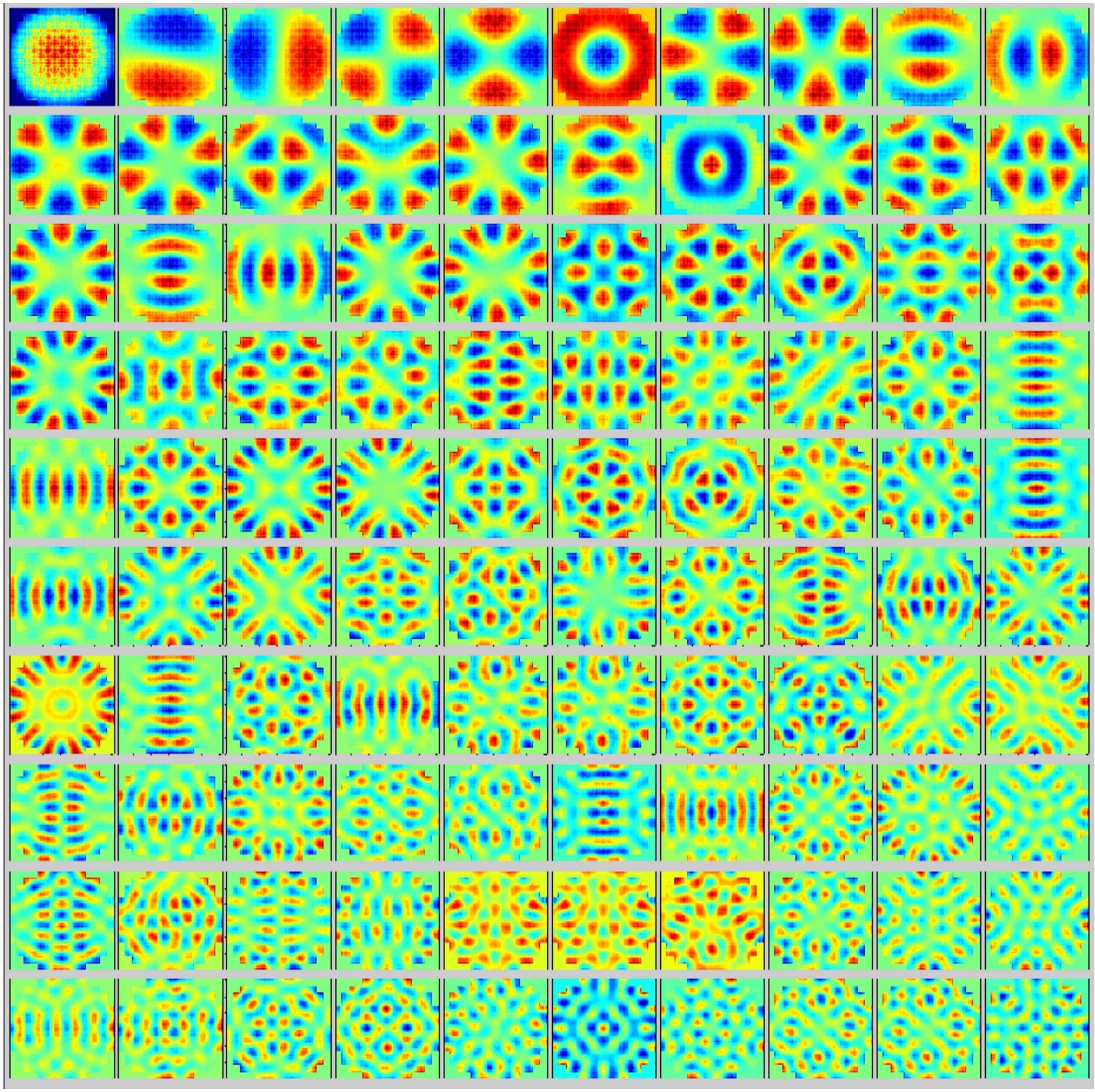
- Fission matrix computed during MCNP k-effective inactive cycles
- Fundamental eigenmode of the fission matrix for a 2D whole-core PWR model, for various spatial meshes used to tally the fission matrix

PWR – Eigenmodes for 120x120x1 Spatial Mesh

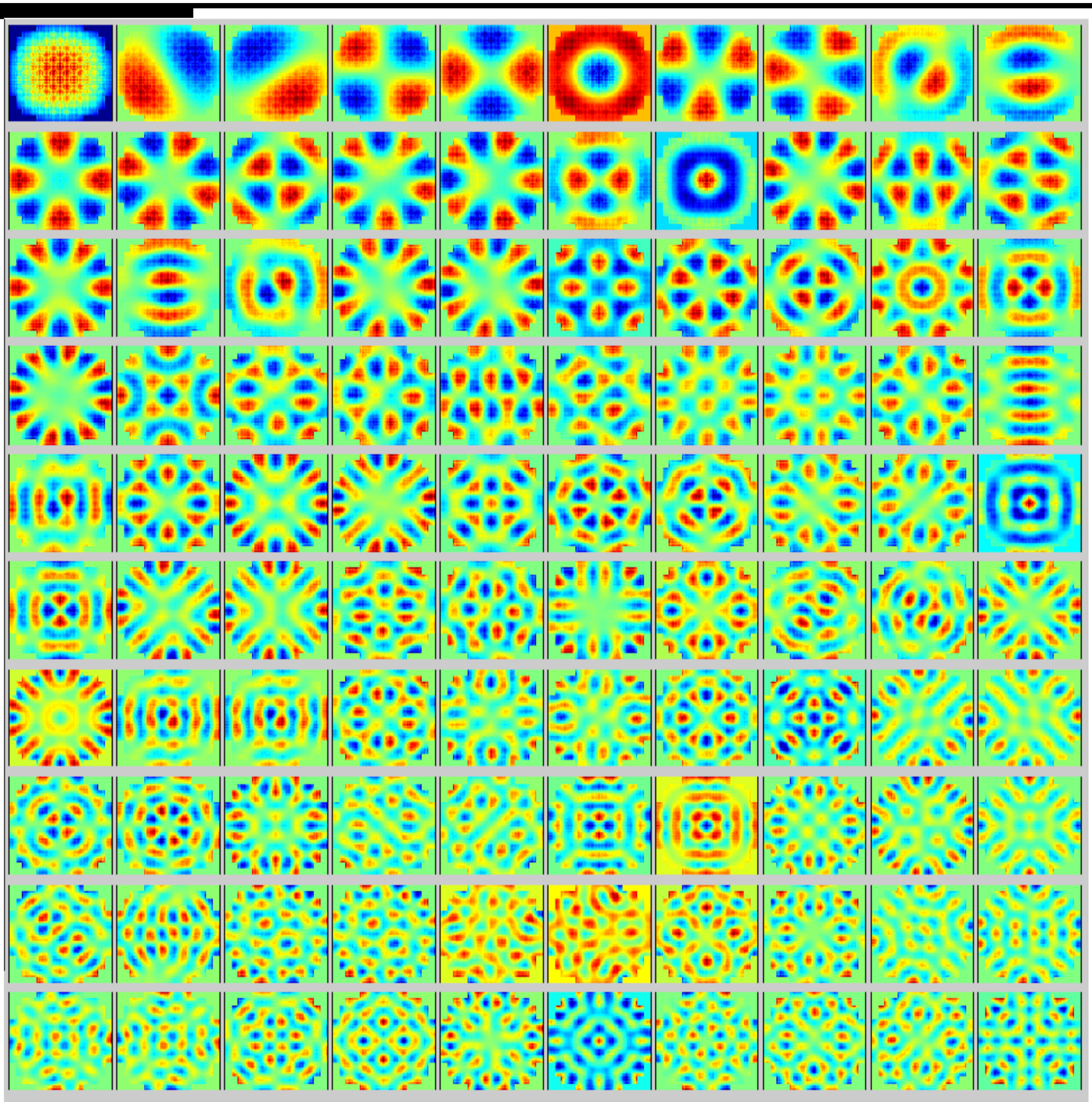


n	K_n
0	1.29480
1	1.27664
2	1.27657
3	1.25476
4	1.24847
5	1.24075
6	1.22160
7	1.22141
8	1.19745
9	1.19743
10	1.18825
11	1.18305
12	1.15619
13	1.14633
14	1.14617
15	1.14584

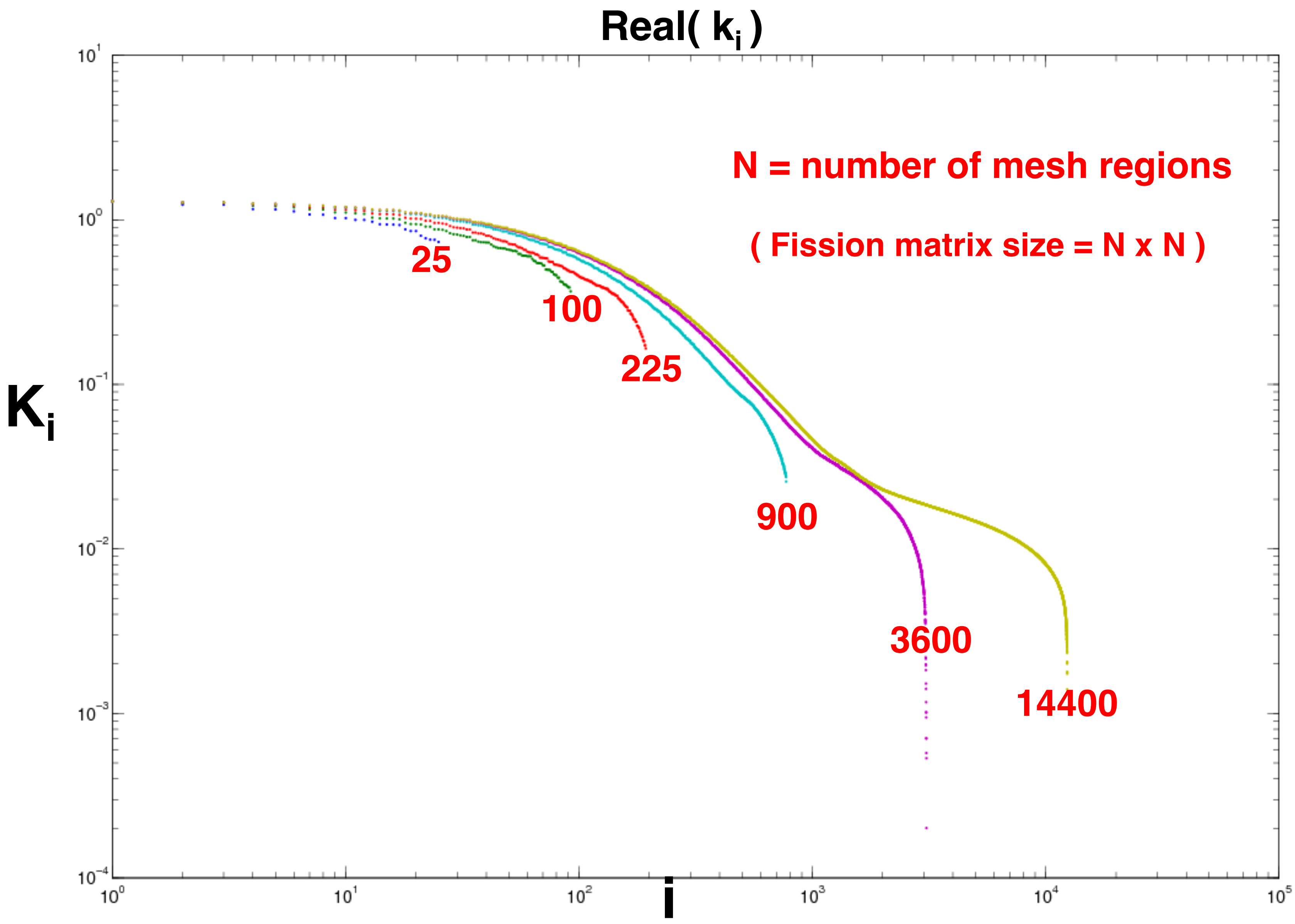
PWR – First 100 Eigenmodes



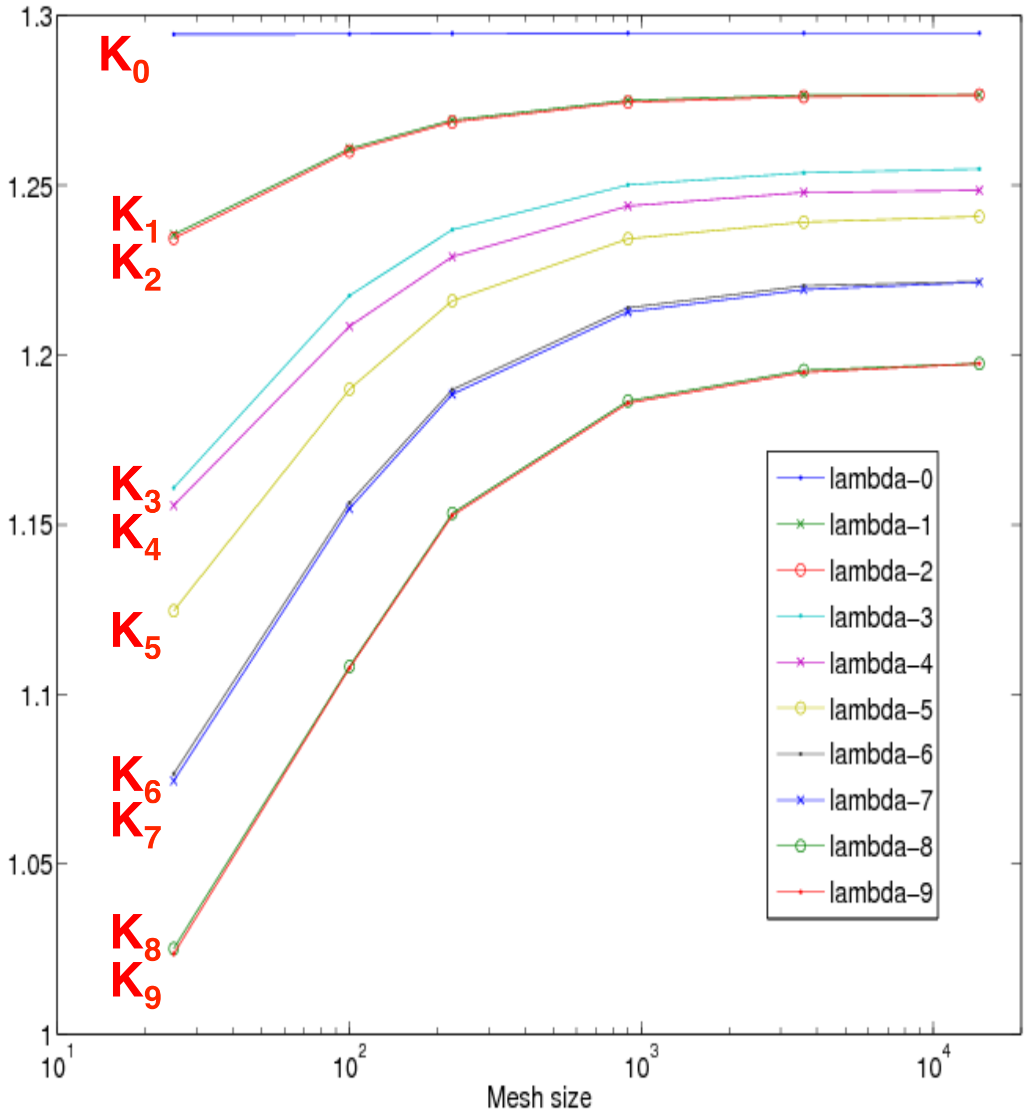
PWR – First 100 Eigenmodes, with More Neutrons



Eigenvalue Spectra with Varying Meshes



Spectrum Convergence from Mesh Refinement

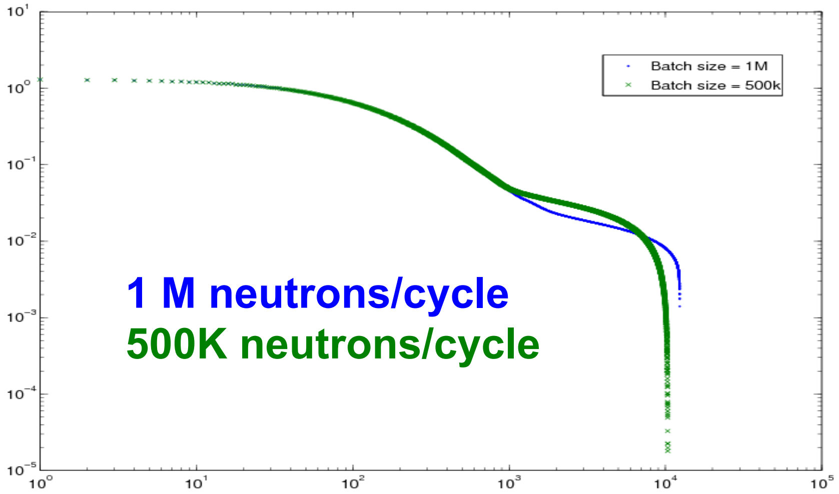


# Mesh Regions			K_0
5x5	=	25	1.29444
10x10	=	100	1.29453
15x15	=	225	1.29469
30x30	=	900	1.29477
60x60	=	3600	1.29479
120x120	=	14400	1.29480

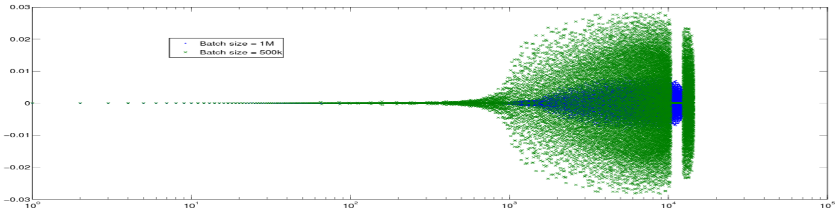
For fine-enough spatial mesh, eigenvalue spectrum converges

Are the Eigenvalues Real or Complex ?

Real(k_i):



Imag(k_i):



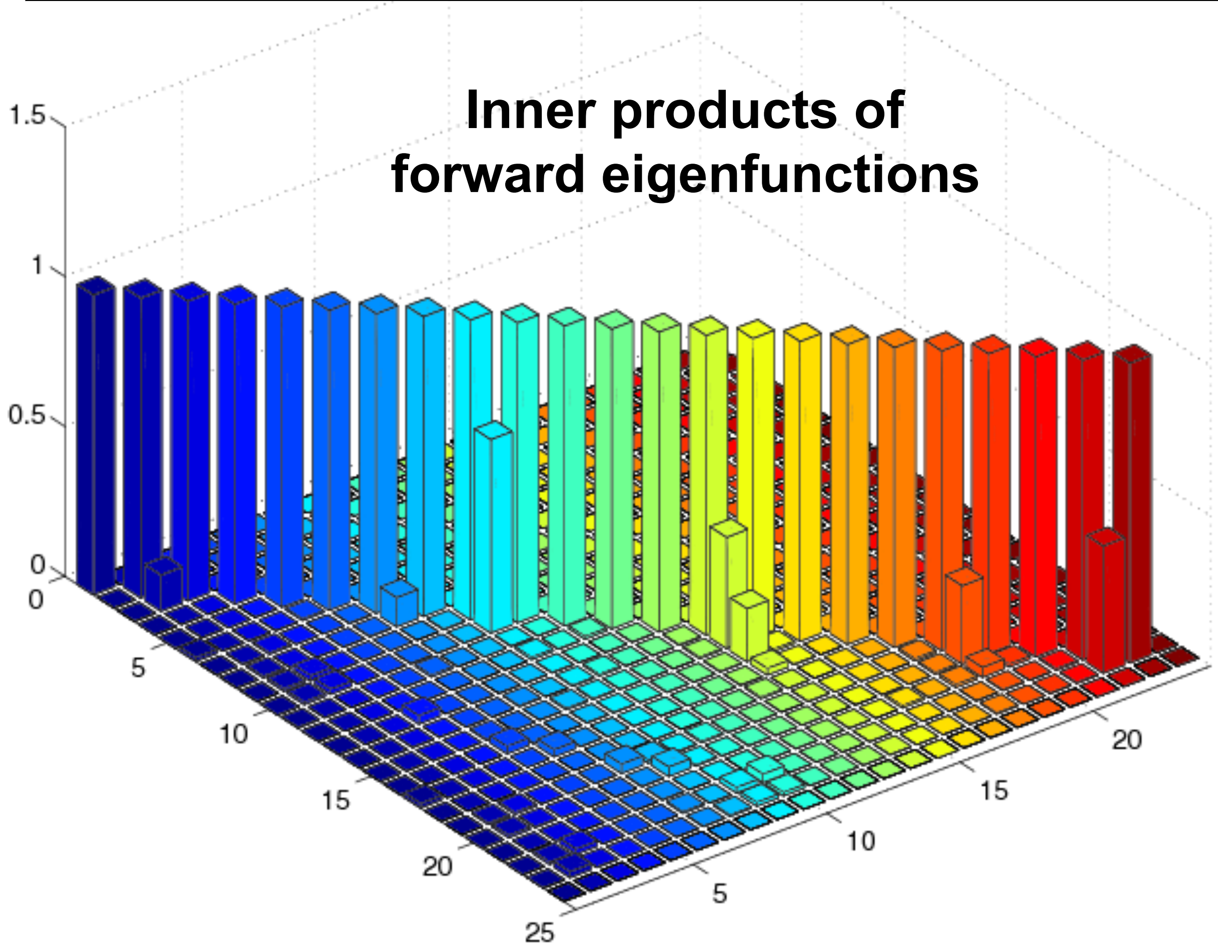
The appearance of complex eigenvalues appears to be strictly an artifact of Monte Carlo statistical noise

When more neutrons/cycle are used to decrease statistical noise, complex components diminish or vanish

The first few 100s or 1000s of discrete eigenvalues are real, and presumably all would be with sufficiently large neutrons/cycle

120 by 120 Spectrum, Varying Neutrons/cycle

PWR – Inner Products of Forward Eigenmodes



$$\int d\vec{r}\,\psi_n(\vec{r})\psi_m(\vec{r})$$
$$= \delta_{nm}\ \ if\ \ fission\,kernel$$
$$is\ self\ adjoint/symmetric$$

Strictly, eigenfunctions of the transport equation are bi-orthogonal.
As shown above, forward eigenfunctions are very nearly orthogonal.

Kord Smith Challenge Problem

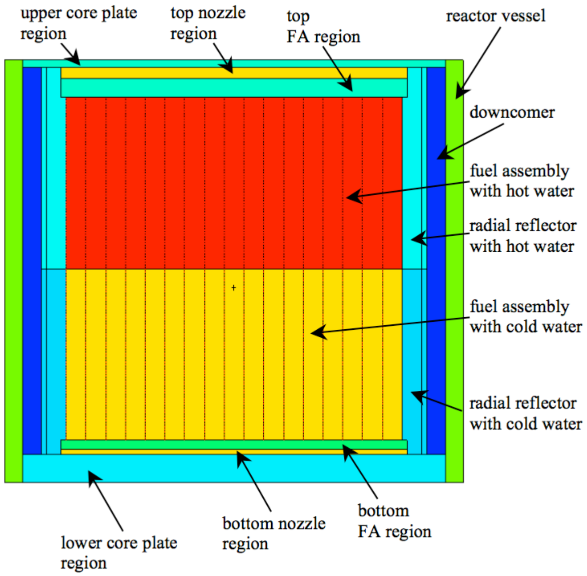
-

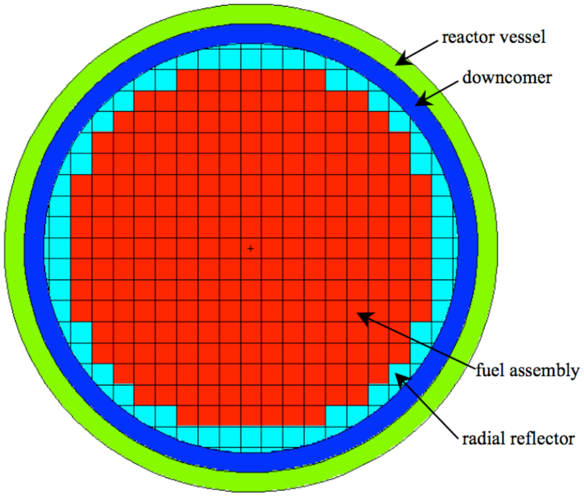
3D Whole-Core PWR

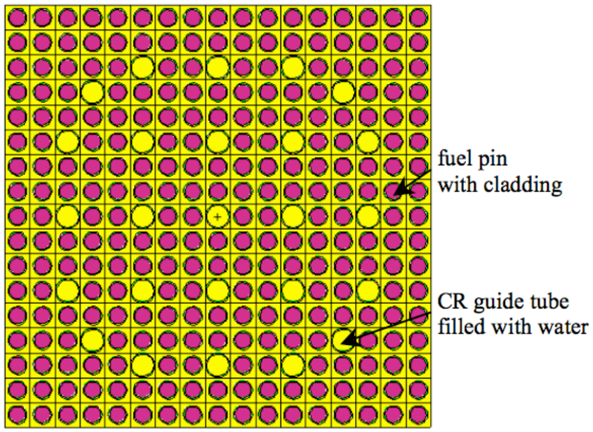
MCNP & the "Kord Smith Challenge"

Full core, 3D benchmark for assessing MC computer performance

- Specified by Hoogenboom & Martin for OECD/NEA (2010)
- LWR model: 241 assemblies, 264 fuel pins/assembly
- Fuel contains 17 actinides + 16 fission products; borated water
- Detailed 3D MCNP model
  - Mesh tallies for pin powers, (63,624 pins) x (100 axial) = 6.3M pin powers
  - Runs easily on deskside computer (Mac Pro, 2 quad-core, 8 GB

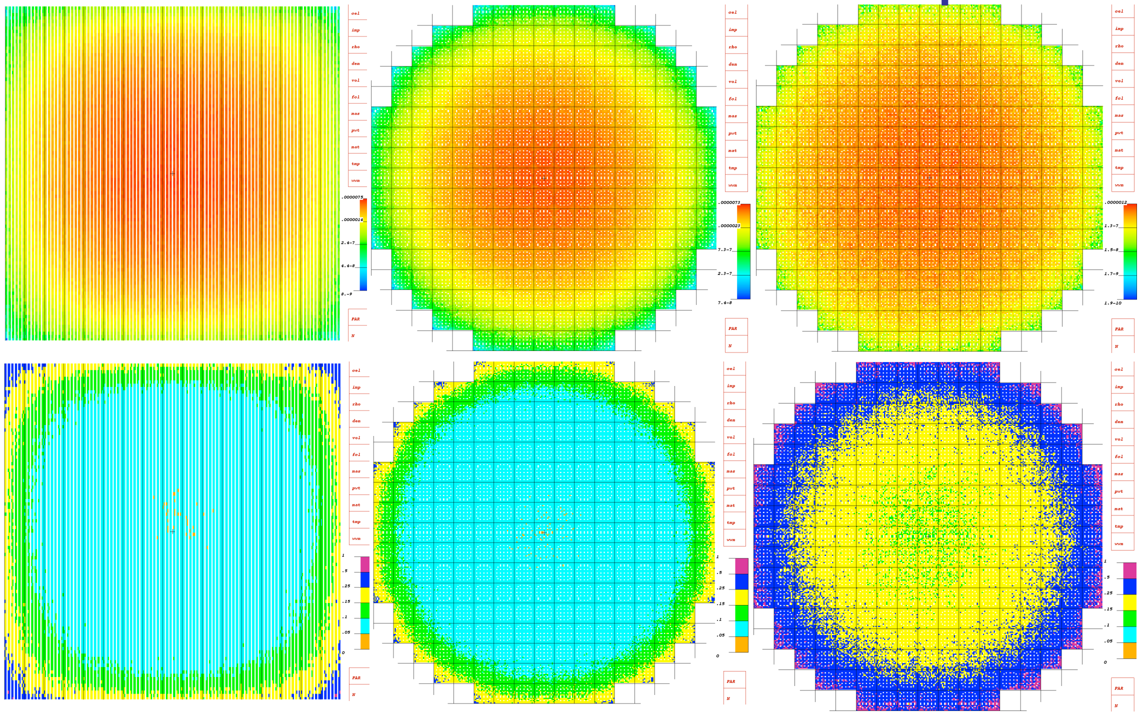






Standard MCNP & the "Kord Smith Challenge"

Pin Powers & Std.Dev

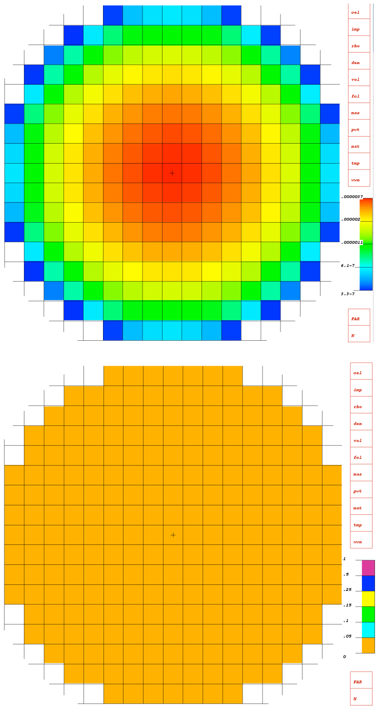


Axial

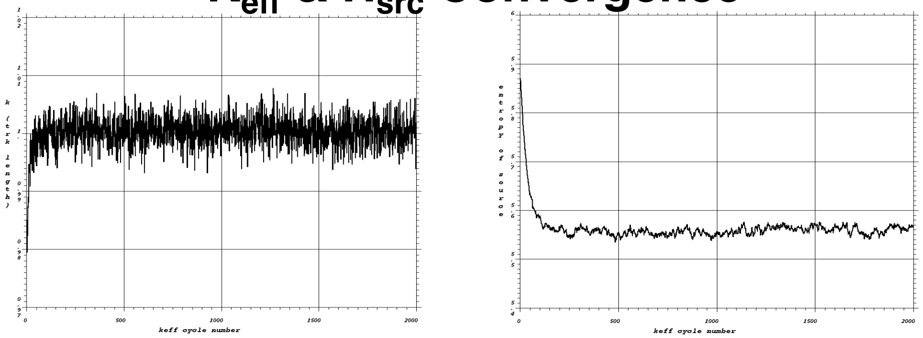
Mid

Top

Assembly Power & Std.Dev



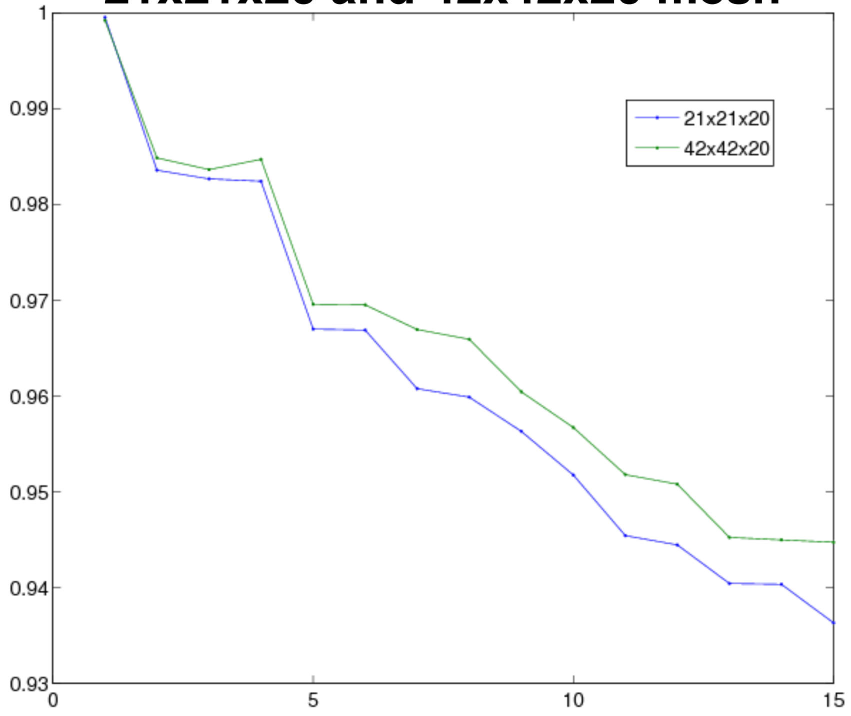
K_{eff} & H_{src} Convergence

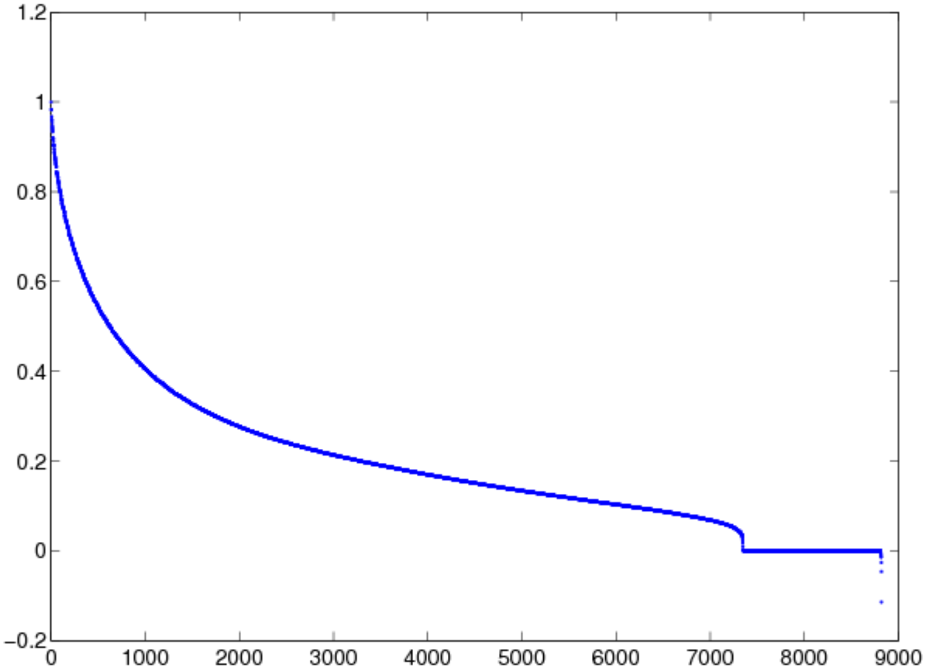


200M neutrons
Mac Pro, 8 cpu

Kord Smith Challenge Eigenvalue Spectrum

First 15 eigenvalues for 21x21x20 and 42x42x20 mesh



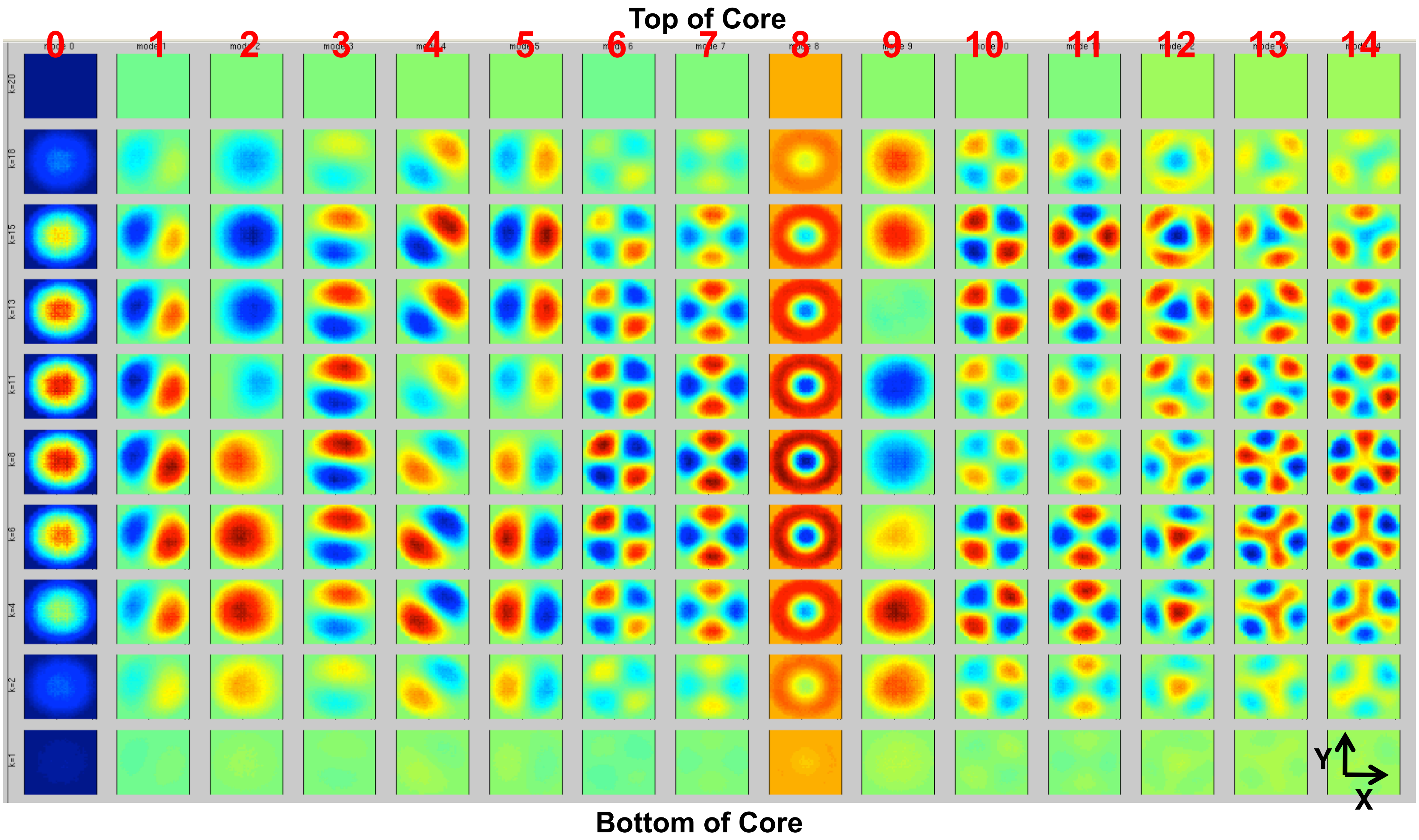


21x21x20 mesh,
Real(K) spectrum

Eigenfunctions from Fission Matrix

XY plots of eigenfunctions at various Z elevations

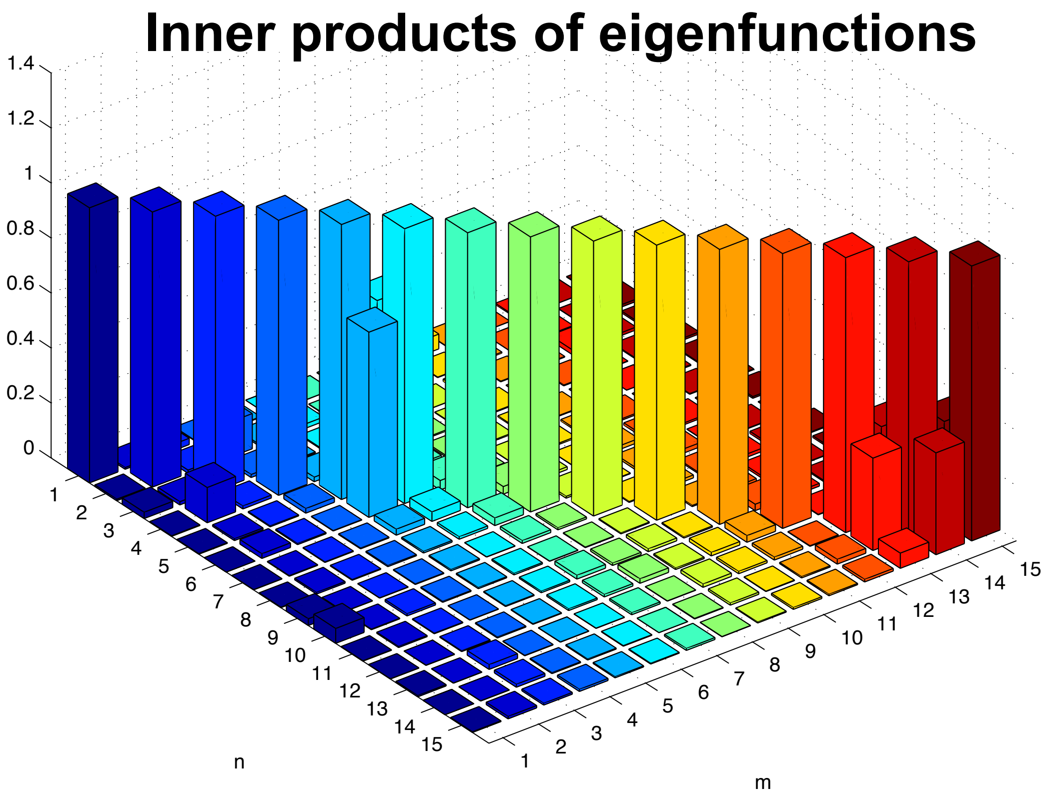
55 cycles, 1 M neutrons/cycle, 42x42x20 mesh, 35280x4913 fission matrix



Eigenvalues & Inner Products of Eigenfunctions

n	K_n
0	0.99919
1	0.98483
2	0.98362
3	0.98469
4	0.96956
5	0.96950
6	0.96693
7	0.96591
8	0.96043
9	0.95671
10	0.95178
11	0.95078
12	0.94524
13	0.94497
14	0.94472

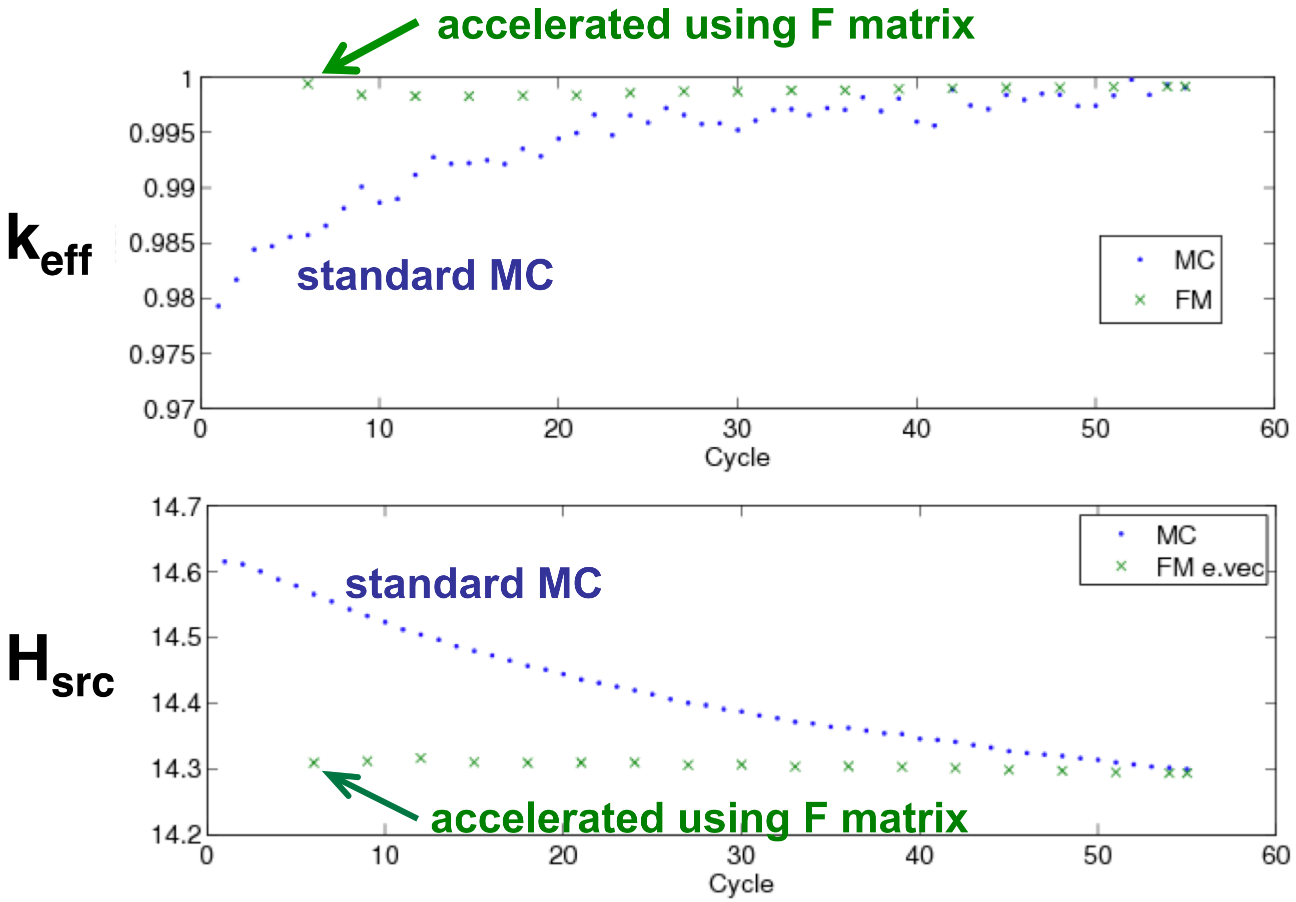
42 x 42 x 20 spatial mesh, 35280 x 4913 fission matrix
55 cycles, 1 M neutrons/cycle
fission matrix tallies for cycles 4-55



Convergence Acceleration Using Fission Matrix

- Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles

- Very impressive convergence improvement



accelerated using F matrix

standard MC

standard MC

accelerated using F matrix

Advanced Test Reactor

Idaho National Laboratory

Advanced Test Reactor

“Serpentine Arrangement of Highly Enrichment Water-Moderated Uranium-Aluminide Fuel Plates Reflected by Beryllium”

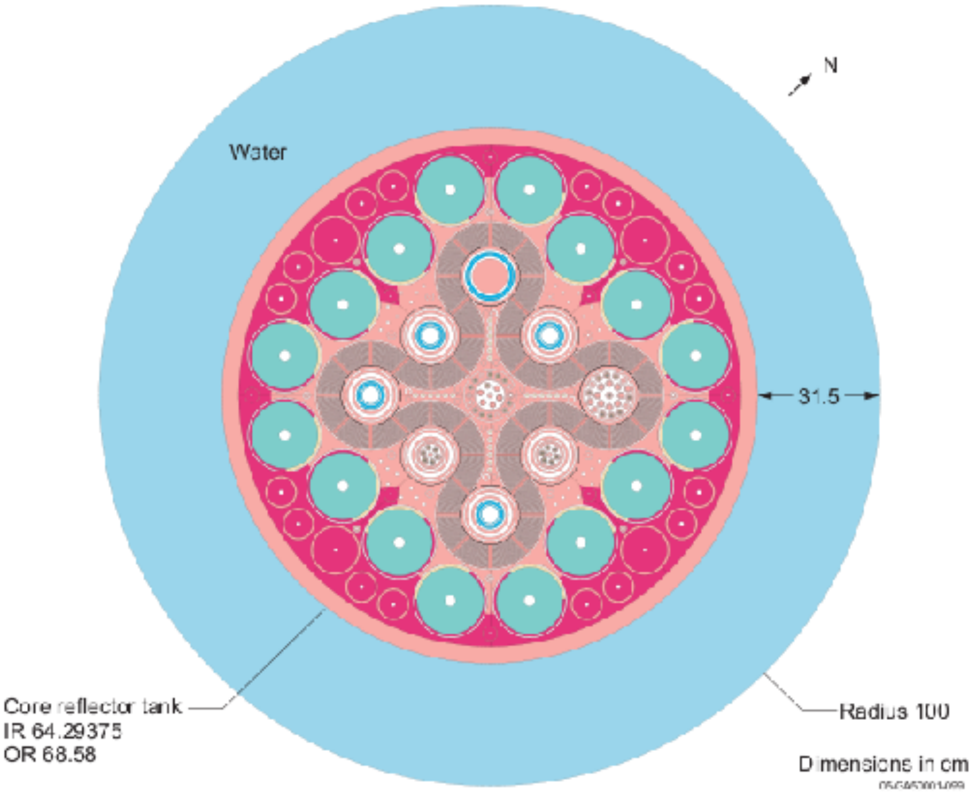
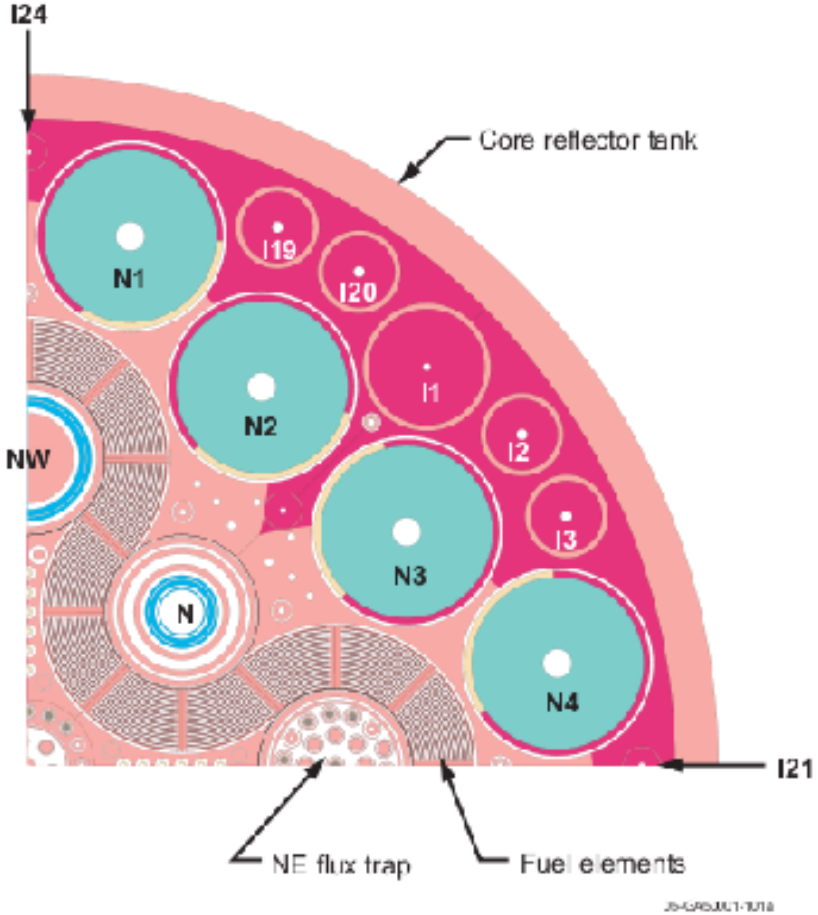


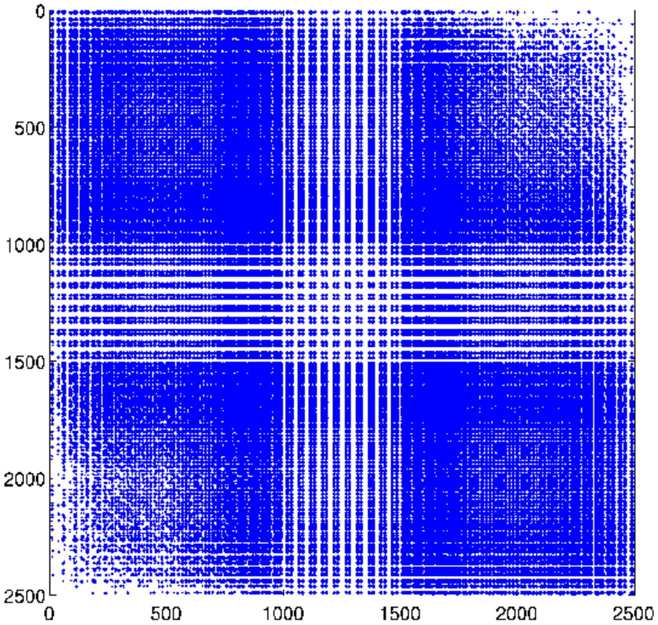
Figure 20. An XY View at x=0,y=0 of the Benchmark Model.



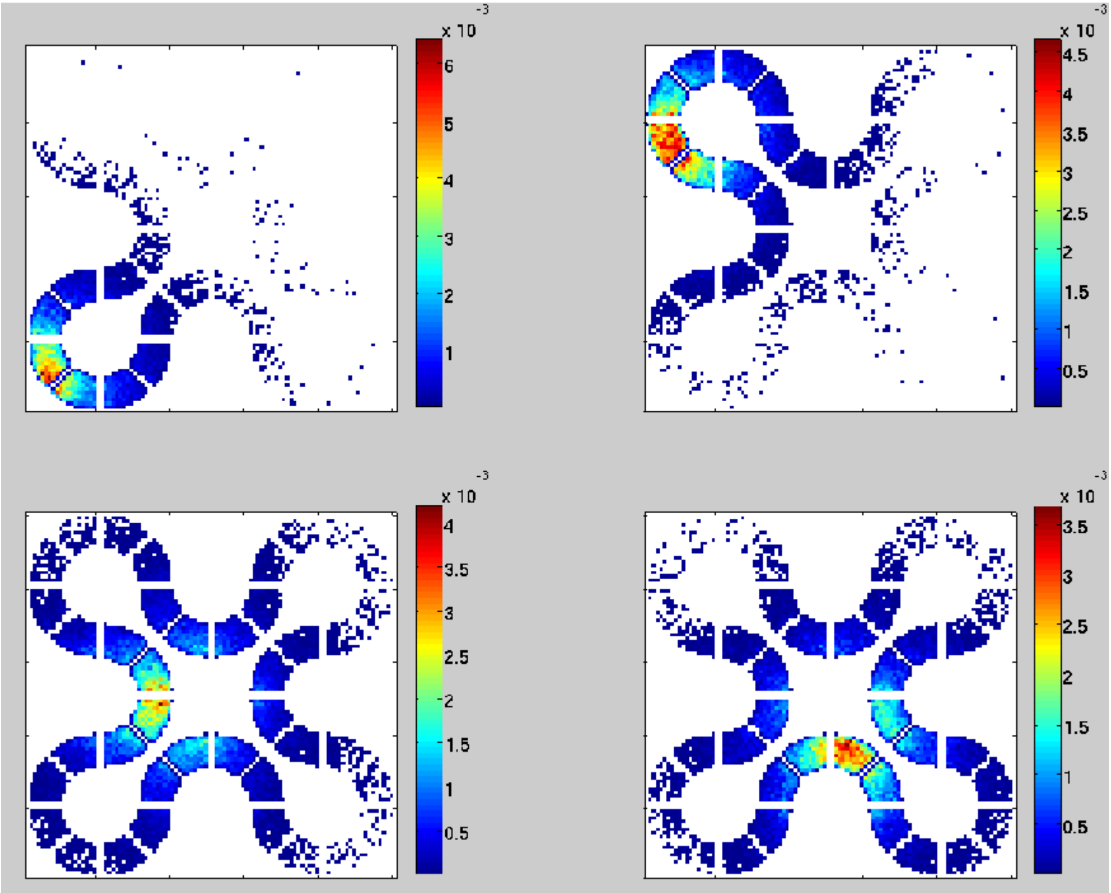
S. S. Kim, B. G. Schnitztler, et. al., “Serpentine Arrangement of Highly Enrichment Water-Moderated Uranium-Aluminide Fuel Plates Reflected by Beryllium”, HEU-MET-THERM-022, Idaho National Laboratory (September 2005).

ATR - Fission Matrix Structure

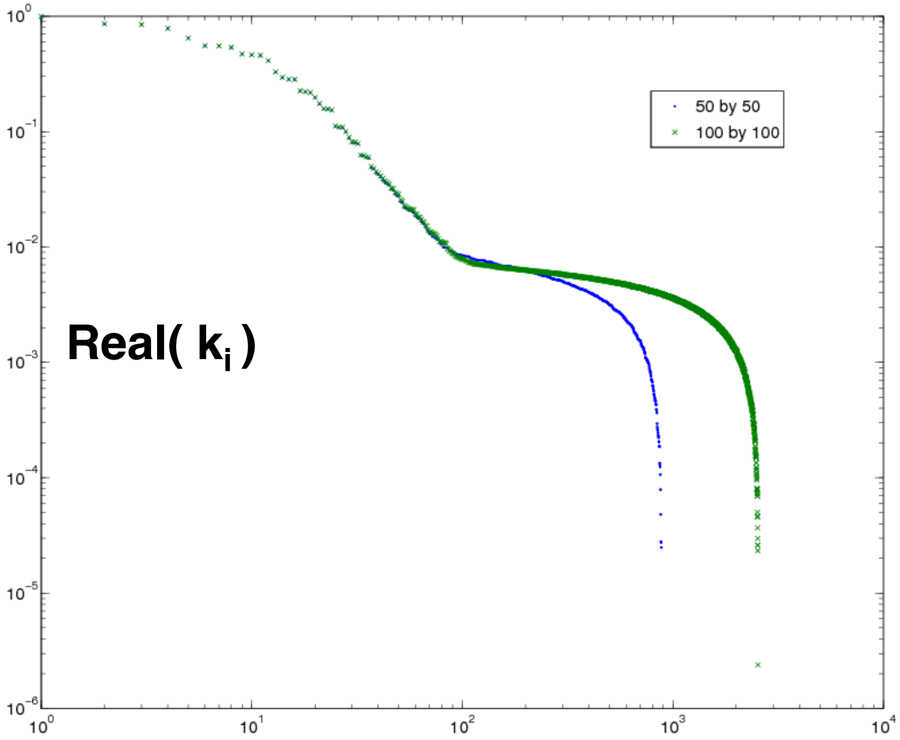
Matrix structure
(50x50 spatial mesh)

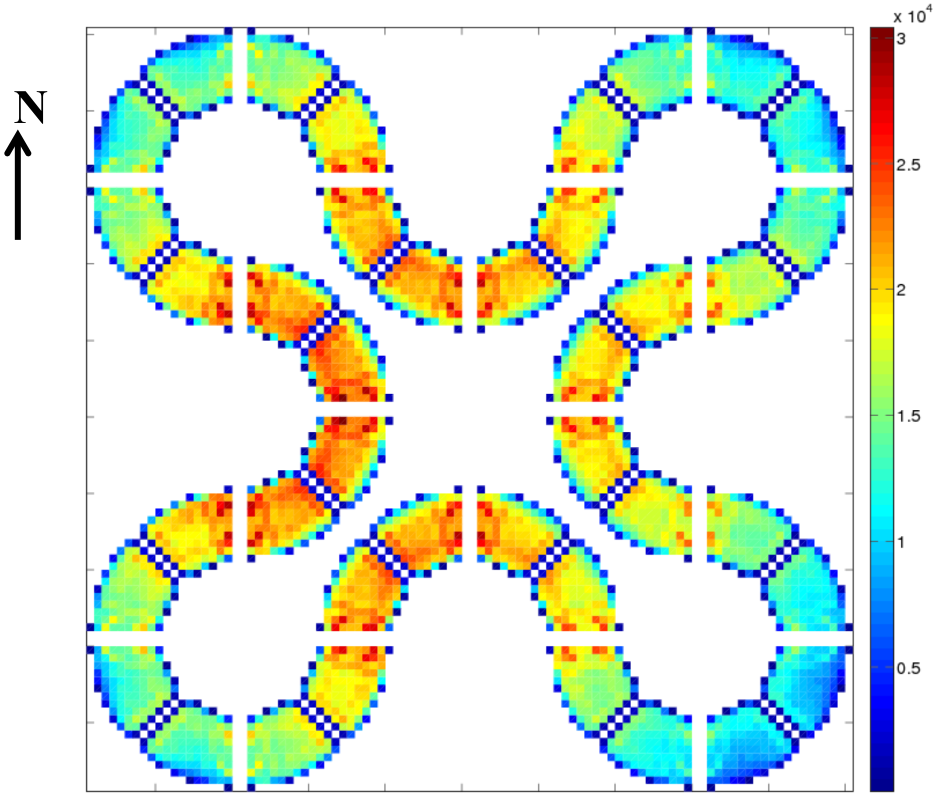


Four matrix columns (100x100 spatial mesh)



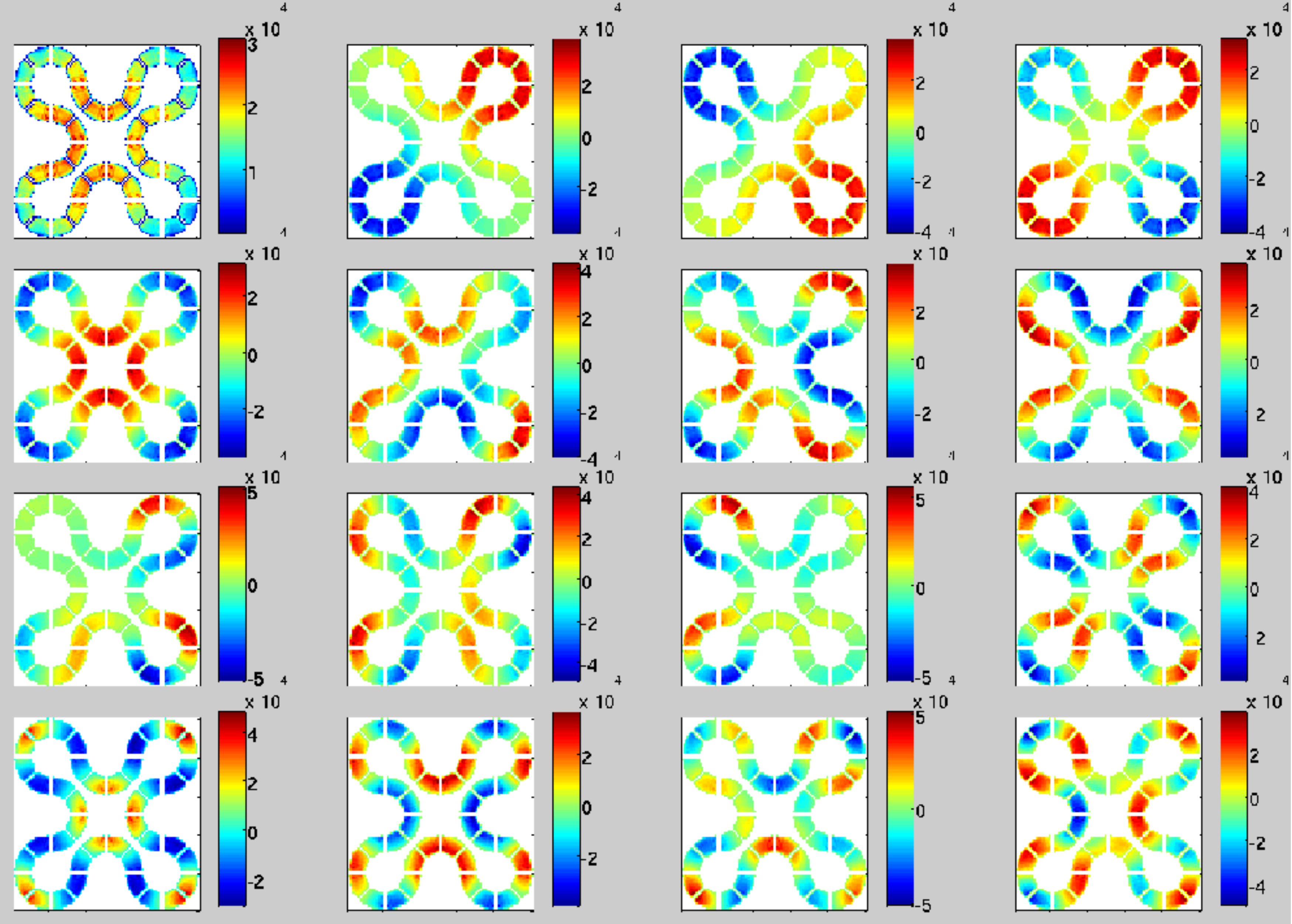
ATR - Fundamental Eigenvector, Eigenvalues





Fundamental mode,
100x100 spatial mesh

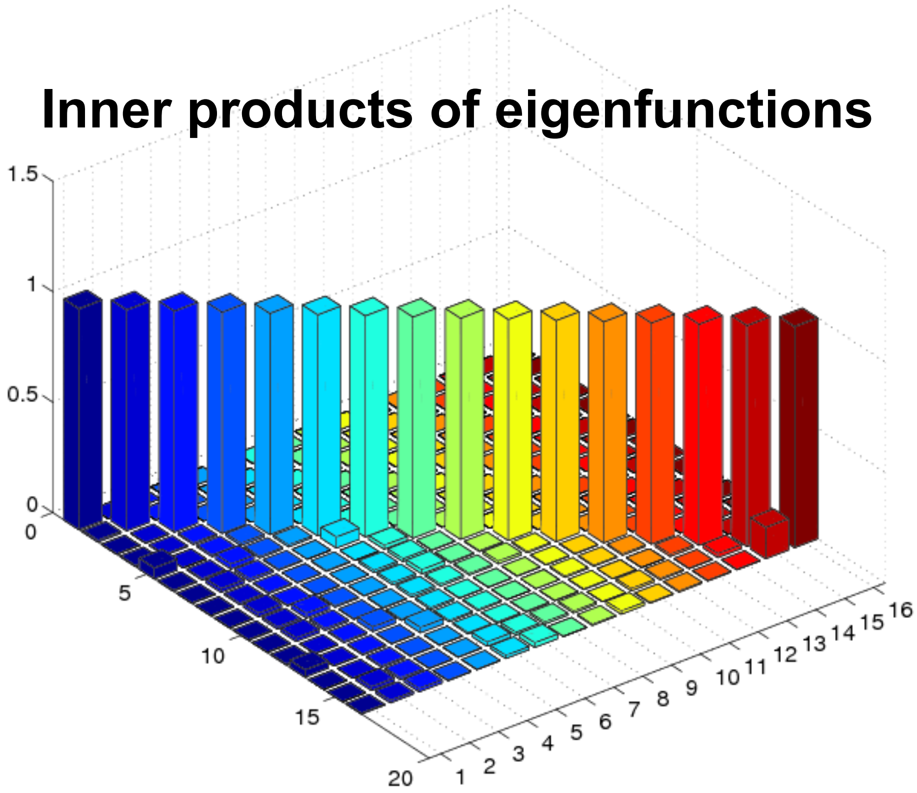
ATR - Eigenmodes (100x100 spatial mesh)



ATR - Fission Matrix Orthogonality

n	K_n
0	0.99490
1	0.85630
2	0.84612
3	0.78265
4	0.64564
5	0.55461
6	0.55207
7	0.53659
8	0.47004
9	0.46173
10	0.45794
11	0.41144
12	0.32865
13	0.29454
14	0.28401
15	0.28327

100 x 100 x 1 spatial mesh, no sparsification
55 cycles, 1 M neutrons/cycle
fission matrix tallies for cycles 4-55


Inner products of eigenfunctions

MCNP Fission Matrix

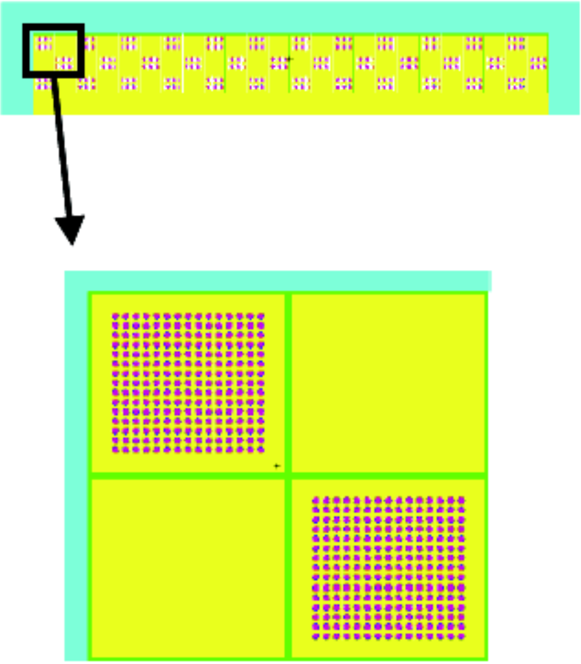
Spent Fuel Storage Vault

(idealized benchmark)

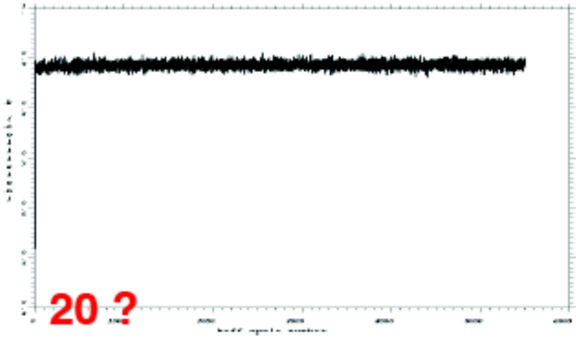
Loosely-Coupled Problem

Fuel Vault Problem

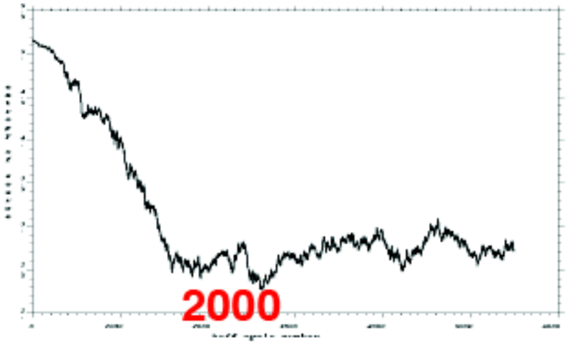
Fuel Storage Vault



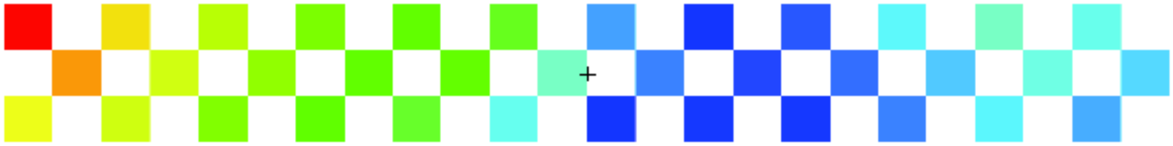
K vs cycle



H_{src} vs cycle



Assembly Heating Distribution

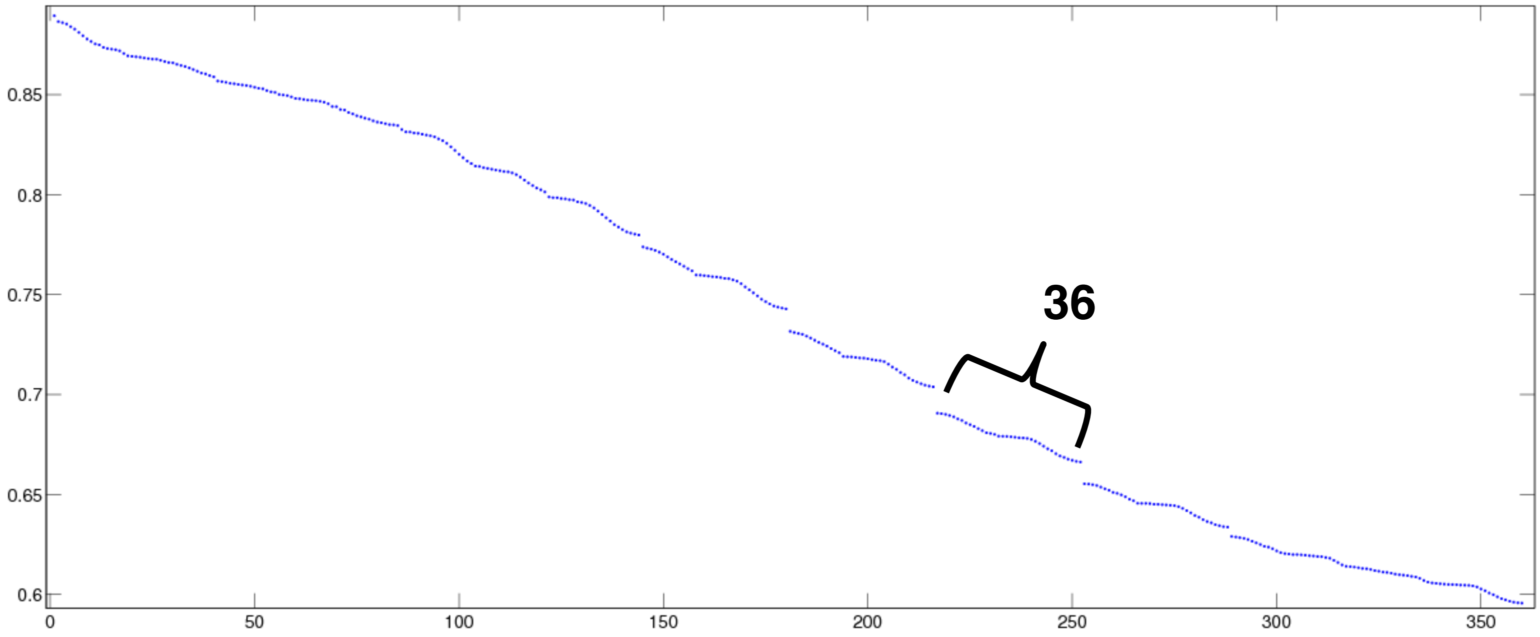


For this calculation,

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

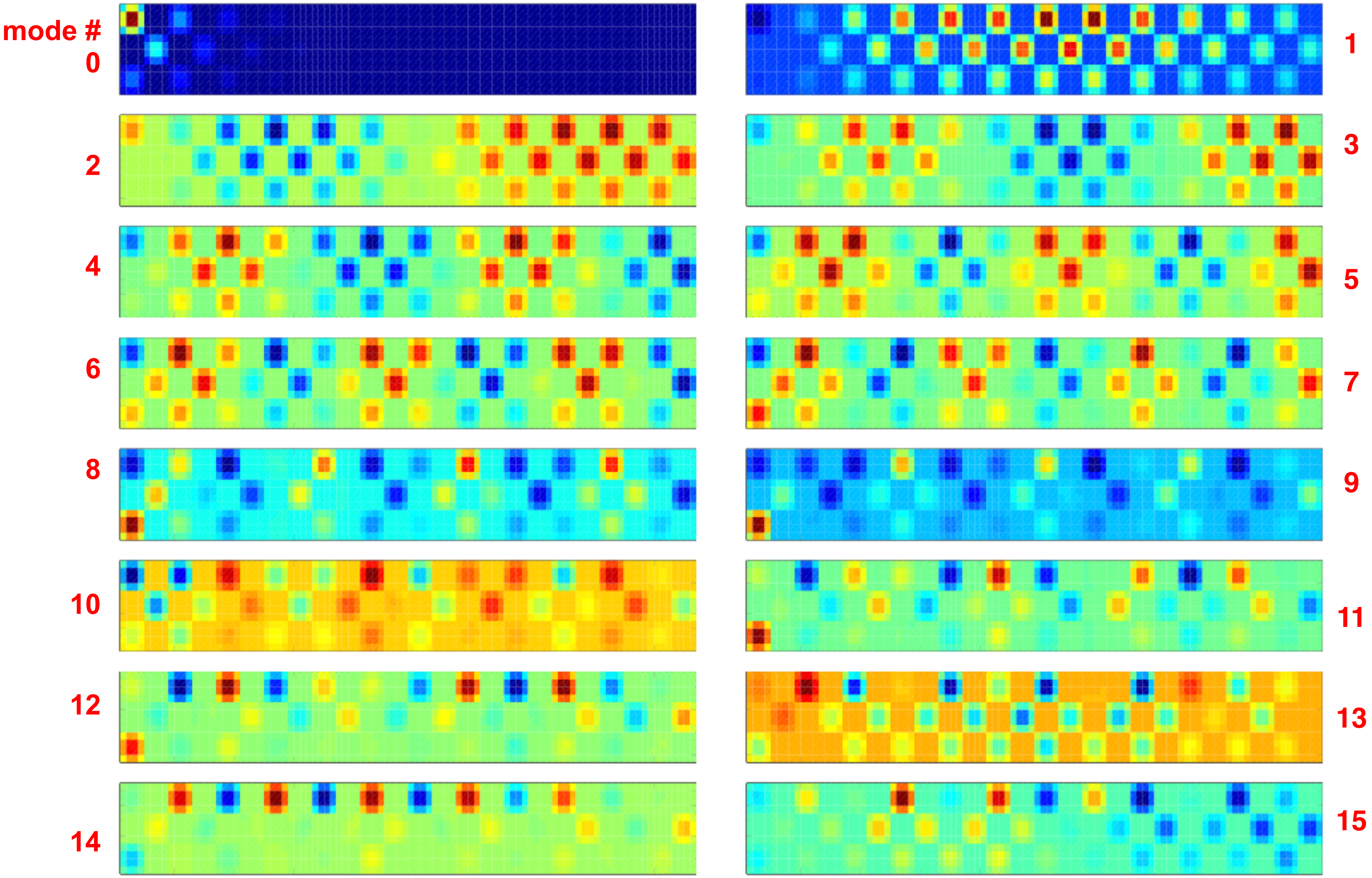
Eigenvalue Spectrum for Fuel Vault Problem- First 360

Real(k_i), i = 1,2,..360



36 semi-coupled assemblies → Mini-groups of 36 in size

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

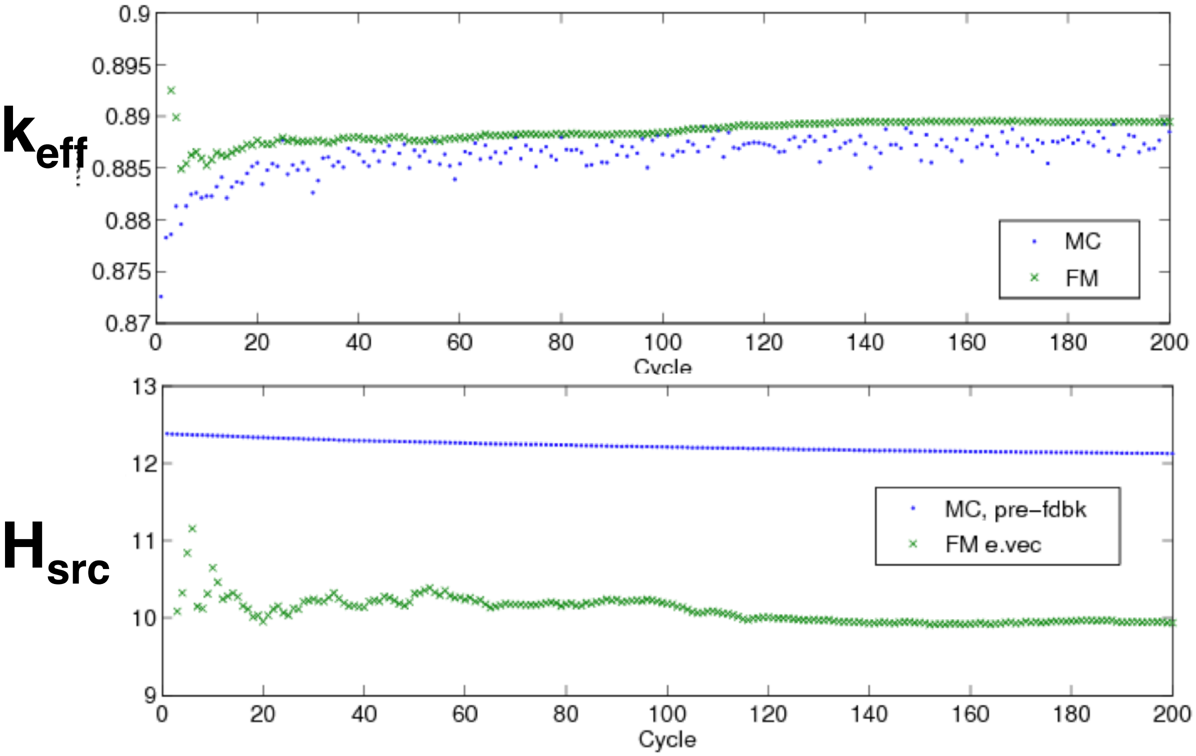


XY planes mid-height. Axial shape is cosine, #10,13,15 have change in sign in z

Fuel Vault Problem - Convergence Acceleration

It takes ~2,000 cycles for standard MC to converge for this problem,

Using the fission matrix for source convergence acceleration, only ~20 cycles are needed



standard MC

accelerated using F matrix

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

Conclusions

- Fission matrix capability has been added to MCNP (R&D for now)
- Tested on variety of real problems (3D, continuous-energy)
- Can obtain fundamental & higher eigenmodes
  - Empirical evidence for: existence of higher modes,
    real, discrete eigenvalues,
    very nearly orthogonal eigenmodes
    (for reactor-like problems)
  - Higher eigenmodes are important for
    BWR void stability,
    Xenon oscillations,
    control rod worth,
    accident behavior,
    higher-order perturbation theory,
    quasi-static transient analysis,
    correlation effects on statistics,
    etc., etc., etc.
- Can provide very effective acceleration of source convergence

LA-UR-12-22277

On-The-Fly Neutron Doppler Broadening for MCNP

Forrest Brown[1], William Martin[2], Gokhan Yesilyurt[3], Scott Wilderman[2]

[1]Monte Carlo Methods (XCP-3), LANL
[2]University of Michigan
[3]Argonne National Laboratory

Abstract

On-The-Fly Neutron Doppler Broadening for MCNP

Forrest Brown, William Martin, Gokhan Yesilyurt, Scott Wilderman

The University of Michigan, ANL, and LANL have been collaborating on a US-DOE-NE University Programs project "Implementation of On-the-Fly Doppler Broadening in MCNP5 for Multiphysics Simulation of Nuclear Reactors." This talk describes the project and provides results from the initial implementation of On-The-Fly Doppler broadening (OTF) in MCNP and testing.

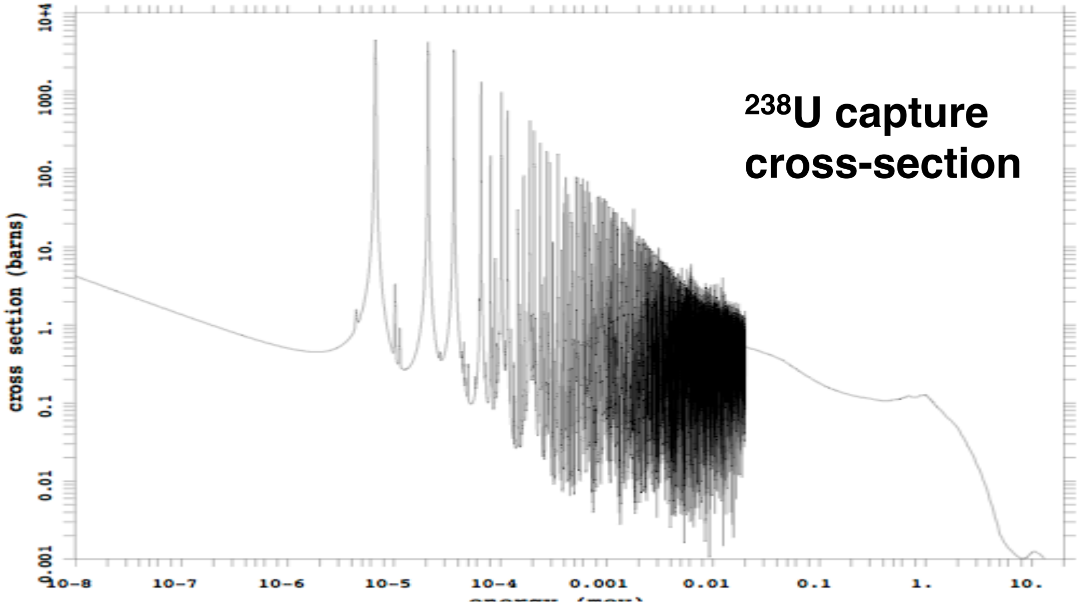
The OTF methodology involves high precision fitting of Doppler broadened cross-sections over a wide temperature range (the target for reactor calculations is 250-3200K). The temperature dependent fits are then used within MCNP during the neutron transport, for OTF broadening based on cell temperatures. It is straightforward to extend this capability to cover any temperature range of interest, allowing the Monte Carlo simulation to account for a continuous distribution of temperature ranges throughout the problem geometry.

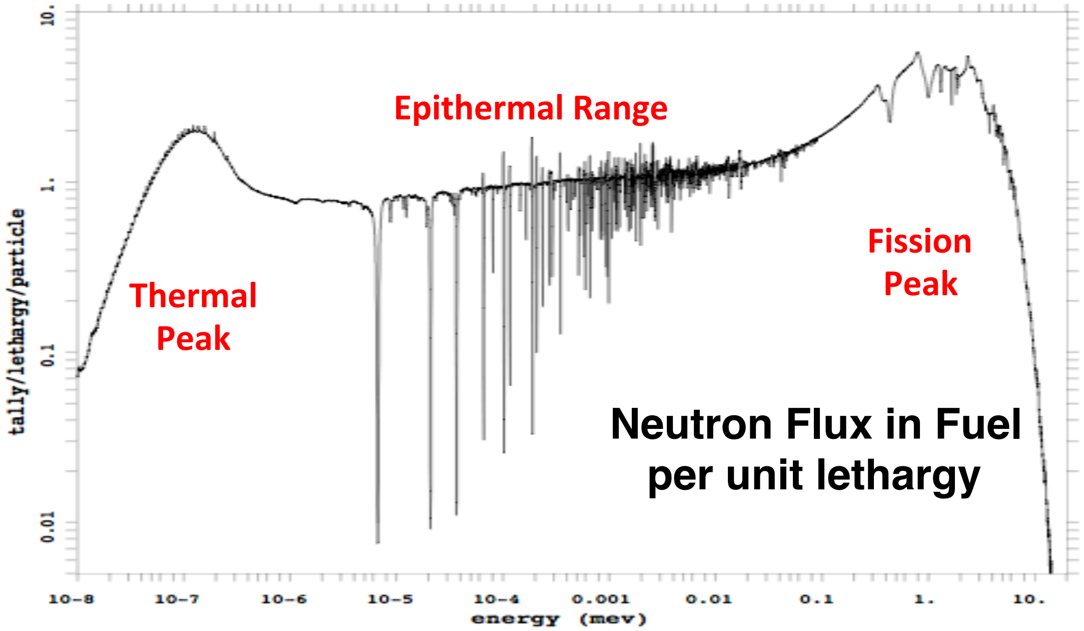
On-The-Fly Neutron Doppler Broadening for MCNP

- **Introduction**
  - Doppler Broadening - Obvious Stuff
  - Methods for Handling Temperature Variations

- **OTF Doppler Broadening in MCNP**
  - OTF Methodology
  - Union Energy Mesh
  - Temperature Fitting
  - OTF Doppler in MCNP
  - Testing
  - Work-in-Progress

Introduction – Doppler Broadening





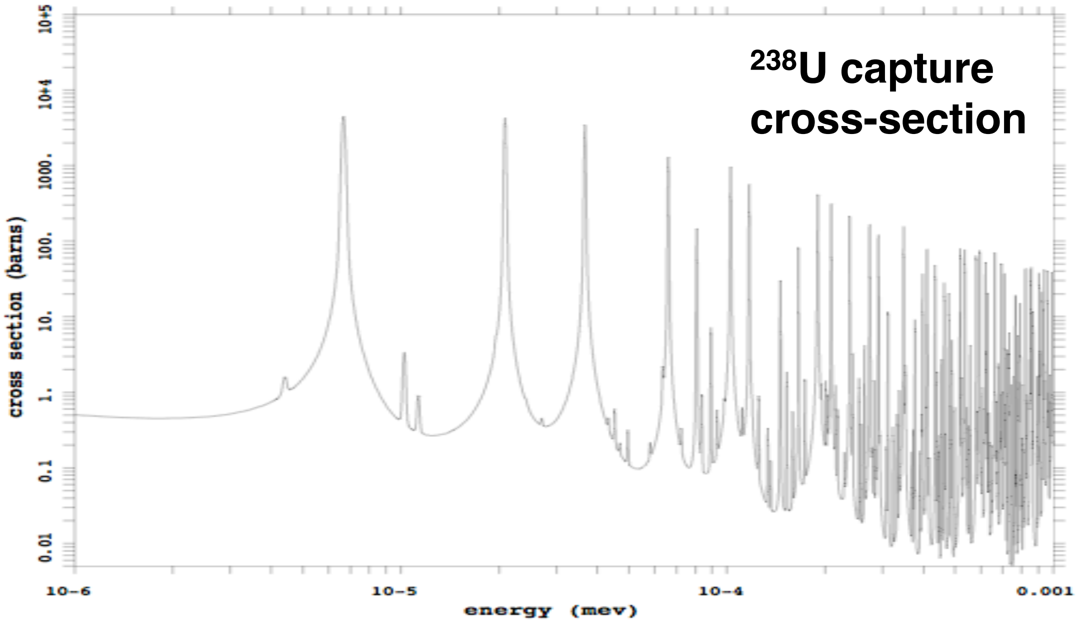
UO_2 Fuel Pin

3.1% Enriched
293.6 °K

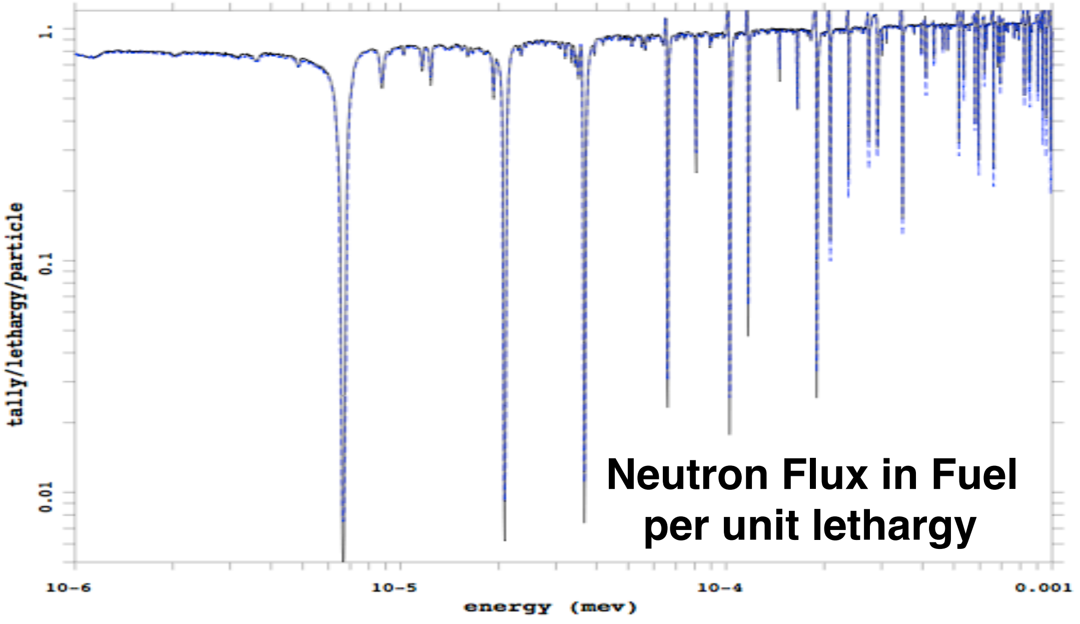
.01 eV – 20 MeV

- Neutrons born in MeV range from fission
- Most fissions caused by thermal neutrons
- 1/3 of neutron losses are due to ^{238}U capture in epithermal energy range during slowing down

Introduction – Doppler Broadening



^{238}U capture cross-section



Neutron Flux in Fuel per unit lethargy

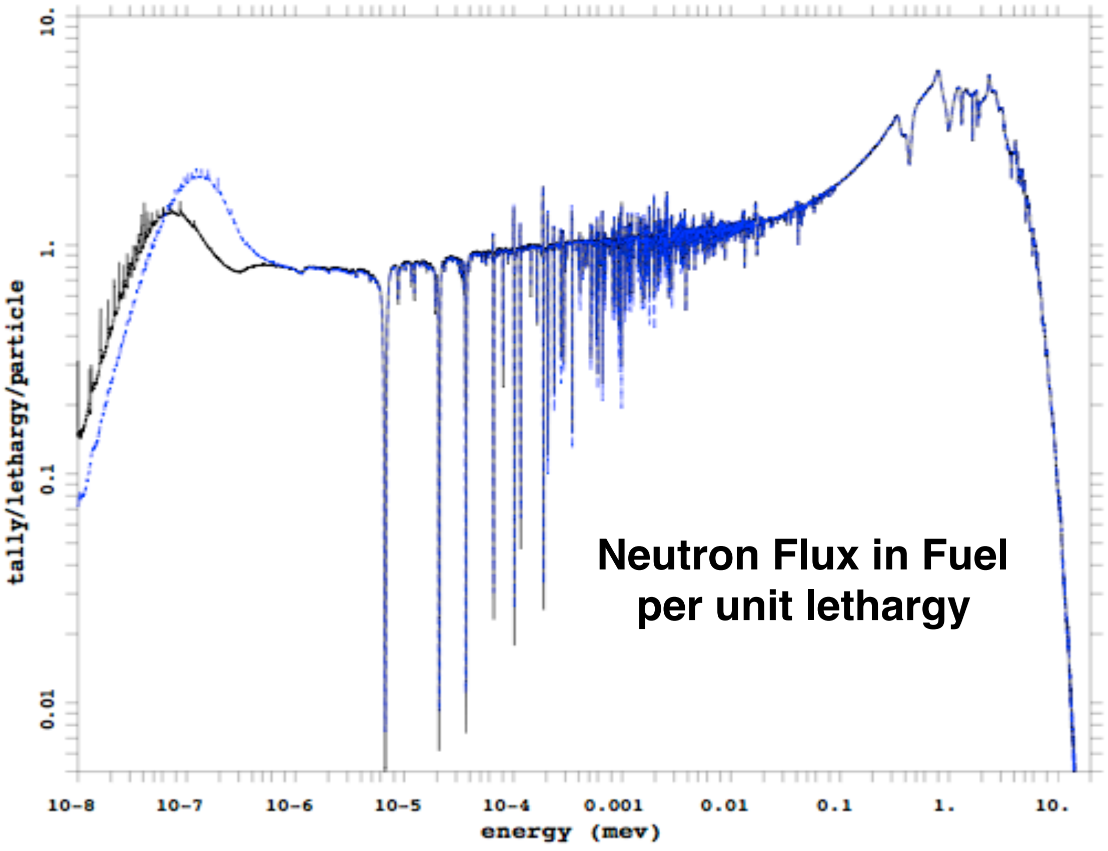
UO_2 Fuel Pin

3.1% Enriched
293.6 °K

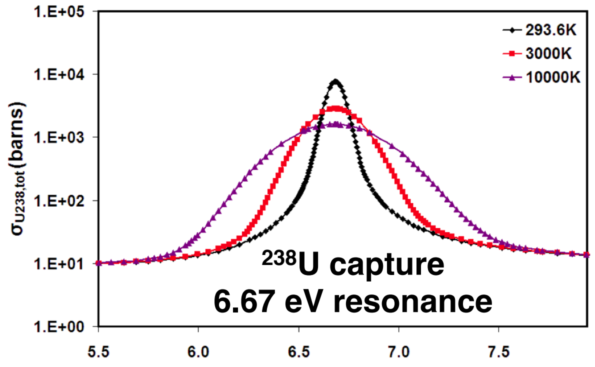
Detail for
1 eV – 1 KeV

1/3 of neutron losses are due to ^{238}U capture at epithermal energies during slowing down

Introduction – Doppler Broadening



Neutron Flux in Fuel per unit lethargy



^{238}U capture
6.67 eV resonance

UO_2 Fuel Pin

3.1% Enriched
293.6 °K vs 900 °K

.01 eV – 20 MeV

Keeping same densities, but changing cross-sections:

k_{inf} (cold) = 1.34498 (8)

k_{inf} (hot) = 1.31167 (8)

At higher temperatures, Doppler broadening of resonance cross-sections increases resonance capture

Introduction

Doppler Broadening

Temperature Variation in Monte Carlo Codes

Neutron - Nucleus Interactions

- **Low neutron energies:**
  - **S(α,β) interaction data is used in modeling collision physics**
    - 2002 data: 10^{-5} eV - **4.46 eV** neutron energies (15 nuclides)
    - 2012 data: 10^{-5} eV - **9.15 eV** neutron energies (20 nuclides)
  - **S(α,β) data accounts for target nucleus chemical binding, molecular binding, crystal structure, thermal motion, etc.**
  - **Nuclides without S(α,β) data: use free-gas model (see below)**

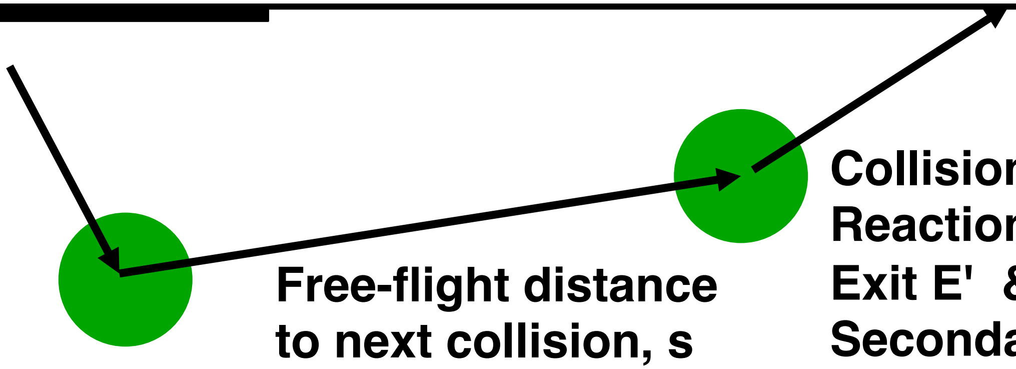
- **High neutron energies:**
  - **Target nucleus thermal motion neglected**
  - **Typical: $E_{neutron}$ > 400 kT for A>1**

- **Epithermal neutron energies:**
  - **Target nucleus thermal motion important**
  - **Free-gas scattering model -- nuclides have Maxwell-Boltzmann energy distribution at temperature T, isotropic direction**

$$f(E_{nuc}) = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{kT} \cdot \left(\frac{E_{nuc}}{kT} \right)^{1/2} e^{-E_{nuc}/kT}$$

Gamma(kT, 3/2),
mean = 1.5 kT
mode = .5 kT

Doppler Broadening



Free-flight distance to next collision, s

Collision isotope,
Reaction type,
Exit E' & (u',v',w'),
Secondary particles

- **Detailed kinematics of collisions must include nucleus E & Ω**

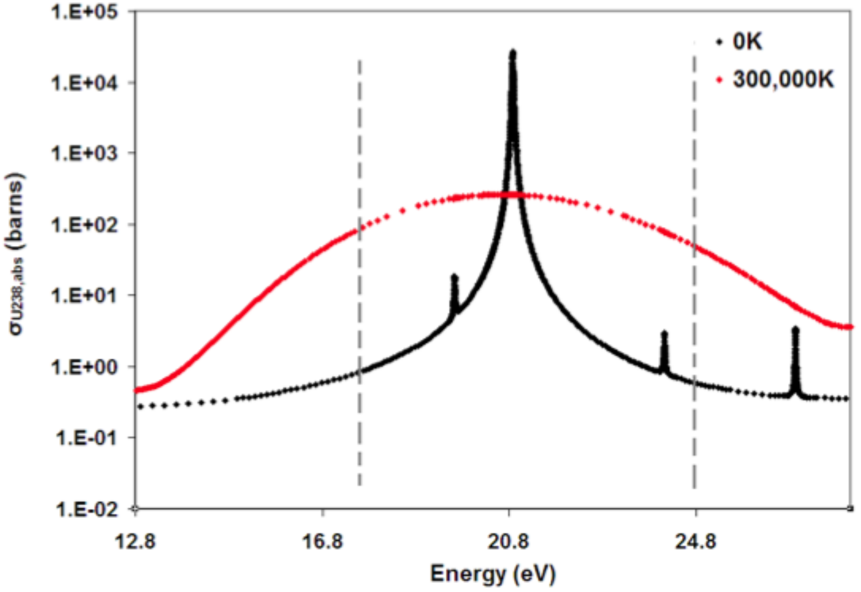
- **For free-flight, selection of collision isotope, & tallies of overall reactions: must use effective cross-sections, averaged over (E, Ω) distribution of nuclides at temperature T**

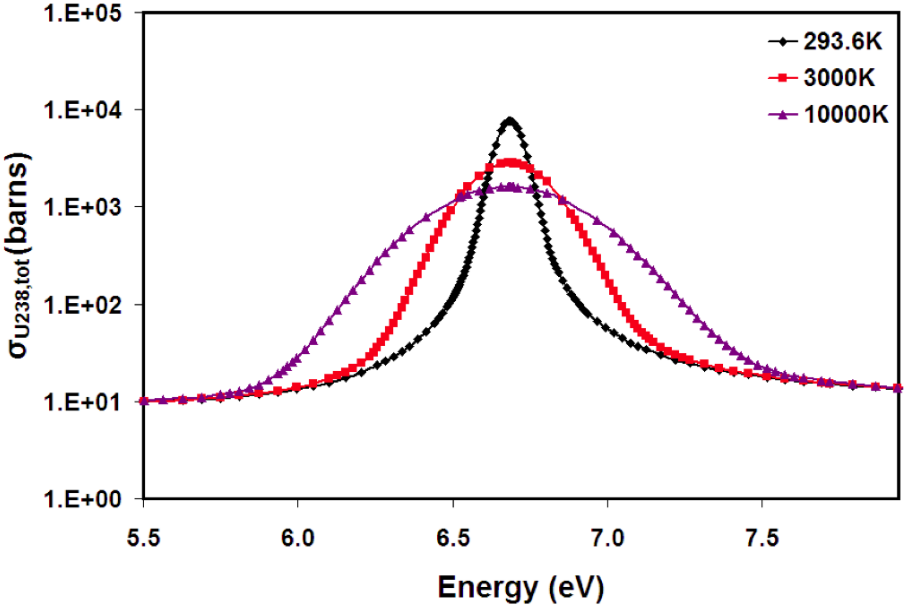
$$\sigma_{eff}(v) = \int \frac{|\vec{v} - \vec{V}|}{v} \sigma(|\vec{v} - \vec{V}|) P(\vec{V}) d\vec{V}, \qquad P(\vec{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

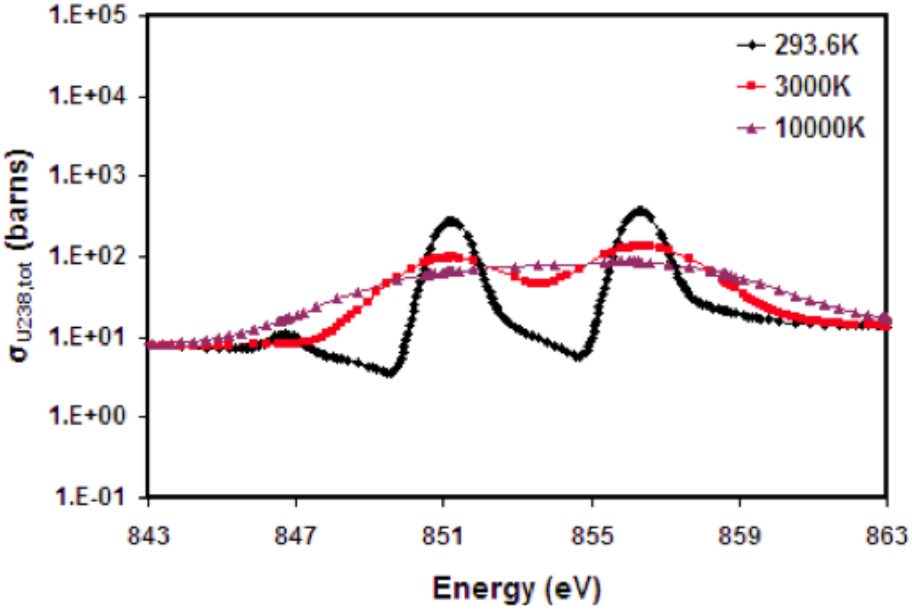
Doppler broadening equation v = neutron, V=nucleus

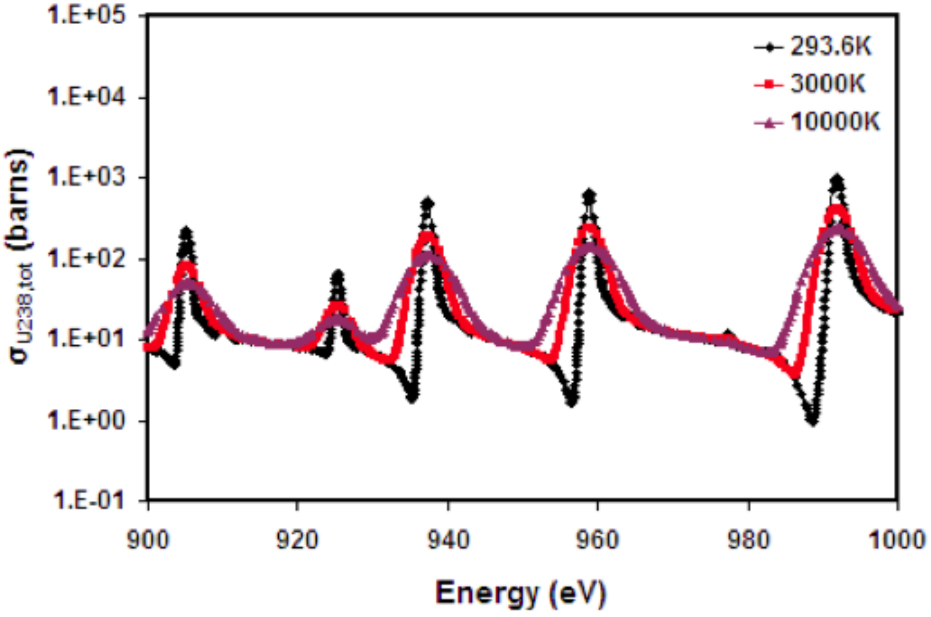
This is a convolution of the cross-section with the target energy or speed distribution.
Smears out & smoothes the cross-section, reduces peak values.

^{238}U Doppler Broadening Examples



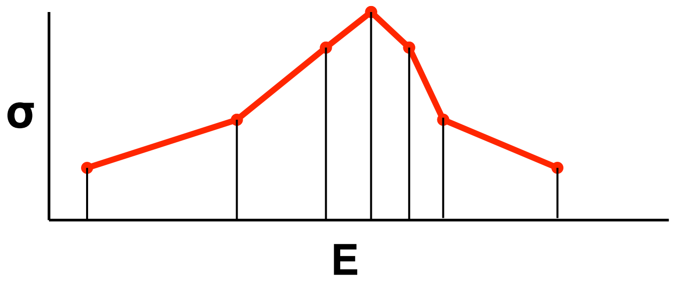






Doppler Broadening - Numerics

- ENDF/B nuclear data is represented by piecewise-linear tabulation of σ(E)



Typically, a linearization tolerance of 0.1% is used

- Doppler Broadened Neutron Cross-sections

$$\sigma_{eff}(v) = \int \frac{|\vec{v}-\vec{V}|}{v} \sigma(|\vec{v}-\vec{V}|) P(\vec{V}) d\vec{V}, \quad P(\vec{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

  – Red Cullen (NSE, 1976) showed how to exactly perform this convolution of Maxwell Boltzmann PDF with piecewise-linear σ(E), called sigma1 method

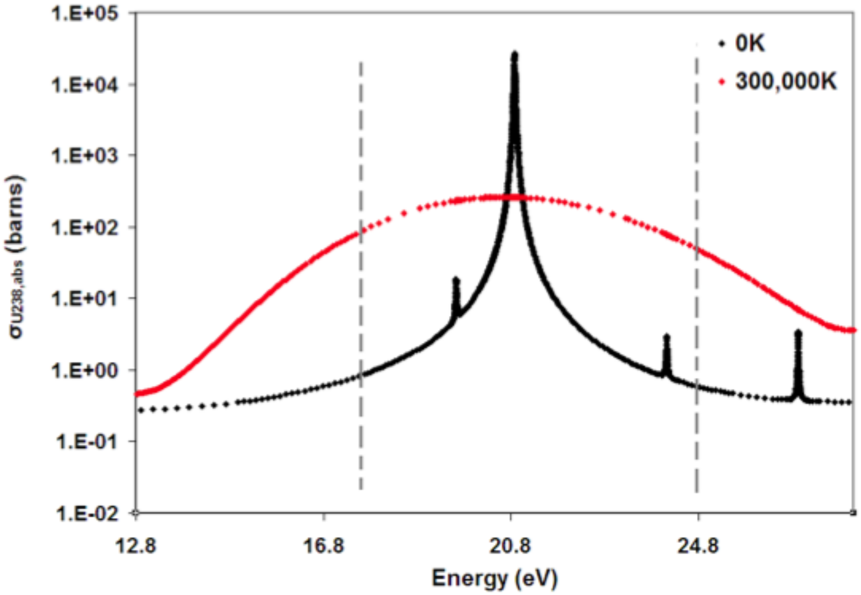
  – NJOY code is similar & adaptively chooses energy points to meet 0.1% accuracy in σ_{eff} at T

  – σ_{eff}(E) has different E-mesh at different T's

  – Very compute-intensive, typically performed prior to Monte Carlo in preparing nuclear data libraries

Doppler Broadening with Adaptive Energy Grid

Temperature Range (K)	Field of Study
77 - 293.6	Cold Neutron Physics
293.6 – 550	Benchmarking Calculations
550 – 1600	Reactor Operation
1600 – 3200	Accident Conditions



NJOY – adaptive E grid for ^{238}U Doppler broadening

	Fractional Tolerance							
	0.1%	*0.3%*	*0.5%*	*1.0%*	*2.0%*	*3.0%*	*4.0%*	*5.0%*
T (K)	**Number of Energy Grid Points**							
0	193131	122935	100646	76856	57347	49659	44955	41676
77	103600	70240	59900	50049	43716	41408	40250	39514
293.6	85247	60192	52352	44810	39965	38089	37104	36494
500	77676	55786	49097	42506	38188	36509	35565	35006
1000	67437	50226	44773	39625	35957	34593	33810	33282
1500	62302	47227	42557	38000	34881	33616	32956	32490
2000	58735	45153	41098	36957	34109	32999	32384	31918
2500	56248	43774	39933	36177	33586	32543	31948	31560
3000	54282	42707	39051	35557	33208	32192	31661	31314

Temperature Variation in Monte Carlo

What if there are 1000s of T's ?

Six approaches:

1. Traditional NJOY+MC (exact)

- NJOY data at specific problem T's
- Each MC region in MC uses specific pre-broadened data
- Exact, very cumbersome, very large amount of xsec data

2. Traditional NJOY+MC (approx.)

- Like (1), but round off T's to nearest 10-20°
- Aproximate, very cumbersome, very large amount of xsec data

3. Stochastic Mixing (approx)

- NJOY data at a few bounding T's
- Set up MC input with a mix of hot & cold data for a nuclide, such that average T for the mix matches problem T
- Run MC, will sometimes get "hot" data, sometimes "cold", average is OK
- Approximate, cumbersome, very large amount of xsec data

(OTF = On-The-Fly)

4. OTF Sigma1 (Monk)

- Use only 1 set of NJOY datafiles
- During MC, use sigma1 method to broaden data as needed
- Exact, but very expensive, ~10x increase in computer time

5. OTF Using Delta-Track (Serpent)

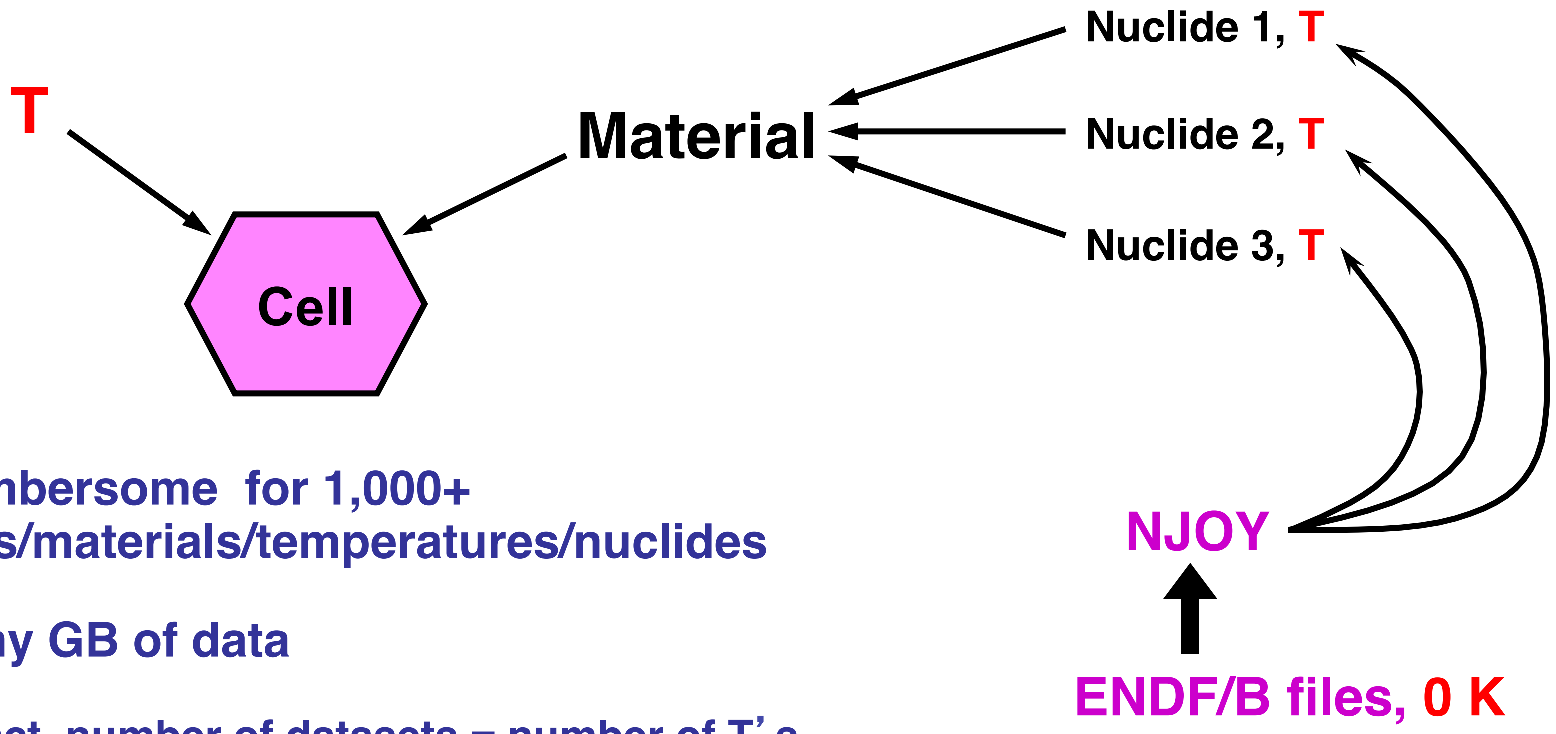
- Use only 1 set of NJOY datafiles
- During MC, use delta-tracking rejection method to broaden data as needed
- Exact, but complex & expensive, ~4x increase in computer time
- Cannot do pathlength MC estimators or point-detector estimators

6. OTF Temp. Fitted Data (MCNP)

- Use only 1 set of NJOY datafiles
- Prior to MC, generate OTF datasets to handle temperature variation
- During MC, Doppler broaden as needed using fitting data
- Exact, extra data for T-fits, ~1.1x increase in computer time

(1)+(2) Traditional NJOY+MC

- **Conventional MCNP problem specification:**
  - Temperatures are assigned to cells (geometry regions)
  - Materials are assigned to cells
  - Doppler broadening for temperature T is performed on nuclides
  - Materials are composed of nuclides



- Cumbersome for 1,000+ cells/materials/temperatures/nuclides
- Many GB of data

(1) Exact, number of datasets = number of T's

(2) Approx., match cell T to closest material with nuclides at T'

(3) Stochastic Mixing

- Often loosely called "stochastic interpolation" or "interpolation"
- This is simply mixing, not interpolation

- MCNP input example:

  – Want this at 500 K: m1000 92235 -.93 92238 -.07

  – Have these datasets from NJOY:

  92235.91c at 300 K, 92238.91c at 300 K
  92235.92c at 600 K, 92238.92c at 600 K

  – For mixing linear in T, mix 1/3 of 300 K data + 2/3 of 600 K data

```
m1000   92235.91c   -.31          92238.91c   -.0233333
        92235.92c   -.62          92238.92c   -.0466667
```

- Cumbersome for 1,000+ cells/materials/temperatures/nuclides (could be scripted…..)

- Many GB of data, 2x nuclides, complex input

(4) OTF Sigma1, (5) OTF Delta, (6) OTF for MCNP

(4) OTF Sigma1

- **Recently implemented in MONK**
- **Numerical sigma1 method OTF during neutron tracking**
- **Increases overall runtime by ~10x**
- **See Davies paper from ICNC-2011**

(5) OTF Delta-tracking

- **Currently being tested in Serpent**
- **Very elegant & innovative, very promising**
- **Increases overall runtime by ~2-4x, may improve**
- **Does not fit with many conventional MC schemes:**
  - No pathlength estimators
  - No point-detector (flux at a point) tallies
  - Requires radical revisions to codes such as MCNP
- **See Viitanen & Leppanen paper from PHYSOR-2012**

(6) OTF for MCNP -- rest of talk

OTF Doppler Broadening

-

U. Michigan + ANL + LANL

DOE NE-UP Project

OTF Methodology

Union Energy Mesh

Temperature Fitting

OTF Doppler in MCNP

Testing

Work-in-Progress

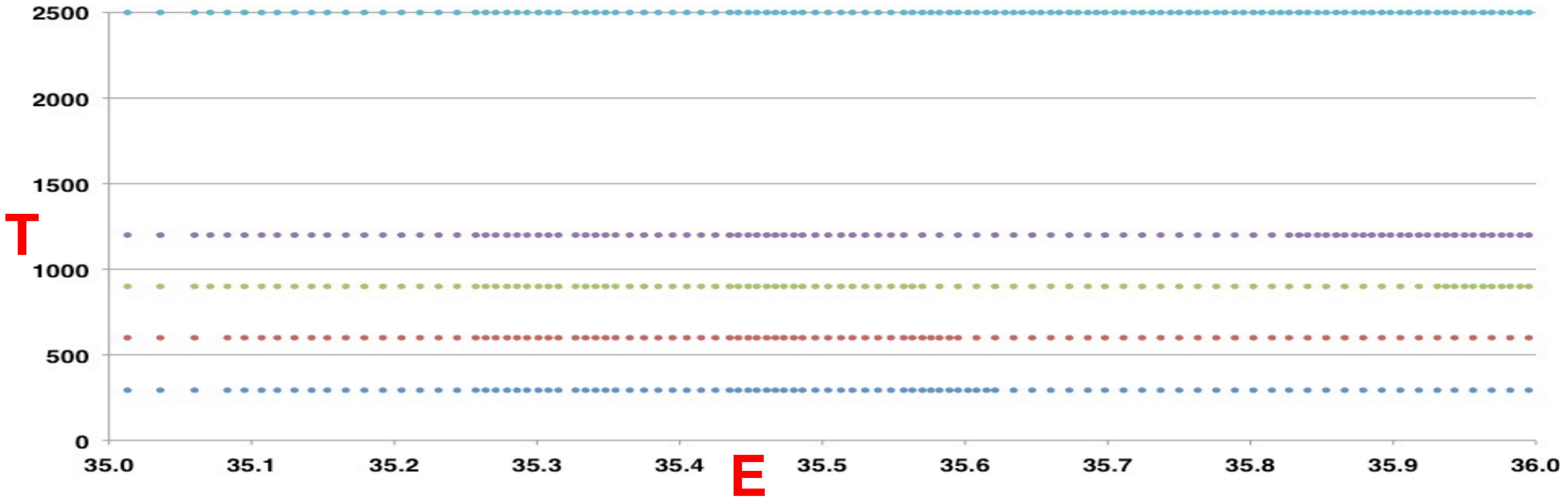
On-The-Fly Neutron Doppler Broadening

- **OTF Methodology (for each nuclide)**
  - **Create union energy grid for a range of temperatures**
  - **Create fits for σ_{eff}(T,E), for range of temperatures, on union E-grid**
  - **MCNP – evaluate σ_{eff}(T,E) OTF during simulation**

- **Comments**
  - **Target application, for now: reactors**
  - **Relies on NJOY methodology**
    - Supplements & extends NJOY
    - Methodology consistent with NJOY
  - **Fitting σ vs temperature (at each E)**
    - High precision, least squares with singular value decomposition
    - Adaptive (for each E, MT, & nuclide)
    - Explicit, direct error checking for fits - fit error < linearization tolerance
    - Threaded parallel, broadening routines called millions of times
    - Over temperature, maintains accuracy consistent with NJOY

OTF Methodology – Union Energy Grid (1)

- ^{238}U energy grid, 35-36 eV, various temperatures (ENDF/B-VII.0)



NJOY adapts the energy grid (for each nuclide, at given T) to preserve linearization tolerance

Temperature (K)	Number of E pts
293.6	157754
600	133964
900	122581
1200	115361
2500	99631

Union E-grid:

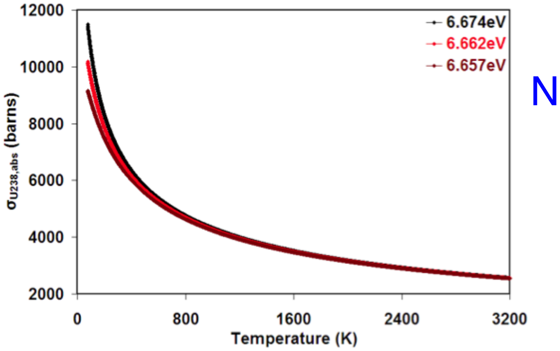
Need to determine 1 energy grid (for each nuclide) that preserves linear interpolation tolerance in E over the entire T range

OTF Methodology – Union Energy Grid

- **For 1 nuclide, determine:**
  - **MT numbers for reactions to be broadened**
  - **Energy range for broadening, E_{min} - E_{max}**
    - Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  - **Temperature range T_{min} – T_{max} & interval ΔT for tolerance testing (input)**
  - **Base set of $\sigma_x(e)$'s from NJOY at T_{base}**
    - "x" = any MT reaction that needs broadening
    - ACE data file from NJOY: Yesilyurt: T_{base}=0 K, Brown: T_{base}=293.6 K
  - **Energy grid from NJOY at T_{min}**

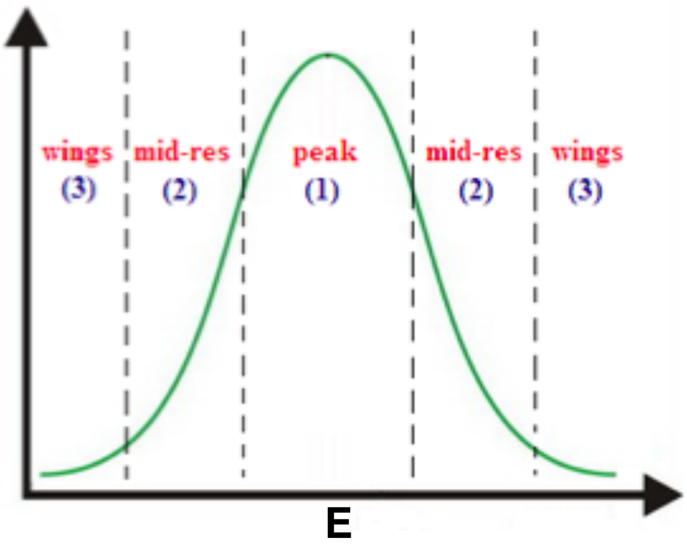
- **For 1 nuclide & a set of T's in range, at each T:**
  - **Adaptively add E points so that 0.1% linear tolerance is maintained**
    - Exact Doppler broadening from T_{base} to T, using sigma1 method
    - Check **all** broadened MT reaction data for each E interval
    - Subdivide E interval until 0.1% linearization tolerance met for all MT's
    - Add E points as needed, do not remove E points
  - **Compute-intensive – millions of calls to sigma1 routine, parallel threads**
  - **Typically expands number of E points by ~10%, for 293-3200 K range**
  - **Result: union E-grid for nuclide, 0.1% linear tolerance over entire T range**

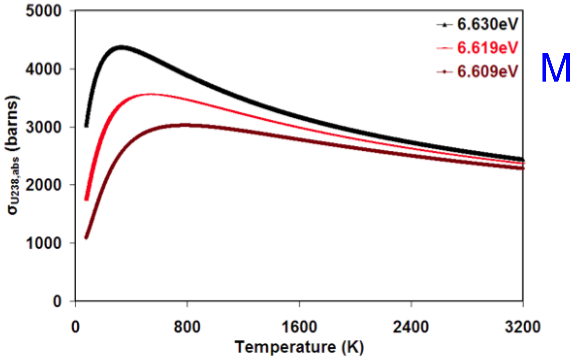
OTF Methodology – Doppler Broadening vs Temperature



Near resonance peaks:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} \frac{d_k}{T^{k/2}}$$



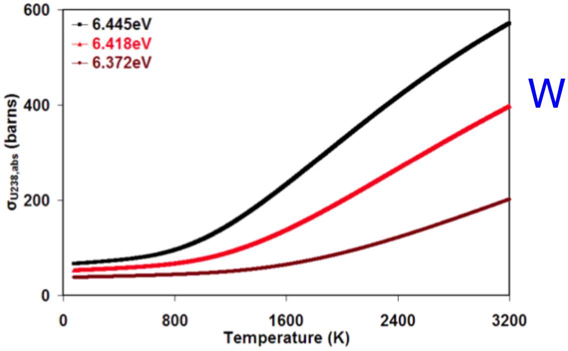


Mid resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} e_k T^{k/2}$$

Combined functional form :

$$\sigma_{T,C,F}(T) \sim \sum_{k=1}^{n} \frac{a_k}{T^{k/2}} + \sum_{k=1}^{n} b_k T^{k/2} + c$$



Wings of resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} f_k T^k$$

- for specific E, MT
- n varies for E, MT
- a_k, b_k, c tabulated for E, MT

Functional forms for temperature fitting based on multilevel Adler-Adler model, with expansions for peak, mid-res, wings

OTF Methodology – Fitting vs T

- **For 1 nuclide, determine:**
  - **MT numbers for reactions to be broadened**
  - **Energy range for broadening, E_{min} - E_{max}**
    - Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  - **Temperature range T_{min} – T_{max} & interval ΔT for tolerance testing (input)**
  - **Base set of $\sigma_x(e)$'s from NJOY at T_{base}**
    - "x" = any MT reaction that needs broadening
    - ACE data file from NJOY: Yesilyurt: T_{base}=0 K, Brown: T_{base}=293.6 K
  - **Union energy grid for this nuclide & T range**
  - **Maximum order for temperature fitting**
    - Adler-Adler based functional form, using powers of $T^{1/2}$ and $1/T^{1/2}$

- **For 1 nuclide, at each point in the union E grid:**
  - **Exact Doppler broadening from T_{base} to all T's in range, using sigma1 method**
  - **Least-squares fitting over T**
    - Singular value decomposition, least squares for temperature dependence
    - **Fitting order chosen adaptively for each energy & reaction so that fits accurate within 0.1% for all T's and all E's in range, for all MT's**
  - **Coefficients saved in files for MCNP use**

OTF Methodology – MCNP OTF

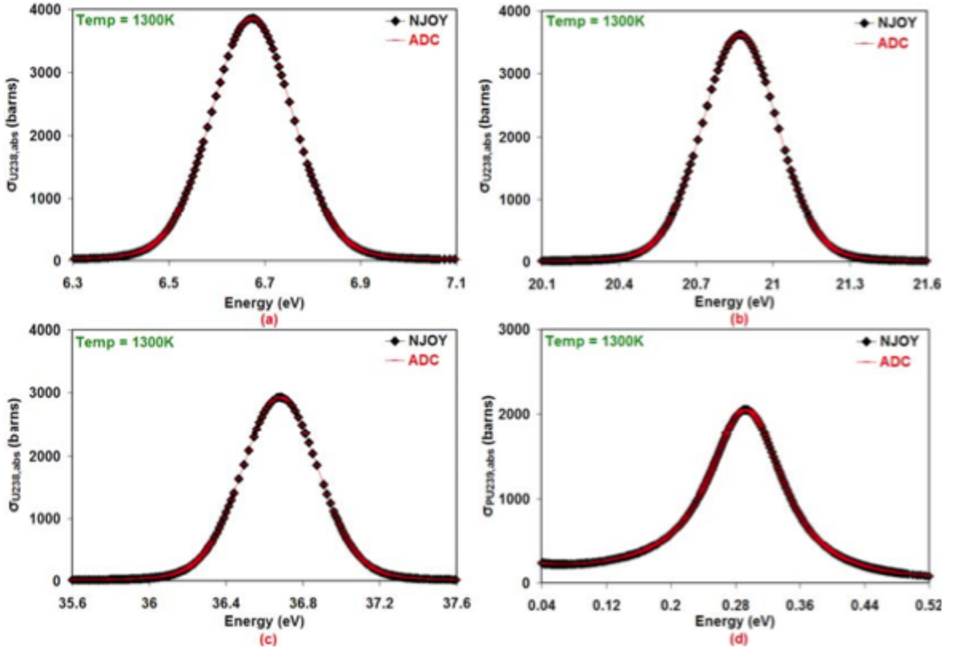
- At problem setup, read in OTF data for various nuclides
  - Each OTF nuclide set can have different fit orders & union E-grid & reactions

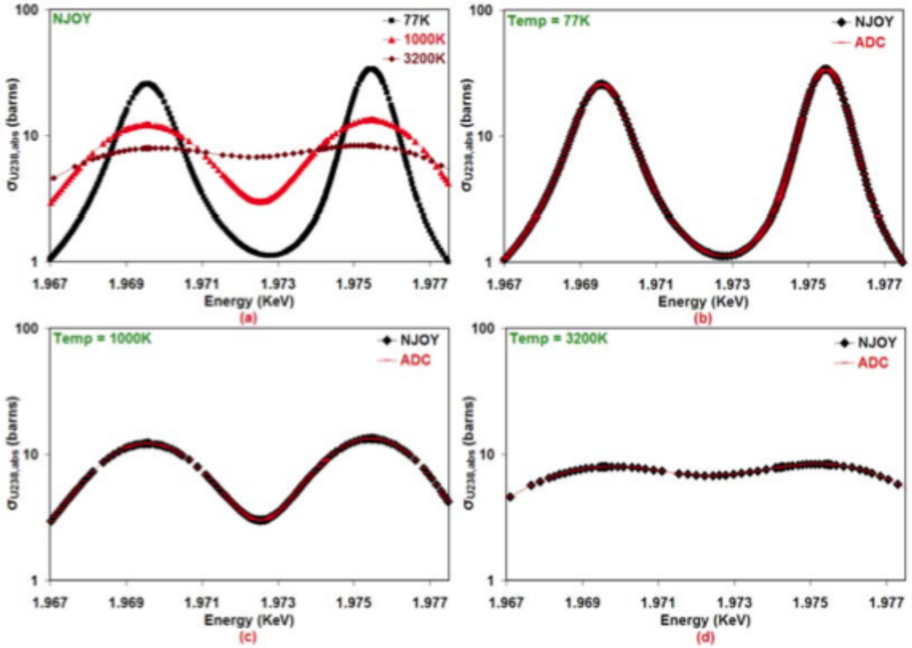
- During simulation, if neutron in E-T range of fits
  - Use OTF data for each nuclide to create on-the-fly Doppler broadened cross-sections at current cell temperature
  - If outside E-T range of OTF data, use standard ACE data
  - Collision physics (exit E & angles) uses standard ACE data

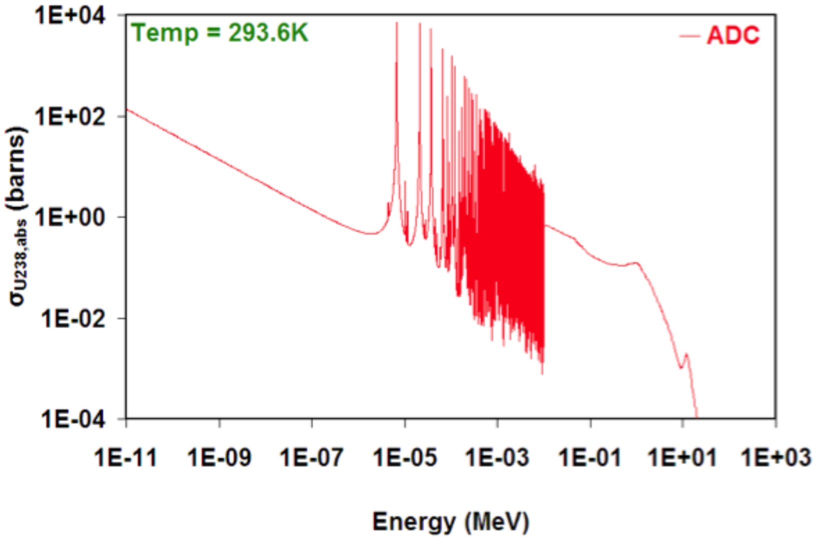
- Only need to generate OTF datasets once, & then use for any problems

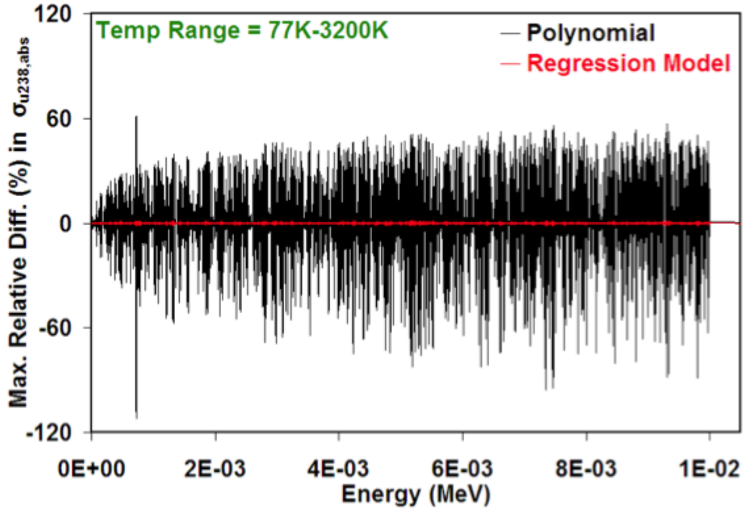
- Cost
  - Extra storage for OTF data
  - Extra computing for evaluating OTF functions (typical <10% runtime)
- Benefit
  - Less storage for ACE data (no need for multiple temperatures)
  - Can solve problems with 1000s of T's or more, no limit
  - Greatly simplifies problem setup

OTF Testing - Yesilyurt

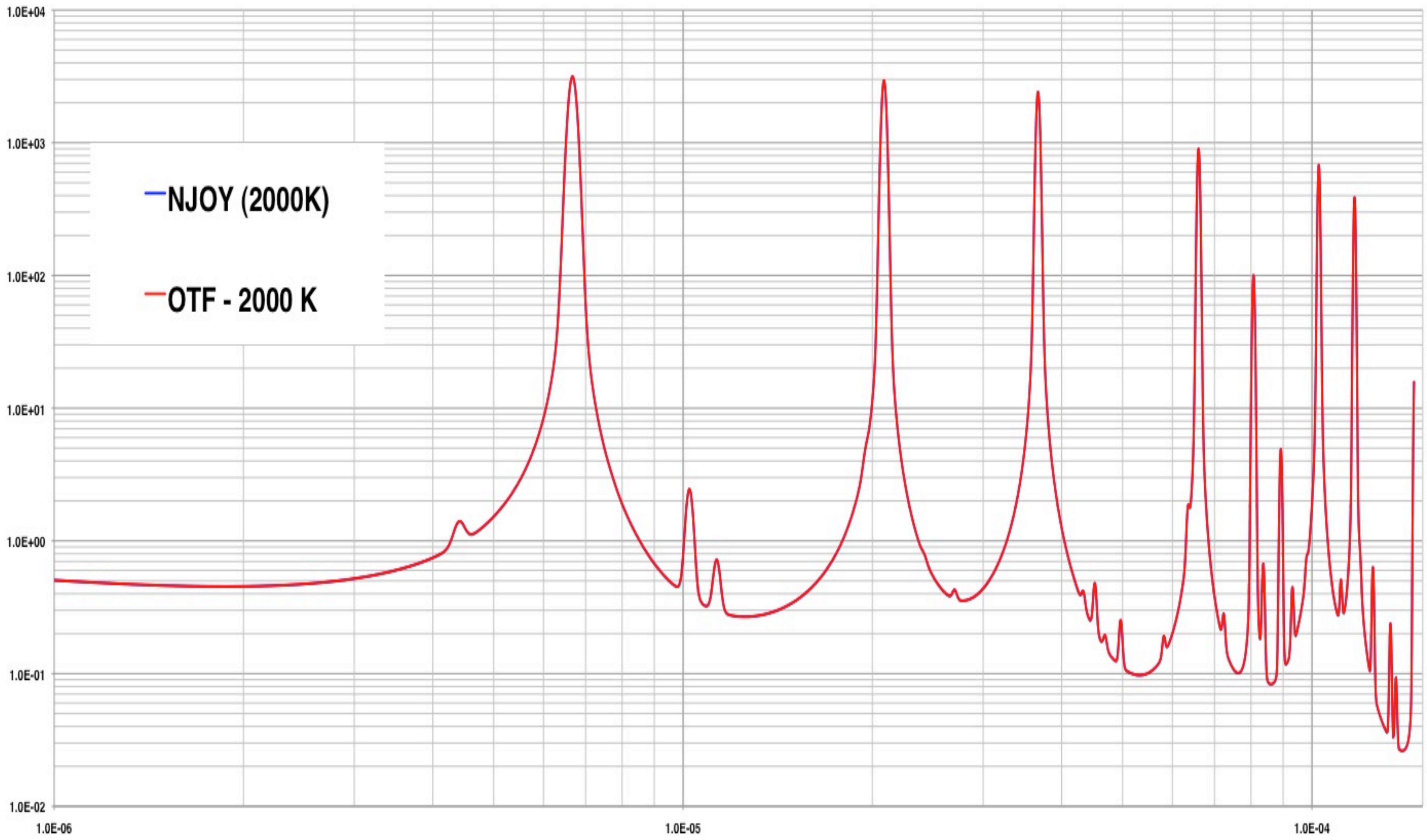








^{238}U Capture – NJOY vs OTF at 2000 K



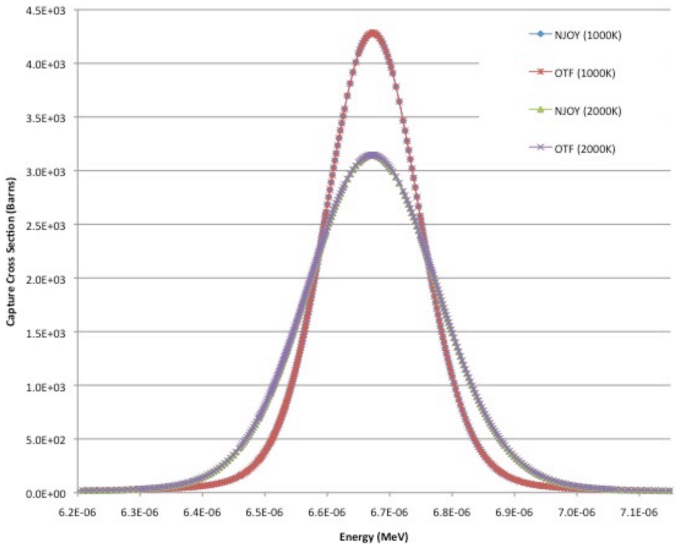
Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies

NJOY vs OTF ^{238}U Capture Cross-Section

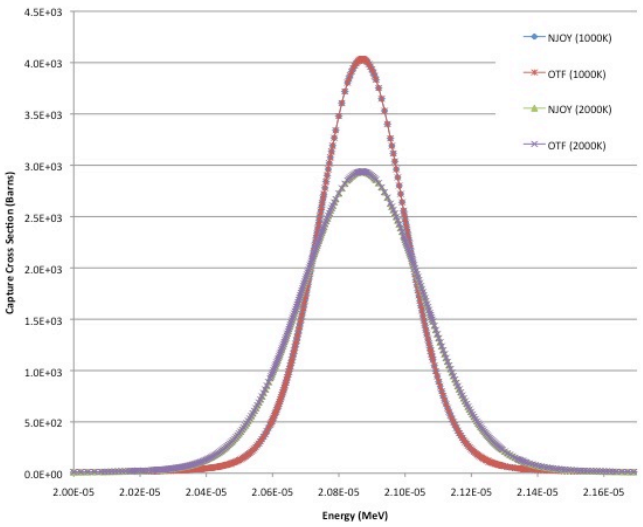
- NJOY vs OTF at 1000 K
  (curves with higher peak)

- NJOY vs OTF at 2000 K
  (curves with lower peak)

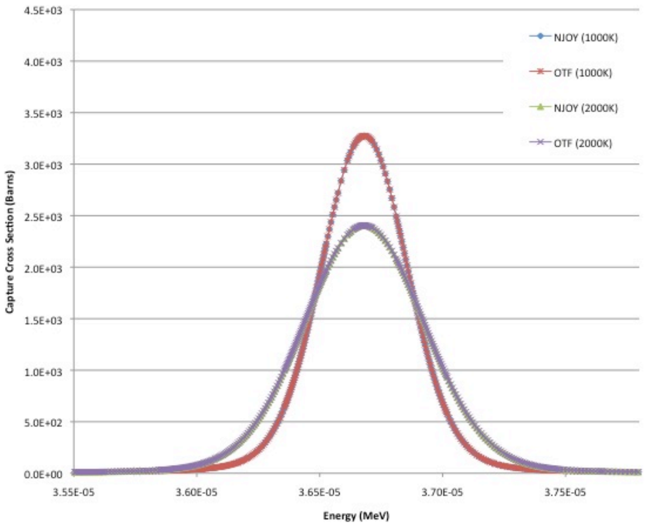
Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies



6.67 eV resonance



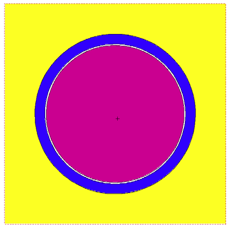
20.9 eV resonance



36.6 eV resonance

MCNP Test Results – Doppler Defect Benchmark

- **Doppler Reactivity Benchmark**
  - **Compare k-effective for HZP (hot, zero power) and HFP (hot, full power) conditions for a unit fuel cell typical of a PWR**
  - **Basic model:**
    - **PWR fuel pin cell** with reflecting BCs, various enrichments
    - **HZP** cases**:** **fuel at 600K**, clad/moderator at 600K
    - **HFP** cases: **fuel at 900K**, clad/moderator at 600K
    - Uniform temperature within each fuel, clad, moderator region.
    - Number densities and dimensions adjusted for the HFP thermal expansion
    - 5M active neutron histories per each of 28 MCNP runs



  - **NJOY+MCNP: NJOY-broadened data at exact temperatures**
  - **OTF+MCNP: OTF data for ^{16}O, ^{234}U, ^{235}U, ^{238}U in fuel**

  - **OTF details**
    - For union E-grid: T_{base}=293.6K, T range 300-1000K, ΔT=100K
    - For OTF fitting: 8th order, T range 300-1000K, ΔT=10K
    - For general production use, would use larger T range & smaller ΔT's

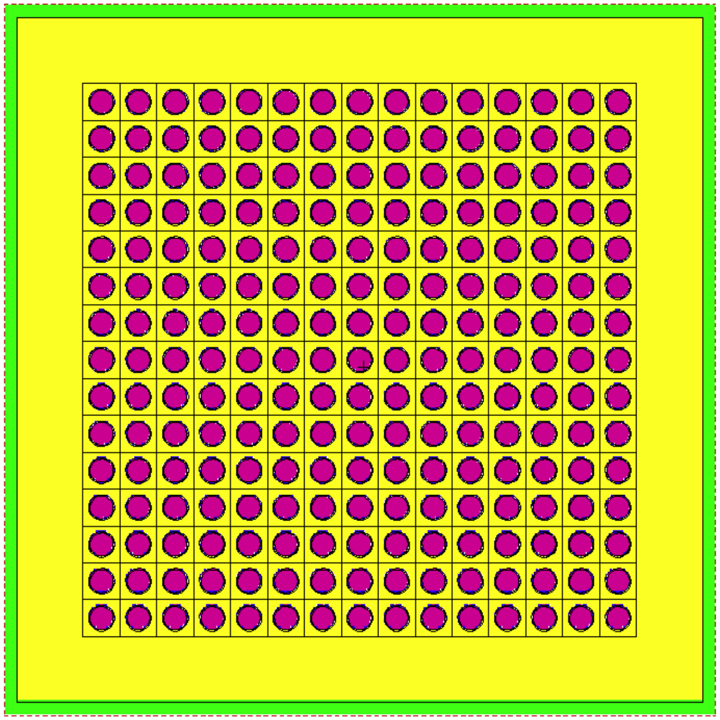
Doppler Defect Benchmark Results

		HZP	HFP	Doppler Coef. pcm/K
UO2 fuel pin	NJOY+MCNP	0.66556 (18)	0.65979 (19)	-4.38 (.20)
0.711% enrichment	OTF+MCNP	0.66567 (18)	0.66022 (19)	-4.13 (.20)
UO2 fuel pin	NJOY+MCNP	0.96094 (26)	0.95293 (25)	-2.92 (.13)
1.60% enrichment	OTF+MCNP	0.96026 (24)	0.95283 (23)	-2.71 (.13)
UO2 fuel pin	NJOY+MCNP	1.09912 (27)	1.08997 (26)	-2.55 (.10)
2.40% enrichment	OTF+MCNP	1.09923 (27)	1.08975 (28)	-2.64 (.10)
UO2 fuel pin	NJOY+MCNP	1.17718 (27)	1.16744 (27)	-2.36 (.09)
3.10% enrichment	OTF+MCNP	1.17703 (30)	1.16767 (30)	-2.27 (.10)
UO2 fuel pin	NJOY+MCNP	1.23967 (27)	1.22920 (30)	-2.29 (.09)
3.90% enrichment	OTF+MCNP	1.23953 (29)	1.22979 (29)	-2.13 (.09)
UO2 fuel pin	NJOY+MCNP	1.27501 (30)	1.26526 (27)	-2.01 (.09)
4.50% enrichment	OTF+MCNP	1.27534 (29)	1.26552 (29)	-2.03 (.09)
UO2 fuel pin	NJOY+MCNP	1.29901 (31)	1.28920 (29)	-1.95 (.08)
5.00% enrichment	OTF+MCNP	1.29907 (28)	1.28938 (29)	-1.93 (.08)

$$\rho = \left(1 / K_{HZP} - 1 / K_{HFP} \right) \times 10^5 / 300 \quad \text{pcm/K}$$

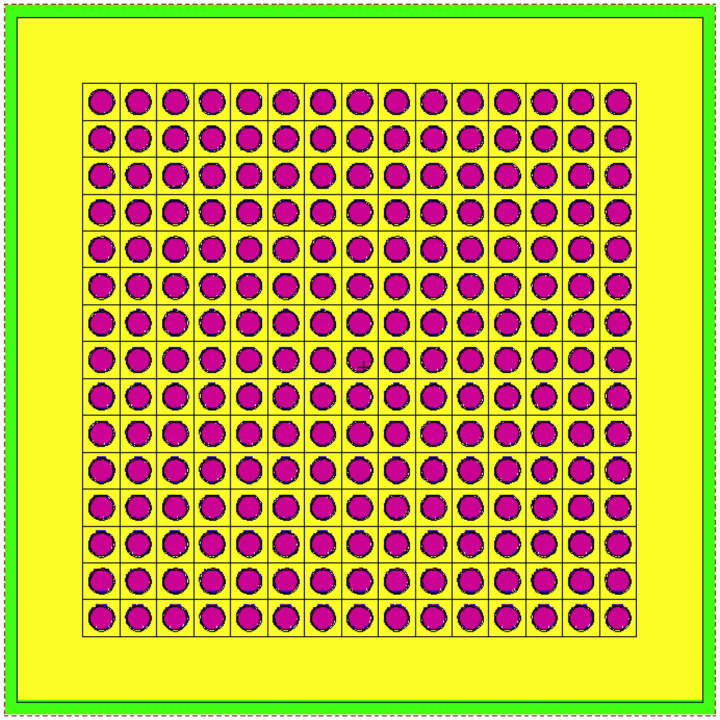
Results – Fuel Assembly I

- Simplified PWR 15 x 15 fuel assembly
  - From OECD/NEA fuel storage vault benchmark
    - Fuel = 900 K
    - Clad & water = 600 K
    - Outer iron rack = 293.6K
  - Standard NJOY+MCNP5:
    - 900K ACE data for fuel,
    - 600K ACE data for clad & mod
    - 293.6K ACE data for iron
  - OTF+MCNP5
    - use 293.6K ACE data for all nuclides
    - OTF data for all nuclides (except iron)
  - MCNP5
    - 20,000 neutrons/cycle,
    - 10 inactive cycles, 1000 active cycle
    - Reflecting BCs



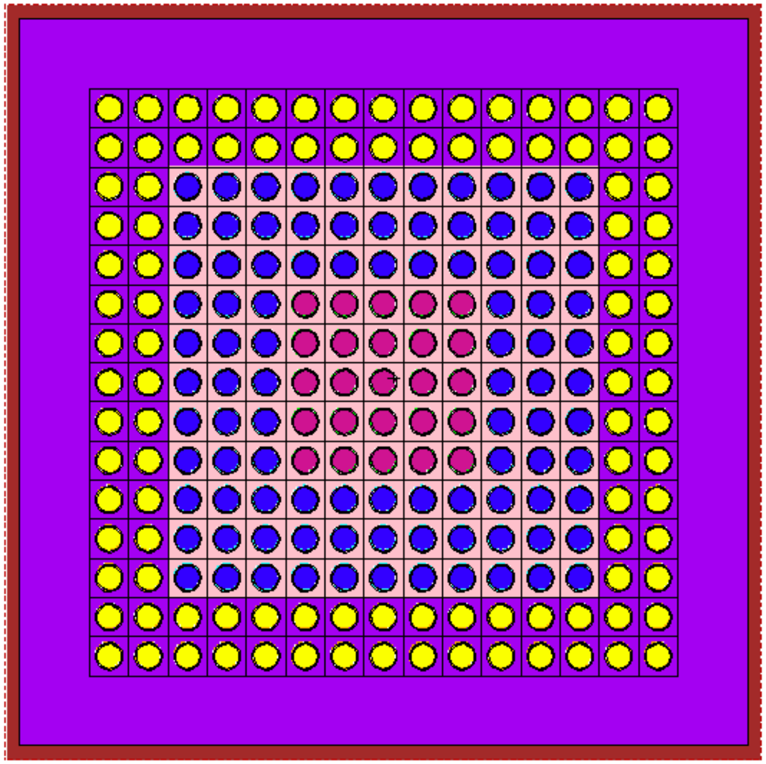
Results - Fuel Assembly I

- K-effective
  - NJOY+MCNP5: 1.13891 (15)
  - OTF+MCNP5: 1.13892 (15)
- Total Fission
  - NJOY+MCNP5: 0.464506 (.02%)
  - OTF+MCNP5: 0.464499 (.02%)
- Total Capture in fuel
  - NJOY+MCNP5: 0.250912 (.02%)
  - OTF+MCNP5: 0.250918 (.02%)
- U235 capture in fuel
  - NJOY+MCNP5: 0.089478 (.02%)
  - OTF+MCNP5: 0.089475 (.02%)
- U238 capture in fuel
  - NJOY+MCNP5: 0.160302 (.03%)
  - OTF+MCNP5: 0.160311 (.03%)
- O16 capture in fuel
  - NJOY+MCNP5: 9.73621e-4 (.11%)
  - OTF+MCNP5: 9.73248e-4 (.11%)



Results – Fuel Assembly II

- **Simplified PWR 15 x 15 fuel assembly, with varying temperatures**
  - **From OECD/NEA fuel storage vault benchmark**
    - Fuel = 900 K, 600 K, 300 K
    - Clad = 900 K, 600 K, 300 K
    - Water = 600 K, 300 K
    - Outer iron rack = 293.6K
  - **Standard NJOY+MCNP5:**
    - ACE data at explicit temperatures
  - **OTF+MCNP5**
    - use 293.6K ACE data for all nuclides
    - OTF data for all nuclides (except iron)
  - **MCNP5**
    - 20,000 neutrons/cycle,
    - 10 inactive cycles, 1000 active cycle
    - Reflecting BCs



Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

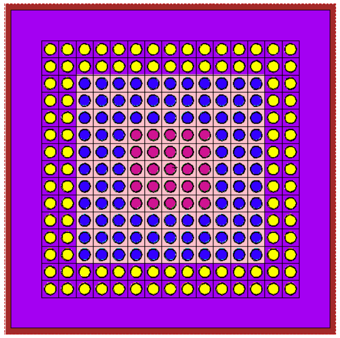
Results – Fuel Assembly II

k-effective:

STD	1.11599 (15)
OTF	1.11592 (15)

Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

		900K	600K	300K
Total fission				
	STD	.045140 (.08%)	.161186 (.04%)	.248782 (.03%)
	OTF	.045081 (.08%)	.161329 (.04%)	.248731 (.03%)
Total capture in fuel				
	STD	.027672 (.09%)	.096276 (.05%)	.116745 (.04%)
	OTF	.027667 (.09%)	.096268 (.05%)	.116829 (.04%)
U235 capture in fuel				
	STD	.008993 (.08%)	.031910 (.04%)	.045998 (.03%)
	OTF	.008983 (.08%)	.031932 (.04%)	.045987 (.03%)
U238 capture in fuel				
	STD	.018547 (.11%)	.063887 (.06%)	.070236 (.05%)
	OTF	.018551 (.11%)	.063858 (.06%)	.070332 (.05%)
O16 capture in fuel				
	STD	1.15E-04 (.23%)	4.18E-04 (.14%)	4.37E-04 (.13%)
	OTF	1.15E-04 (.23%)	4.16E-04 (.14%)	4.37E-04 (.13%)



OTF Work in Progress

- Better integration into MCNP (optimization)

- FIT_OTF fitting program
  - Investigate scaling & Chebychev, for better numerical stability
  - Investigate regression, to vary fit order by energy & reaction [done]

- U. Michigan work
  - Create OTF libraries for all nuclides in ENDF/B-VII.0
  - Test various applications: fuel assemblies, 3D whole core, LWR, HTGR, ...

- Methodology for Unresolved Resonances & S(α,β) data
  - Probable 1st cut – tables with temperature interpolation
  - Possible thesis topic for PhD student

- Implement corrected free-gas scatter model
  - Demonstrated, needs robust implementation

- Easy to extend to any temperature range
  - Need to investigate broadening for high-threshold reactions

References

- **F.B. Brown, W.R. Martin, G. Yesilyurt, S. Wilderman**, "Progress with On-The-Fly Neutron Doppler Broadening in MCNP", *Trans. Am. Nuc. Soc.* 106 [also LA-UR-12-00423] (2012).

- **G. Yesilyurt**, "Advanced Monte Carlo Methods for Analysis of Very High Temperature Reactors: On-the-Fly Doppler Broadening and Deterministic / Monte Carlo Methods," *PhD thesis*, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI (2009).

- **G. Yesilyurt, W.R. Martin, F.B. Brown**, "On-The-Fly Doppler Broadening for Monte Carlo Codes", accepted for publication, *Nuclear Science & Engineering.*

- **F.B. Brown, B.C. Kiedrowski, W.R. Martin, G. Yesilyurt**, "Advances in Monte Carlo Criticality Methods", Invited Workshop for M&C-2009, Saratoga Springs, NY, May 3-7 [also, LA-UR-09-02442] (2009)

- **R.D. Mosteller**, "Computational Benchmarks for the Doppler Reactivity Defect", ANS Joint Benchmark Committee [LA-UR-06-2968] (2006).

- **R.E. Macfarlane and D.W. Muir**, ""NJOY99.0 - Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data,"" *PSR- 480/NJOY99.00*, Los Alamos National Laboratory, Los Alamos (2000).

- **T. Viitanen, J. Leppanen**, "Explicit Temperature Treatment in Monte Carlo Neutron Tracking Routines – First Results", PHYSOR-2012, Knoxville, TN (2012).

Fit_OTF Example (1)

```
====================================================================
 =  Fit_OTF:  Command-line options:
 =
 =       perform_fitting  =  T
 =
 =       zaid             = 92238.70c
 =       ace_file         =
 =       ugrid_file       = ugrid_92238.70c.txt
 =       otf_file         = otf_file.txt
 =       fit order min    =           1
 =       fit order max    =           8
 =       fit   min temp   =    293.600000000000       (if > ACE temp)
 =       fit   max temp   =    1000.00000000000
 =       fit   inc temp   =    10.0000000000000
 =
 =       print n-th lines =          20
 =
 =       create ugrid     =  F
 =
 =       testing?         =  T
 =       test_emin        =   5.500000000000000E-006
 =       test_emax        =   7.500000000000000E-006
 ====================================================================
```

Fit_OTF Example (2)

```
.....read ACE file =
    92238.70c
        xsdir = /Volumes/fbb/fbrown/LANL/MCNP_DATA/xsdir
        file  = /Volumes/fbb/fbrown/LANL/MCNP_DATA/endf70j
   ................................................................................
   Info from ACE data file for ZAID = 92238.70c

        Number of energies  =   157754
        Atomic weight ratio = 236.005800 amu
        Temperature         =  2.530100E-08 MeV,     293.6 K
        Date                = 08/25/07
        Info                = 92-U -238 at 293.6K from endf/b-vii.0 njoy99.248
        endf MAT            = mat9237

        MT reactions (std+gpd+mtlist), n= 52
                 1  101    2  301  202   16   17   18   37   51
                52   53   54   55   56   57   58   59   60   61
                62   63   64   65   66   67   68   69   70   71
                72   73   74   75   76   77   78   79   80   81
                82   83   84   85   86   87   88   89   90   91
               102  444
        MT reactions for fission, n=  1
                18

        URR-probability tables are present
             energy range:  2.000001E-02 MeV -  1.490287E-01 MeV

        Doppler broadening info:
             energy range:  1.000000E-11 MeV -  2.000001E-02 MeV
             MT reactions for Doppler broadening, n=  8
                      1  101    2  301  202   18  102  444
   ................................................................................
```

Fit_OTF Example (3)

```
 .....read ugrid

 .....  ugrid e pts =       168626
 .....  ugrid min e =   9.999999999999999E-012
 .....  ugrid max e =   2.074926000000000E-002



Broadening & fitting info:
     number of ugrid pts =   168603
     min energy          =  1.000000E-11 MeV
     max energy          =  2.000001E-02 MeV
     number of temps     =       71
     min temp            =    293.6 K
     max temp            =    993.6 K
     temp increment      =     10.0 K
     number of reactions =   8
     MT numbers          =     1  101    2  301  202   18  102  444
     MT for tot fission  =  18

     fitting order is variable, to meet tolerance
       min order         =   1
       max order         =   8
       max number coefs  =  17
```

Fit_OTF Example (4)

```
                                           MT-order for kprt lines. Errors given if >tolerance.

    k=   460, e=  5.60999     ev:      1-1  101-2    2-3  301-1  202-4   18-1  102-5  444-1
    k=   480, e=  6.03017     ev:      1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
    k=   500, e=  6.28893     ev:      1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
    k=   520, e=  6.41344     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-1
    k=   540, e=  6.47134     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-1
    k=   560, e=  6.50794     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
    k=   580, e=  6.53025     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
    k=   600, e=  6.55195     ev:      1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-8
    k=   620, e=  6.57375     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
    k=   640, e=  6.59798     ev:      1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
    k=   660, e=  6.65659     ev:      1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
    k=   680, e=  6.70483     ev:      1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
    k=   700, e=  6.76322     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
    k=   720, e=  6.79844     ev:      1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-8
    k=   740, e=  6.85025     ev:      1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
    k=   760, e=  6.89968     ev:      1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-1
    k=   780, e=  6.98755     ev:      1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-1
    k=   800, e=  7.18240     ev:      1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
 >>>>> e-points/minute =     3624.46836348410
```

Fit_OTF Example (5)

```
Overall error checks:
     mt=  1  max-err= 0.100%     for   e=  2883.54     eV,  t=  303.6 K
     mt=101  max-err= 0.100%     for   e=  5967.96     eV,  t=  313.6 K
     mt=  2  max-err= 0.097%     for   e=  20.2401     eV,  t=  313.6 K
     mt=301  max-err= 0.079%     for   e=  7089.62     eV,  t=  313.6 K
     mt=202  max-err= 0.026%     for   e=  2664.37     eV,  t=  313.6 K
     mt= 18  max-err= 0.002%     for   e=  723.161     eV,  t=  333.6 K
     mt=102  max-err= 0.005%     for   e=  4264.86     eV,  t=  333.6 K
     mt=444  max-err= 0.000%     for   e=  20.6344     eV,  t=  333.6 K

     Overall maximum error              =  0.100%

     Number of energies with err > 0.10% =      0

  nctot_max =     22930008
  nctot     =     11074134
```

Monte Carlo Depletion Tutorial

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

From: FB Brown, WR Martin, RD Mosteller, "Monte Carlo - Advances and Challenges",
PHYSOR'08 Monte Carlo Workshop, LA-UR-08-03328 (2008)

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
SERPENT, 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 the PHYSOR-2008 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"**

Introduction

- **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

➜ Repeat (1) & (2) for each time step

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

Definitions

$N_k = N(t_k)$

= vector of all the number densities for each isotope of every region in the problem at time t_k

$\varphi_k = \varphi(t_k) = \varphi(N_k)$

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

$B_k = B(t_k, \Delta t, N_k, \varphi, A, F, \lambda)$

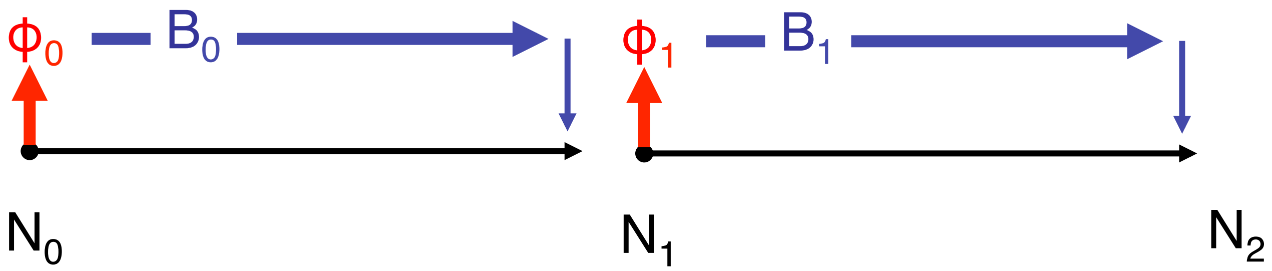
= burnup calculation from time t_k to $t_k+\Delta t$, using N_k, φ_k, A_k, F_k, λ_k

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

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

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

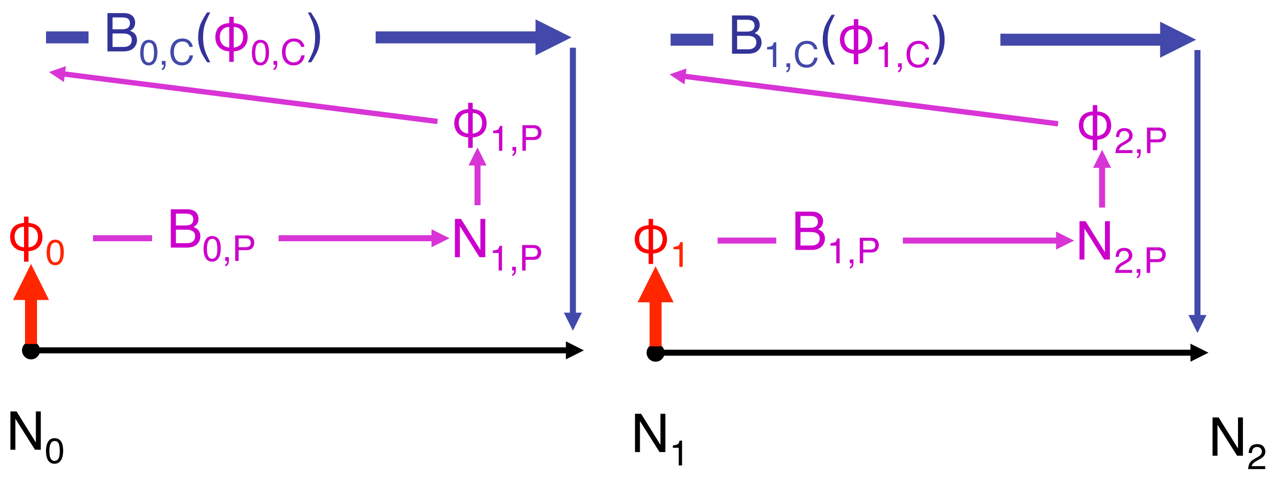
Simple MC Depletion



- **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**

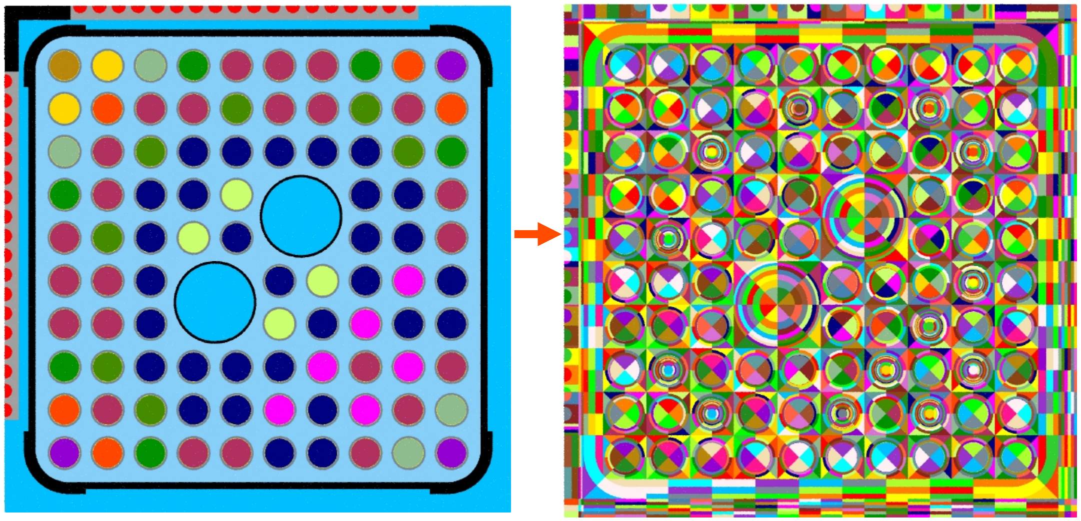
- **Better accuracy, can use much longer time steps**
- **2 MC's & 2 depletions per timestep**
- **Other prescriptions could be used for corrector flux, $\varphi_{J,C}$ (eg, linear, …)**
- **Could iterate until predictor-corrector N's are close**

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

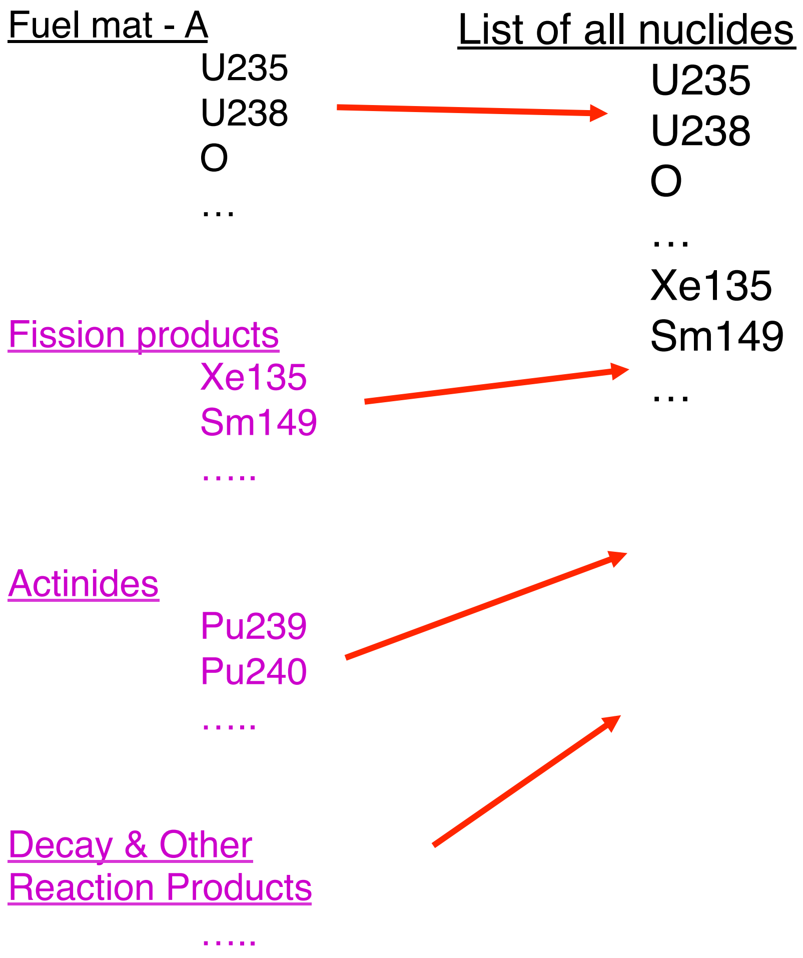


- Most MC depletion codes can't handle this level of detail (yet) for the entire reactor
- If the depletion regions are too large, errors will be introduced

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



Fuel mat - A

U235
U238
O
…

Fission products

Xe135
Sm149
…..

Actinides

Pu239
Pu240
…..

Decay & Other Reaction Products

…..

List of all nuclides

U235
U238
O
…
Xe135
Sm149
…

Cross-section Treatment

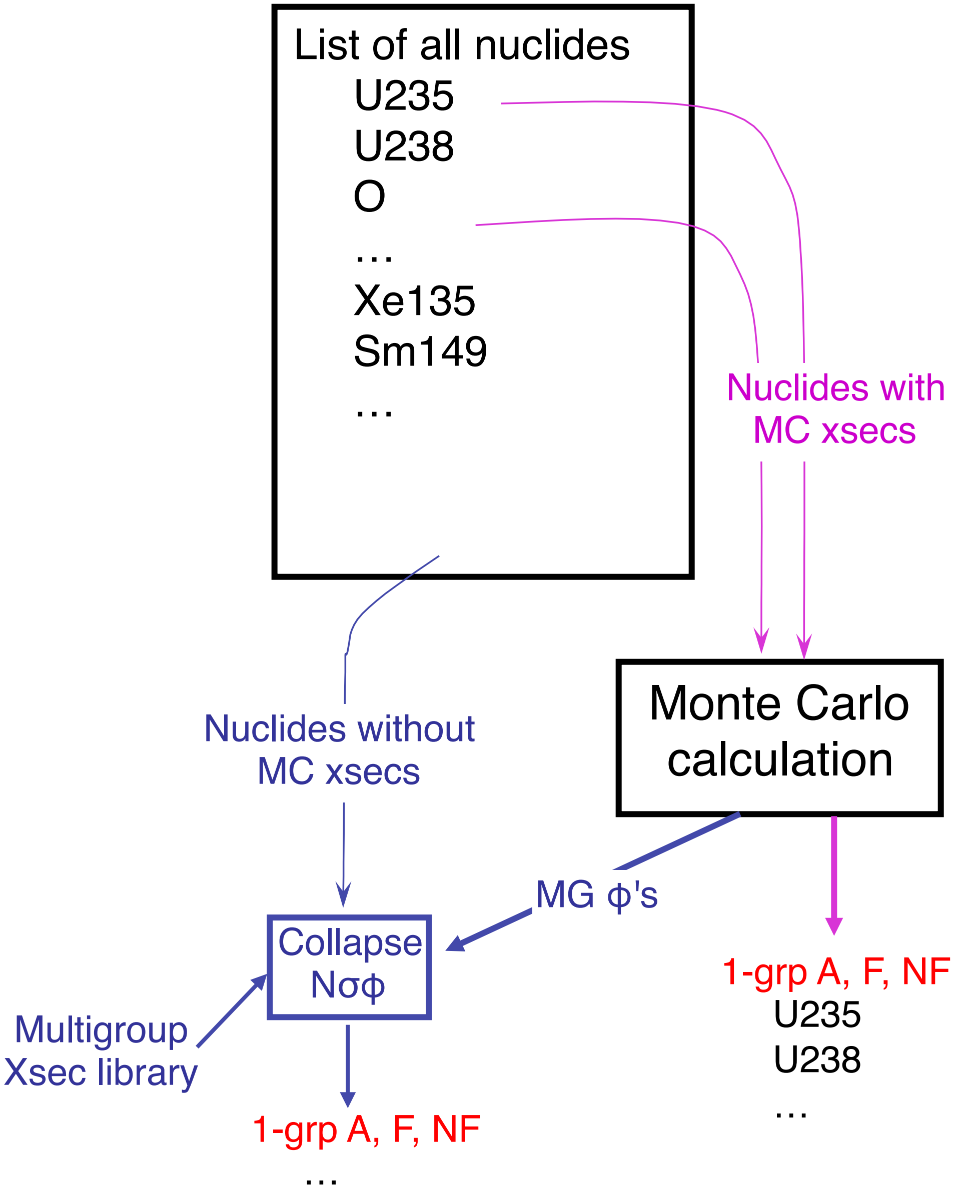
- **For depletion calculation, just need overall (1-group) absorption & fission in each nuclide**
  - **These can be computed directly in the MC, if cross-sections are available**

- **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



List of all nuclides
U235
U238
O
…
Xe135
Sm149
…

Nuclides with MC xsecs

Monte Carlo calculation

1-grp A, F, NF
U235
U238
…

Nuclides without MC xsecs

MG ϕ's

Collapse Nσϕ

Multigroup Xsec library

1-grp A, F, NF
…

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 $K_{eff} \neq 1$ 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 En*ergy 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

HTGR Modeling

HTGR Modeling with MCNP5
MCNP5 Stochastic Geometry
HTGR Physics & Modeling

Outline

- Introduction
- HTGR Modeling with MCNP5
  - MCNP Geometry - Universes, Lattices
  - HTGR Models - Fuel Kernels, Compacts, Pebbles, Core
- MCNP5 Stochastic Geometry
  - Random Translations for Stochastic Universes
  - Discussion & Limitations
- HTGR Physics & Modeling
  - Fuel Kernel Modeling
  - Stochastic Effects
  - Compact or Pebble Modeling
  - Full-core Calculations
- Conclusions

Introduction

- High Temperature Gas-Cooled Reactor
  - One of the Next Generation Reactors ("Gen-IV")
  - Coolant temperatures above 900 C, fuel temperatures above 1250 C
    - Higher energy conversion efficiency
    - Thermochemical hydrogen production
  - Fuel kernels with several layers of coatings
    - Contain fission products
    - Safety aspects …

- Two types of Reactor Design
  - Prismatic fuel type reactor design, with fuel "compacts"
  - Pebble bed fuel type reactor design
  - Double Heterogeneity problem
    - Fuel kernels inside fuel compacts or pebbles in the core
    - Fuel kernels randomly located within fuel elements
    - Challenging computational problem

- Monte Carlo codes can faithfully model HTGRs
  - Full 3D geometry
  - Multiple levels of geometry, including embedded lattices
  - Random geometry ?????

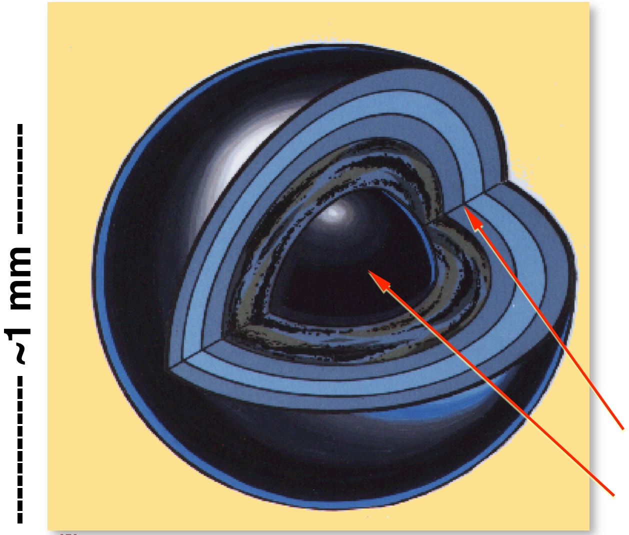
TRISO Coated Fuel Particles

TRISO Coated Fuel Particles:

- Lots of cladding - extremely strong
- Little fuel - fully encapsulated

Each fuel particle forms a separate pressure containment vessel for the fuel kernel

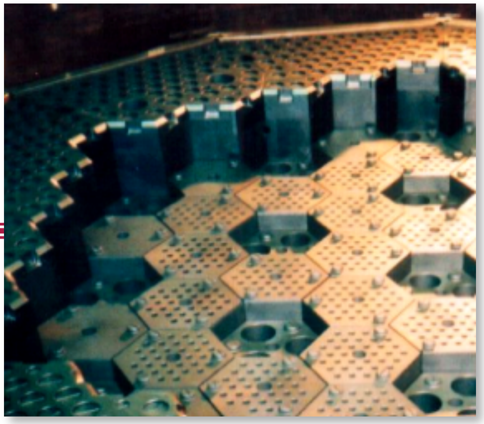
Fuel concept is same for block or pebble bed



PARTICLES

COMPACTS

FUEL BLOCK

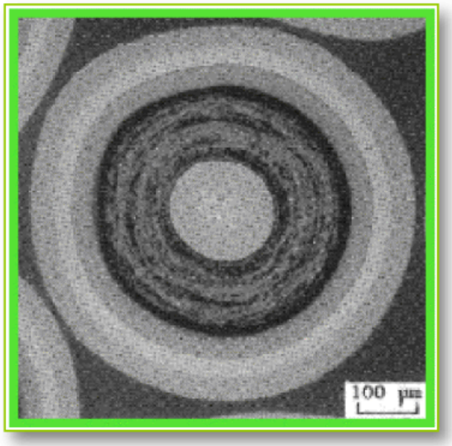


CORE

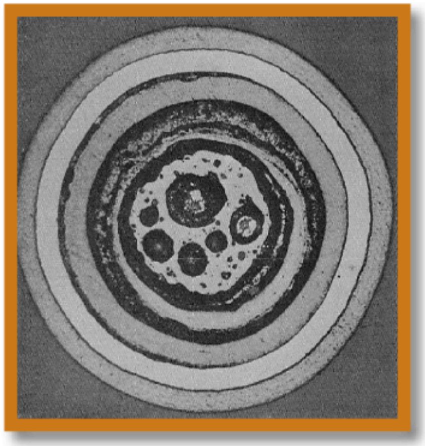
(From INL)

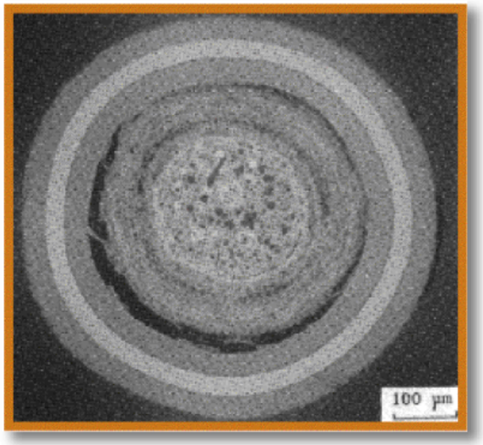
TRISO Coated Fuel Particles - Burnup

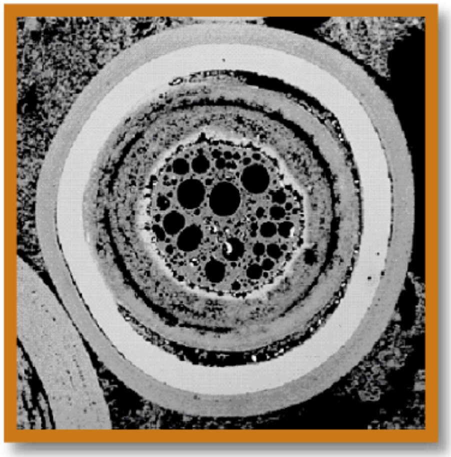
Fresh TRISO Fuel

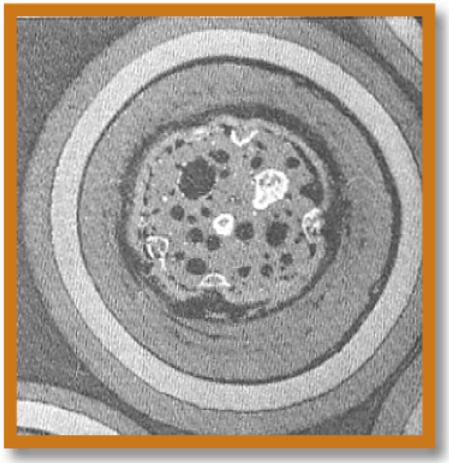


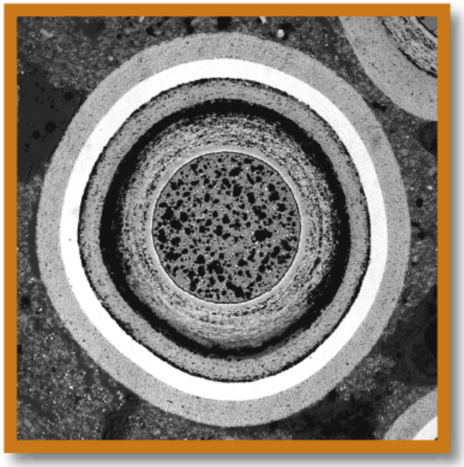
Very High Burnup











TRISO Fuel

- Fission product gases trapped within the layers of coatings

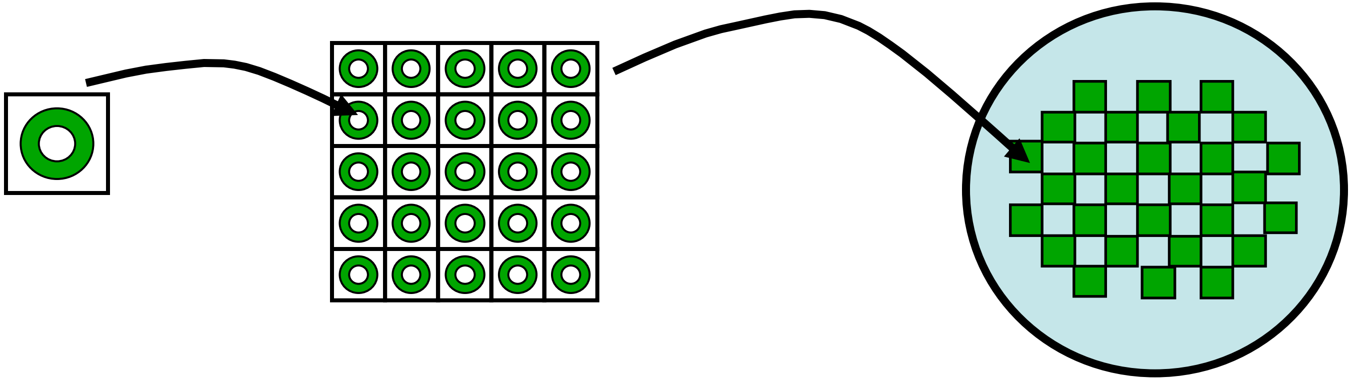
- Coatings remain intact, even with very high burnup

(From General Atomics)

HTGR Modeling With MCNP5

Embedded Geometry - Universes

- In most real-world applications, there is a need for modeling detailed geometry with many repeating units



- All production Monte Carlo codes provide capabilities for multiple levels of nested geometry
  - Called universes & lattices in MCNP
  - A collection of cells may be grouped into a universe
  - Universe may be embedded in another cell,
    with the universe 'clipped' by the cell boundaries

Prismatic HTGR

Plukiene, R. and Ridikas, D., Modelling of HTRs with Monte Carlo: from a homogeneous to an exact heterogeneous core with microparticles. Annals of Nuclear Energy 30, 1573-1585 (2003).

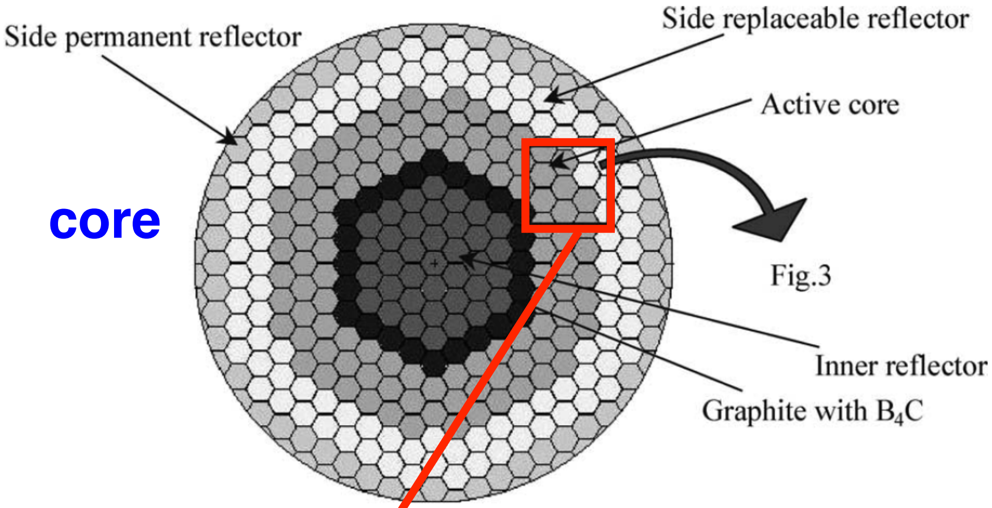


Fig. 2. A cross-section of the GT-MHR homogeneous core with hexagonal structure (HTR1).

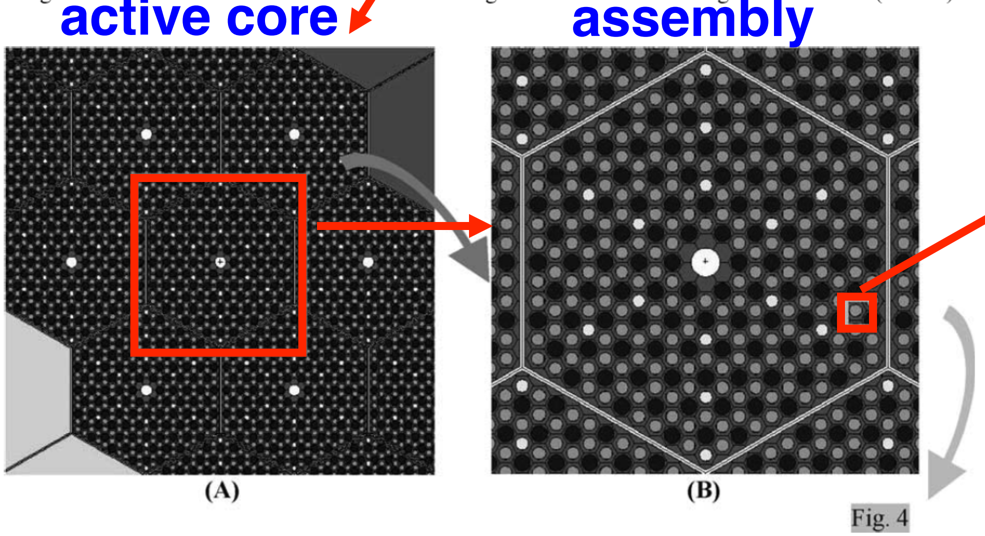


Fig. 3. Fragments of single-heterogeneous GT-MHR (HTR2): (A) an active core structure: three rings of hexagonal fuel columns; (B) magnified view of a separate fuel assembly. Fuel compacts are presented in small grey circles, burnable poison compacts in light grey. Bigger diameter holes stand for He channels, while the rest material represents the graphite matrix.

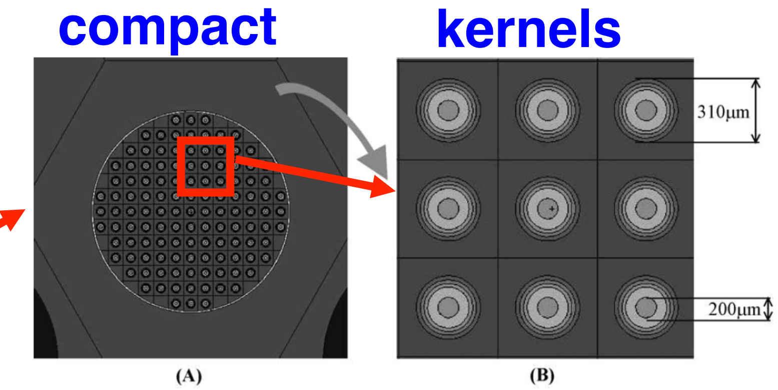


Fig. 4. Fragments of double-heterogeneous GT-MHR (HTR3): (A) fuel element (compact) cross section with coated fuel particles; (B) magnified view of coated fuel particles: spherical kernels of PuO_{2-x} are surrounded by protective coatings made of PyC_{buffer}, PyC I, SiC and PyC II layers correspondingly. The same structure is valid for particles containing burnable poison—natural Er_2O_3.

Pebble Bed HTGR

Core

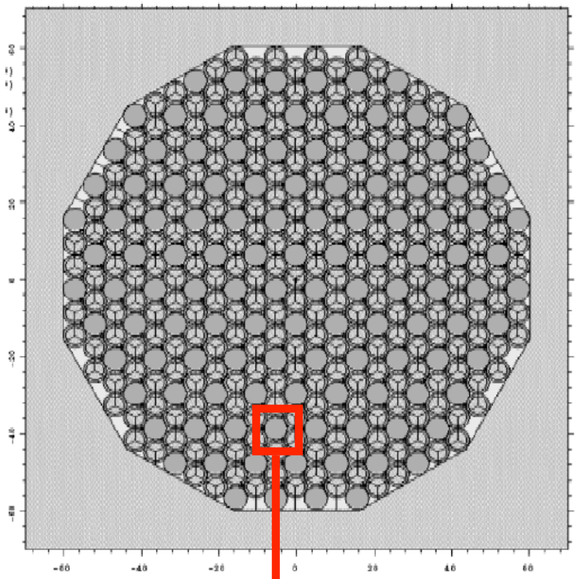


Fig. 3. Cross section of the odd layers of the hcp configurations, case 4 with polyethylene rods. The fi
with the visualization tools of the MCNP program.

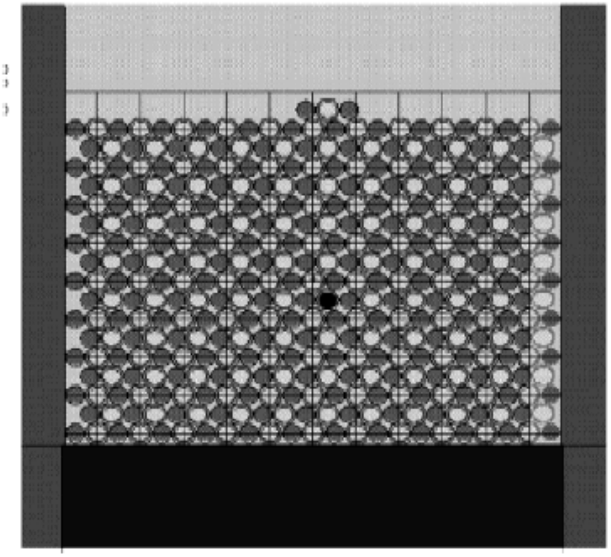


Fig. 5. Case 4, vertical cross section. The black pebble (fuel type) appears magnified in Figs. 6, 7, and 8 to show the heterogeneous details of the fuel pebble.

Difilippo, F.C., Monte Carlo Calculations of Pebble Bed Benchmark Configurations of the PROTEUS Facility. Nucl. Sci. Eng. 143, 240-253 (2003).

Pebbles

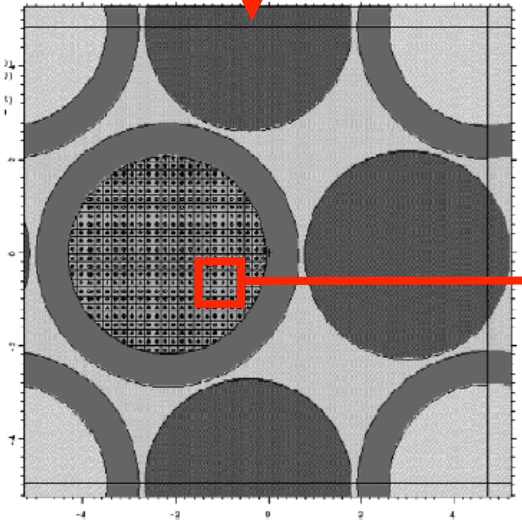


Fig. 6. Magnified fuel pebble of Fig. 5.

Fuel kernel lattice

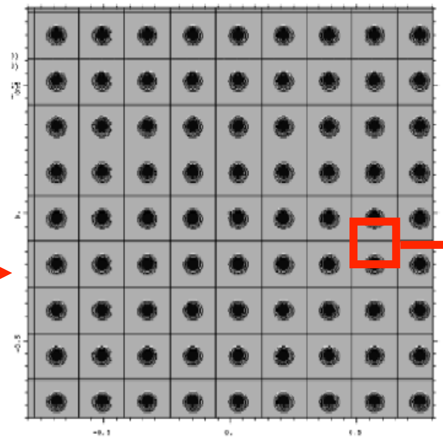


Fig. 7. Details of the cubic lattice of fuel kernels inside the pebble of Fig. 5.

Fuel kernel

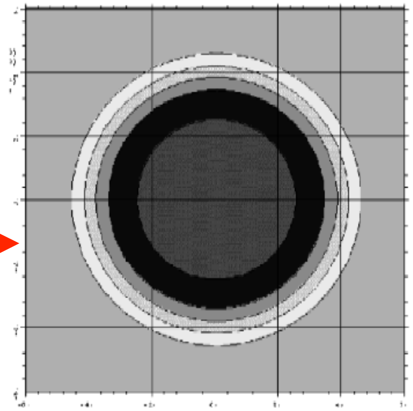
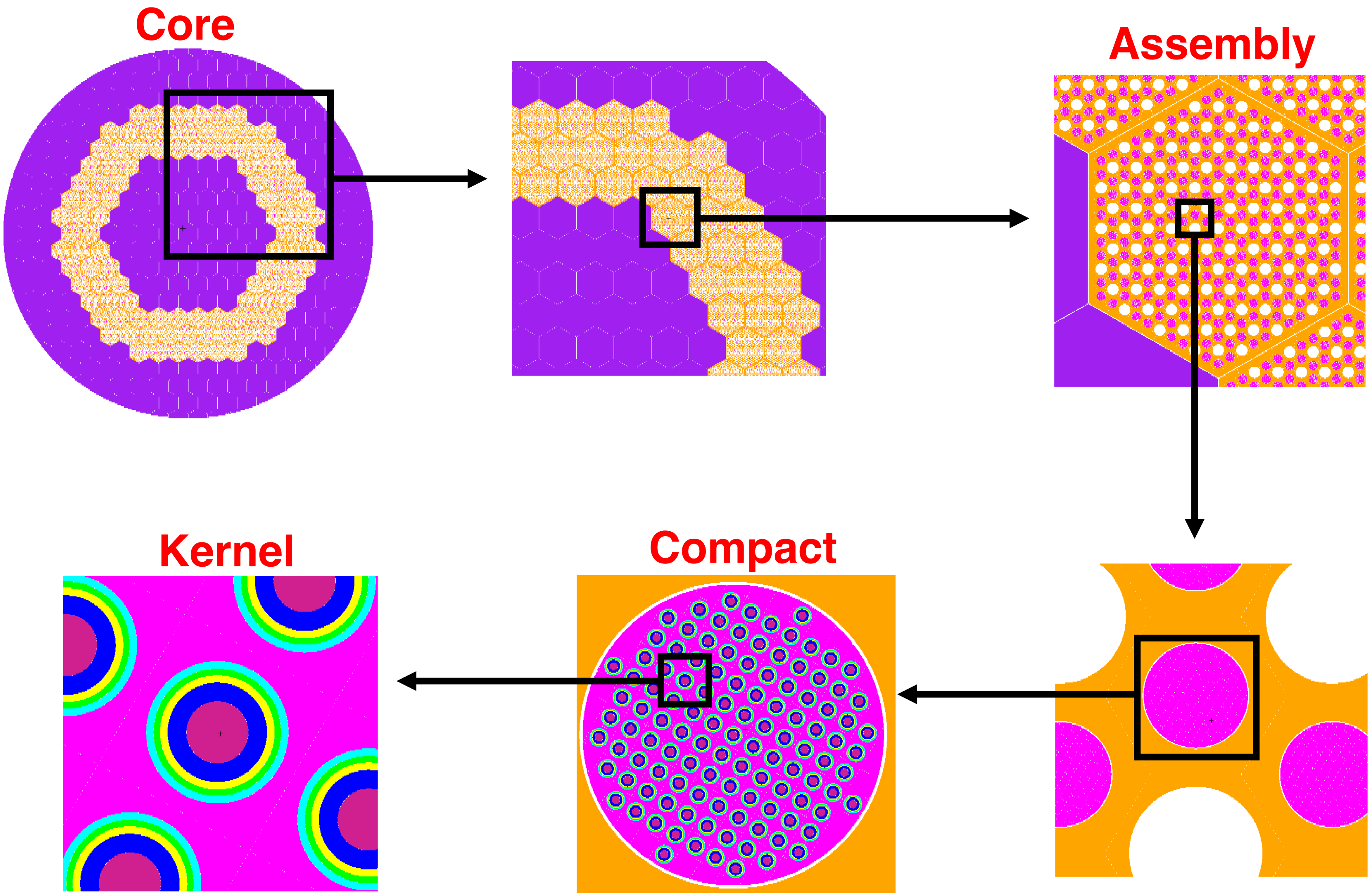


Fig. 8. Fuel kernel with the four coatings at each location of the cubic lattice and inside the fuel region of the pebble shown in Fig. 6.

Very High Temperature Gas-cooled Reactor



MCNP5
Stochastic Geometry

MCNP Models for HTGRs

- Existing MCNP geometry can handle:
  - **3D description of core**
  - **Fuel compacts or lattice of pebbles**
    - Typically, **hexagonal lattice** with close-packing of spherical pebbles
    - Proteus experiments: ~ 5,000 fuel pebbles
~ 2,500 moderator pebbles
  - **Lattice of fuel kernels within compact or pebble**
    - Typically, **cubic lattice** with kernel at center of lattice element
    - Proteus experiments: ~ 10,000 fuel kernels per pebble
~ 50 M fuel kernels, total
  - **Could introduce random variations in locations of a few thousand cells in MCNP input, but not a few million.**
  - **See papers by: Difilipo, Plukiene et al, Ji-Conlin-Martin-Lee, etc.**

MCNP5 Stochastic Geometry

- When a neutron enters a new lattice element, a transformation is made to the neutron's position & direction to the local coordinates of the universe embedded in that lattice element. [standard MCNP]

- Users can flag selected universes as "stochastic" [new]
  – A neutron entering a lattice element containing a stochastic universe undergoes the normal transformations.

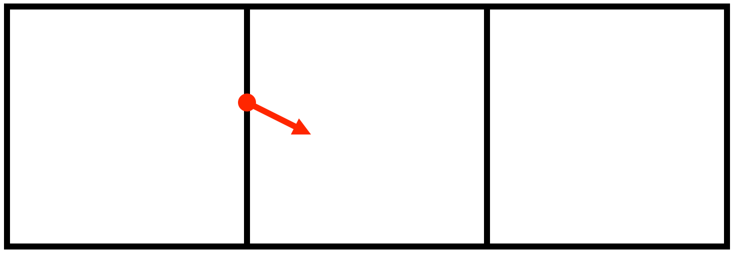
  – Then, additional random translations are made:

$$x \leftarrow x + (2\xi_1 - 1) \cdot \delta_x$$
$$y \leftarrow y + (2\xi_2 - 1) \cdot \delta_y$$
$$z \leftarrow z + (2\xi_3 - 1) \cdot \delta_z$$

  – Then, tracking proceeds normally, with the universe coordinates fixed until the neutron exits that lattice element

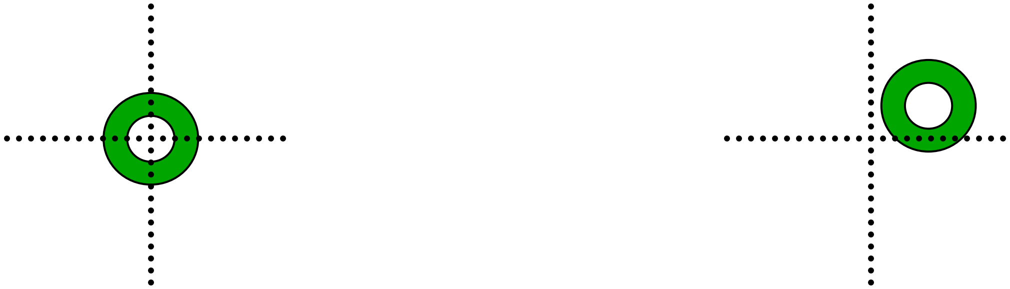
MCNP5 Stochastic Geometry

- **Neutron on lattice edge, about to enter embedded universe**

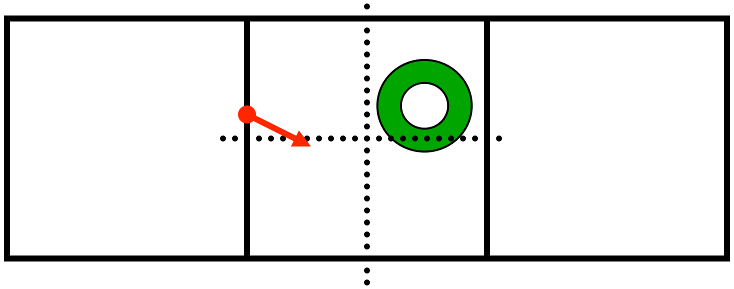


- **Embedded universe,**

before **random translation** after **random translation**



- **Track normally, until neutron exits the lattice element**

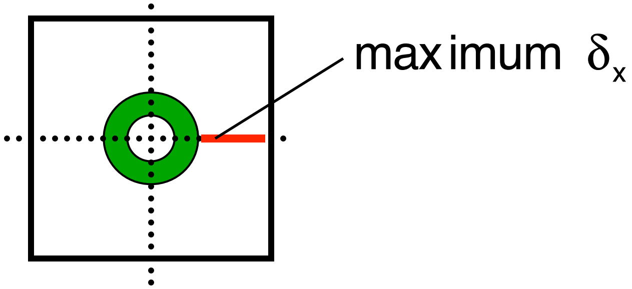


MCNP5 Stochastic Geometry

- On-the-fly random translations of embedded universes in lattice
  - Does not require any extra memory storage
  - Very little extra computing cost -
    only 3 random numbers for each entry into a stochastic universe

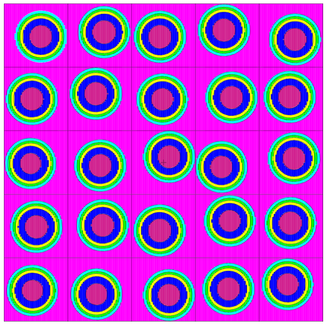
- For K-effective calculations (KCODE problems)
  - If fission occurred within fuel kernel, should have source site in next cycle be at same position within fuel kernel
  - Need to save $\delta_x, \delta_y, \delta_z$ along with neutron coordinates in fission bank
  - On source for next cycle, apply $\delta_x, \delta_y, \delta_z$ after neutron pulled from bank

- To preserve mass exactly, rather than on the average stochastically, must choose $\delta_x, \delta_y, \delta_z$ so that fuel kernels are not displaced out of a lattice element



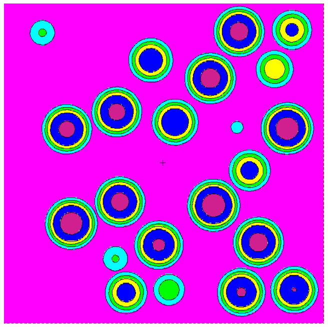
MCNP5 Stochastic Geometry - Testing

- MCNP5 stochastic geometry



Fuel kernels displaced randomly on-the-fly within a lattice element each time that neutron enters

- RSA placement of fuel kernels



Fuel kernels placed randomly in job input, using Random Sequential Addition
Standard MCNP5 - geometry is fixed for entire calculation (Does not use stochastic geometry)

MCNP5 Stochastic Geometry - Testing

MCNP5 Results for Infinite Lattices of Fuel Kernels

Method	K-effective
Fixed lattice with centered spheres	1.1531 ± 0.0004
Fixed lattice with randomly located spheres ("on the fly")	1.1515 ± 0.0004
Multiple (25) realizations of lattice with randomly located spheres	1.1513 ± 0.0004
Multiple (25) realizations of randomly packed (RSA) fuel "box"	1.1510 ± 0.0003

- Small but significant effect from stochastic geometry, -.15% Δk
- New MCNP5 stochastic geometry matches multiple realizations
- New MCNP5 stochastic geometry matches true random (RSA)

HTGR Physics & Modeling

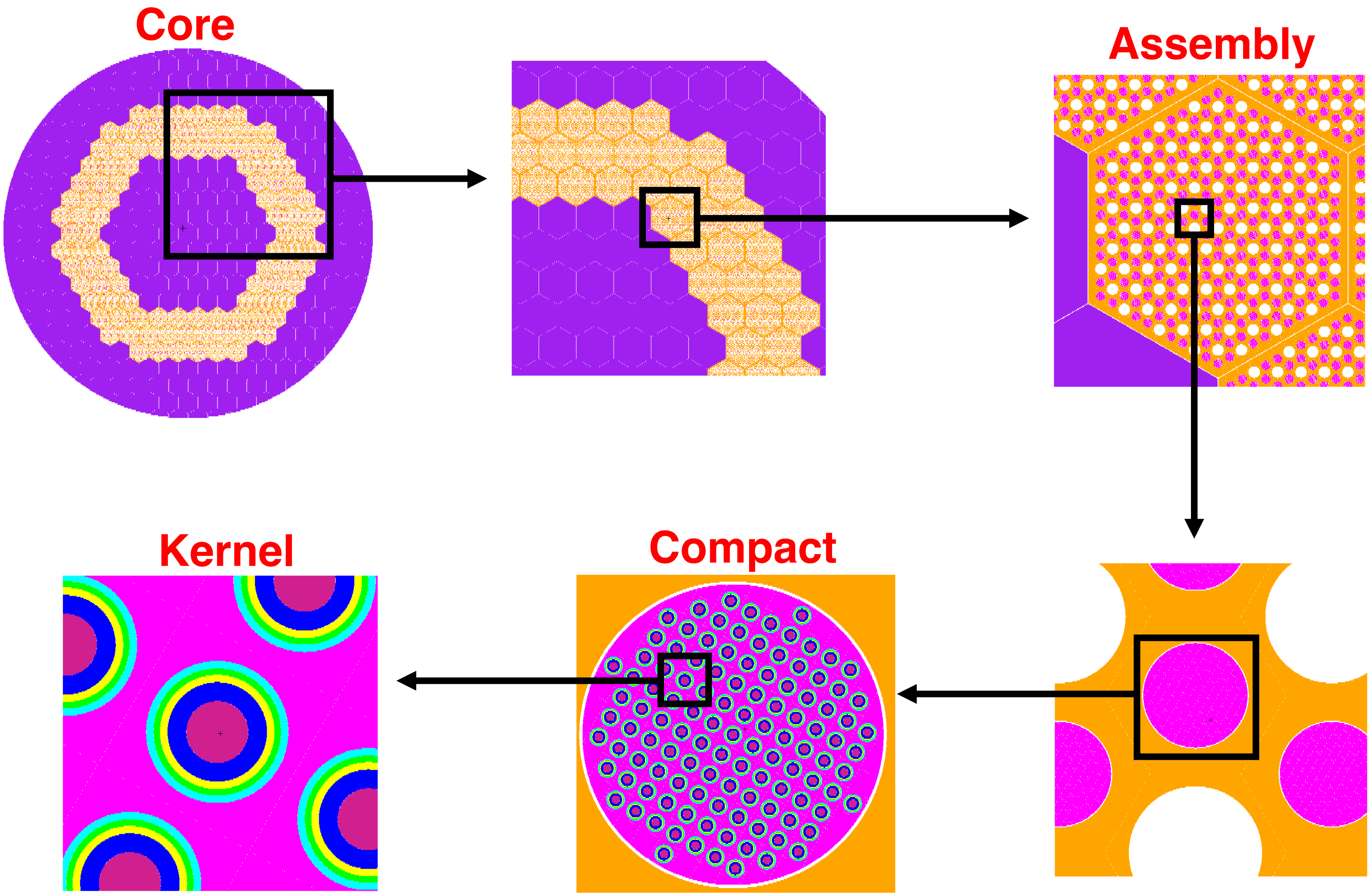
HTGR Modeling with MCNP5

- Modeling HTGR core & assembly geometry is relatively straightforward using standard MCNP5 features

- We have examined in detail some of the fine-points of modeling
  - Fuel kernels embedded in the graphite matrix
    - Lattice arrangements
    - Stochastic effects
  - Compacts or pebbles
    - Embedding a lattice of fuel kernels

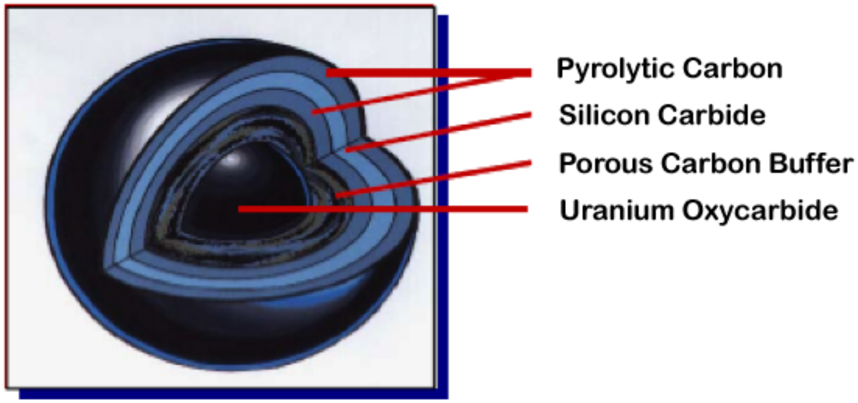
- We have run full-core HTGR calculations to examine the effects of detailed modeling techniques

HTGR Modeling with MCNP5



Fuel Kernels

- **TRISO fuel kernels in graphite matrix**
  - **Fuel kernel geometry & composition taken from the NGNP Point Design (MacDonald et al. 2003)**

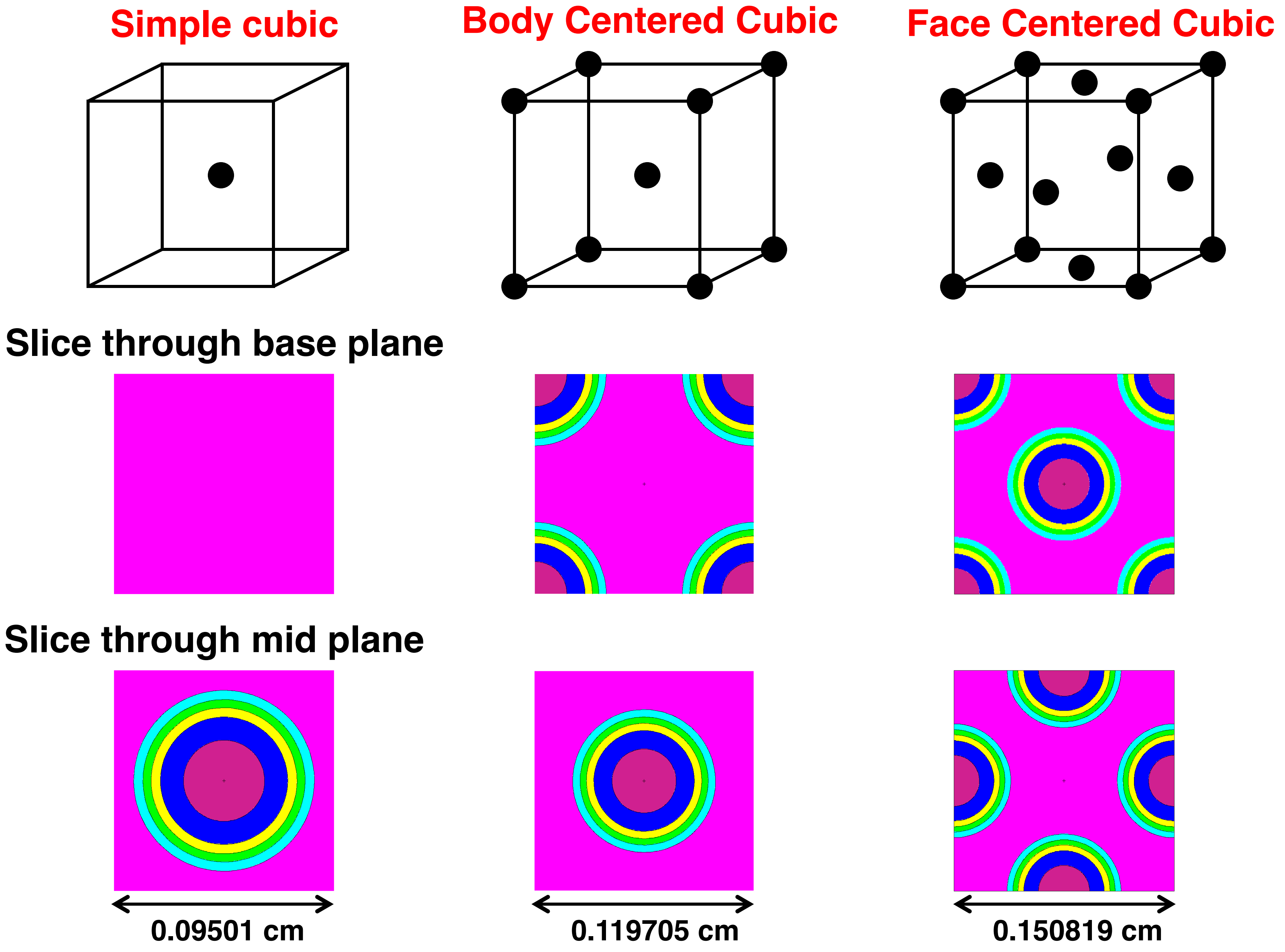


TRISO Fuel Kernel Geometry and Composition

Region #	Name	Outer radius (μ)	Composition	Density (g/cc)
1	Uranium oxycarbide	175	UCO ($UC^{.5}O^{1.5}$)	10.5
2	Porous carbon buffer	275	C	1.0
3	Inner pyrolytic carbon	315	C	1.9
4	Silicon carbide	350	SiC	3.2
5	Outer pyrolytic carbon	390	C	1.9

Fuel kernel packing fraction = .289

Fuel Kernel Modeling - Lattices



Simple cubic

Body Centered Cubic

Face Centered Cubic

Slice through base plane

Slice through mid plane

0.09501 cm

0.119705 cm

0.150819 cm

Fuel Kernel Modeling - Results

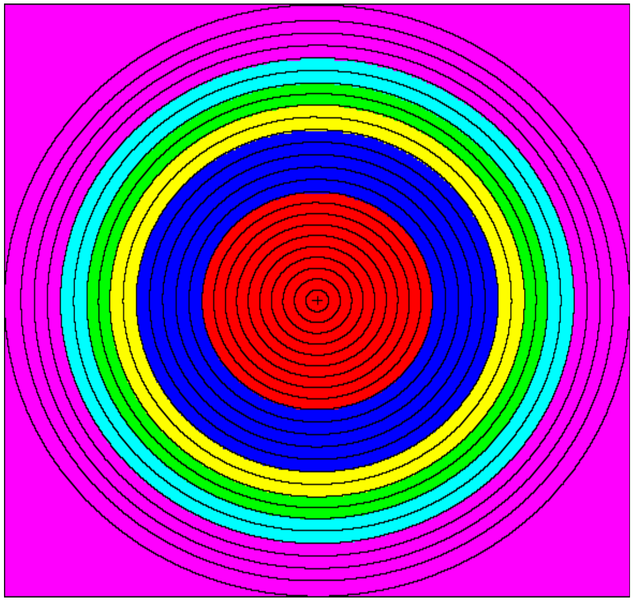
- MCNP5 calculations for infinite geometry, fuel kernels in graphite matrix

Configuration	K-effective ± 1σ
Homogenized matrix & fuel kernel	1.0996 ± .0008
Simple cubic lattice pitch = 0.09501 cm	1.1531 ± .0004
Body centered cubic lattice pitch = 0.119705 cm	1.1534 ± .0003
Face centered cubic lattice pitch = 0.150819 cm	1.1526 ± .0003

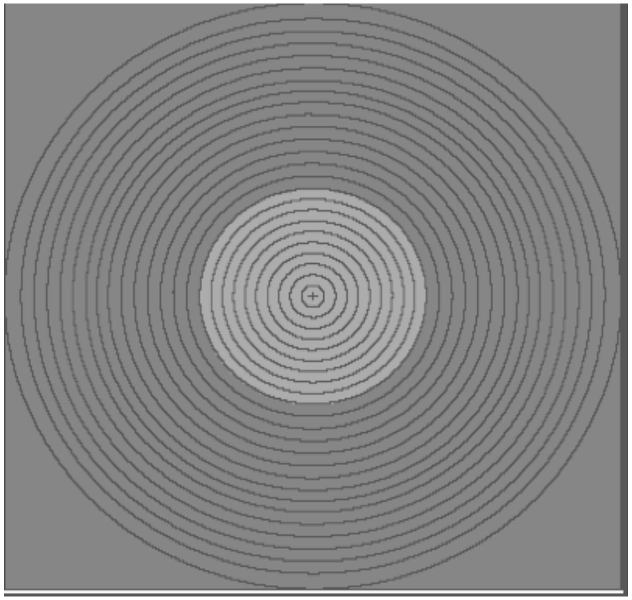
➜ Large errors for homogenized model

➜ Essentially same results for all lattice models

Fuel Kernels - Radial Flux Profiles



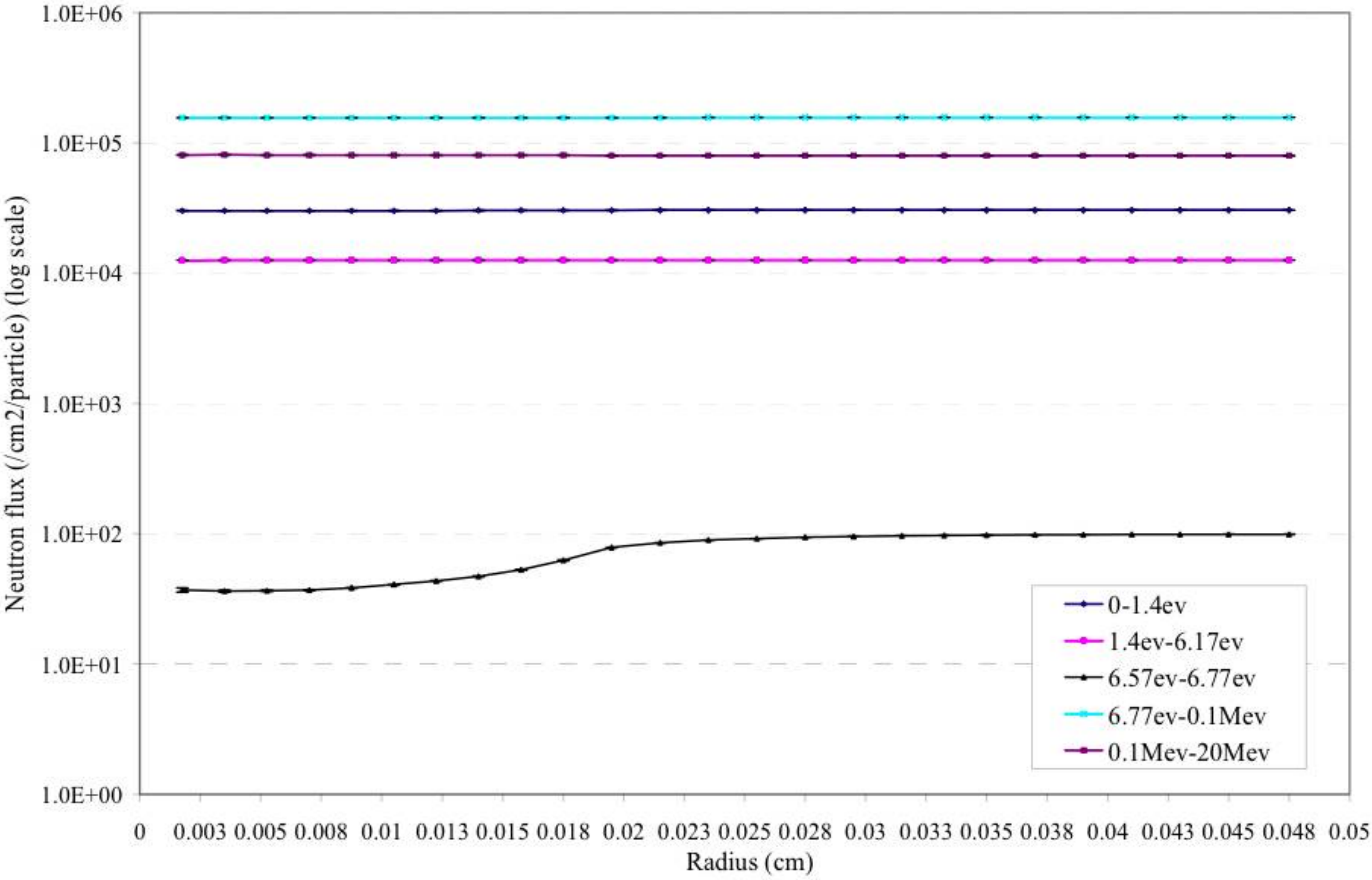
Six-Region Heterogeneous



Two-Region Heterogeneous

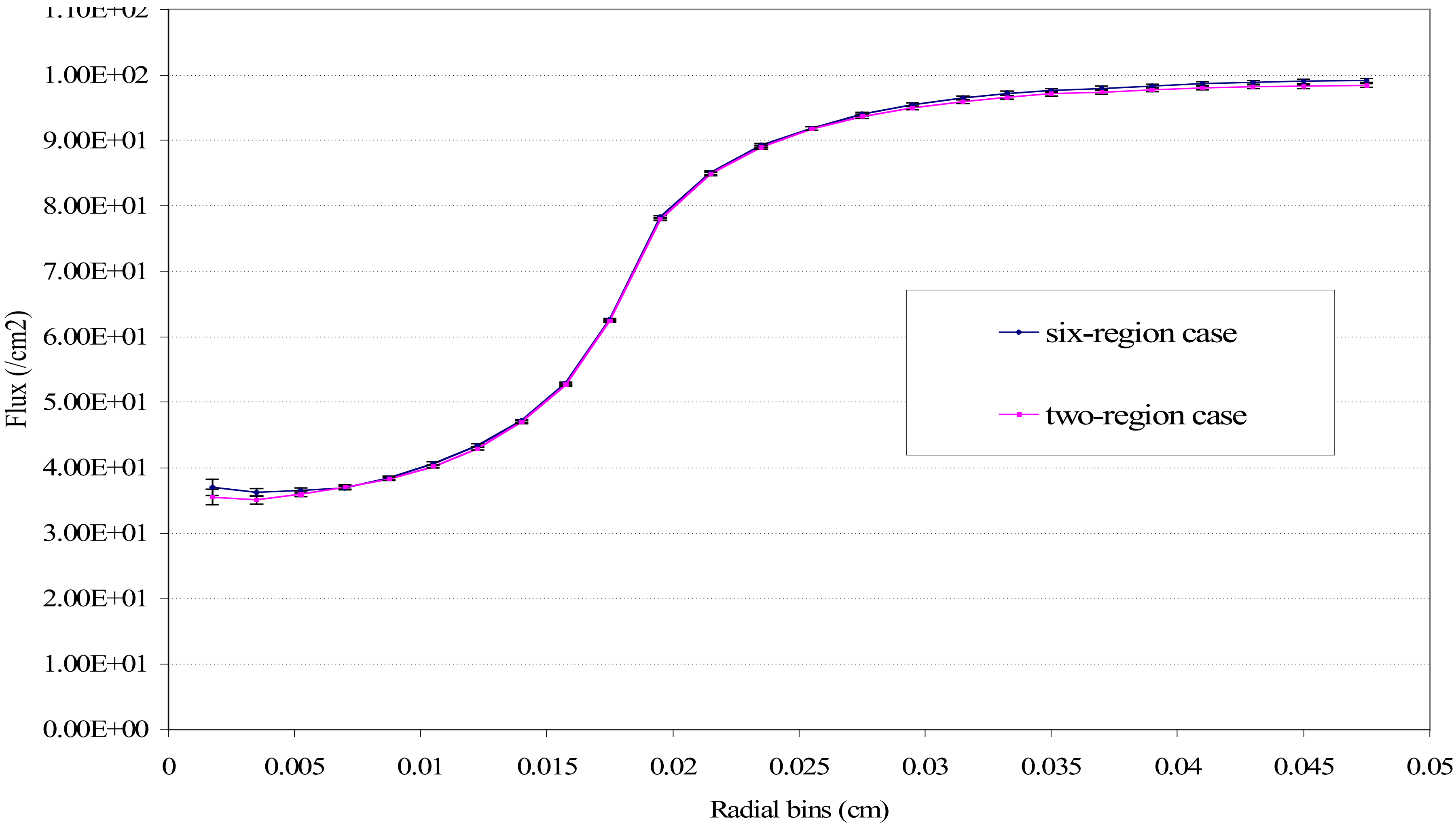
Reflecting b.c. on all sides of cubes

Radial Neutron Flux Profile in 6-region Kernel



Radial Neutron Flux in Resonance Range

- Resonance Energy Range: 6.57eV - 6.77eV



MCNP5 Simulations of Fuel Kernels

Configuration	Kernel location	keff	std dev
Homogeneous microsphere cell	- - -	1.0995	.0004
Two-region heterogeneous microsphere cell	Centered	1.1535	.0004
Six-region heterogeneous microsphere cell	Centered	1.1533	.0003

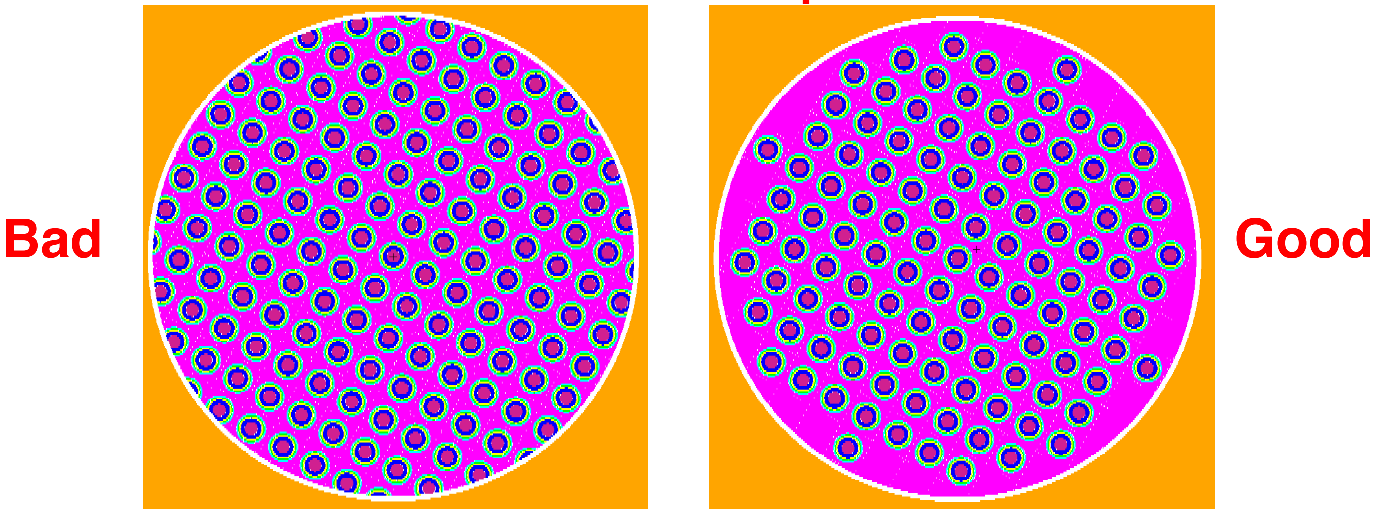
- Essential to model the microsphere heterogeneity
- Homogenizing the coatings into the matrix does not introduce any significant errors, & can reduce model complexity
- Adequate to explicitly represent just the UCO spheres

Compact or Pebble Modeling

- If an infinite lattice of fuel kernels is embedded in a compact or pebble, **clipping** by the enclosing cylinder or sphere results in fragments of kernels. **This is not correct modeling - does not preserve mass**

- **A finite lattice of fuel kernels should be used, so that there are no fragments. Vertical pitch of the lattice should be adjusted to preserve total mass or packing fraction.**

HTGR Fuel Compact



Infinite lattice of kernels, truncated by cylinder

Finite lattice of kernels, no intersections with cylinder

Full-core Calculations

- **Heterogeneous core, with simple cubic** infinite **lattice of kernels** (with partial kernels **at cylinder boundary)**
- **Heterogeneous core, with simple cubic** finite **lattice of kernels** (with no partial kernels **at cylinder boundary)**

Case	Configuration	K-effective ± 1σ
E	Heterogeneous core, with simple cubic fixed infinite lattice (with partial kernels at cylinder boundary)	1.0948 ± .0002
F	Heterogeneous core, with simple cubic fixed finite lattice (with no partial kernels at cylinder boundary)	1.0974 ± .0002

➜ **Correct modeling of compacts, using a finite lattice to avoid partial kernels at boundary, is important**

Full-core Calculations

- **Heterogeneous core, simple cubic infinite lattice**
- **Heterogeneous core, simple cubic infinite lattice, with new MCNP5** stochastic **geometry**

Case	Configuration	K-effective ± 1σ
F	Heterogeneous core, with simple cubic fixed finite lattice (with no partial kernels at cylinder boundary)	1.0974 ± .0002
G	New MCNP5 stochastic geometry, on-the-fly random location of kernels within simple cubic finite lattice elements (with no partial kernels at cylinder boundary)	1.0968 ± .0002

➜ Stochastic effects are small for full-core calculations, may or may not be important

Conclusions

- The new stochastic geometry treatment for MCNP5 provides an accurate and effective means of modeling the particle heterogeneity in TRISO particle fuel
- Homogenizing the fuel or core introduces very large errors (~8%)
- Double heterogeneity important only in resonance energy range
  - Increased resonance self-shielding due to "particle shadowing".
  - Effect is more pronounced for fuel kernel or compact calculations, and decreases as one goes to full core due to increased moderation hence decreased effect of resonance absorption
- The effect of choosing either centered fixed spheres or randomly located spheres is small
- Can introduce significant errors by using an infinite lattice truncated by compact or pebble (clipped), rather than a finite lattice
- Homogenizing the fuel coatings into the graphite matrix is a reasonable approximation

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- **Z. Karriem, C. Stoker, and F. Reitsma, "MCNP Modeling of HTGR Pebble-Type Fuel,"** ***Proc. Monte Carlo 2000 Conference*****, Lisbon, 841-846 (2000).**
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Coupled Monte Carlo & Thermal-Hydraulics Calculations

From: FB Brown, WR Martin, RD Mosteller, "Monte Carlo - Advances and Challenges",
PHYSOR'08 Monte Carlo Workshop, LA-UR-08-03328 (2008)

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

Accounting for Temperature Effects in MCNP

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.

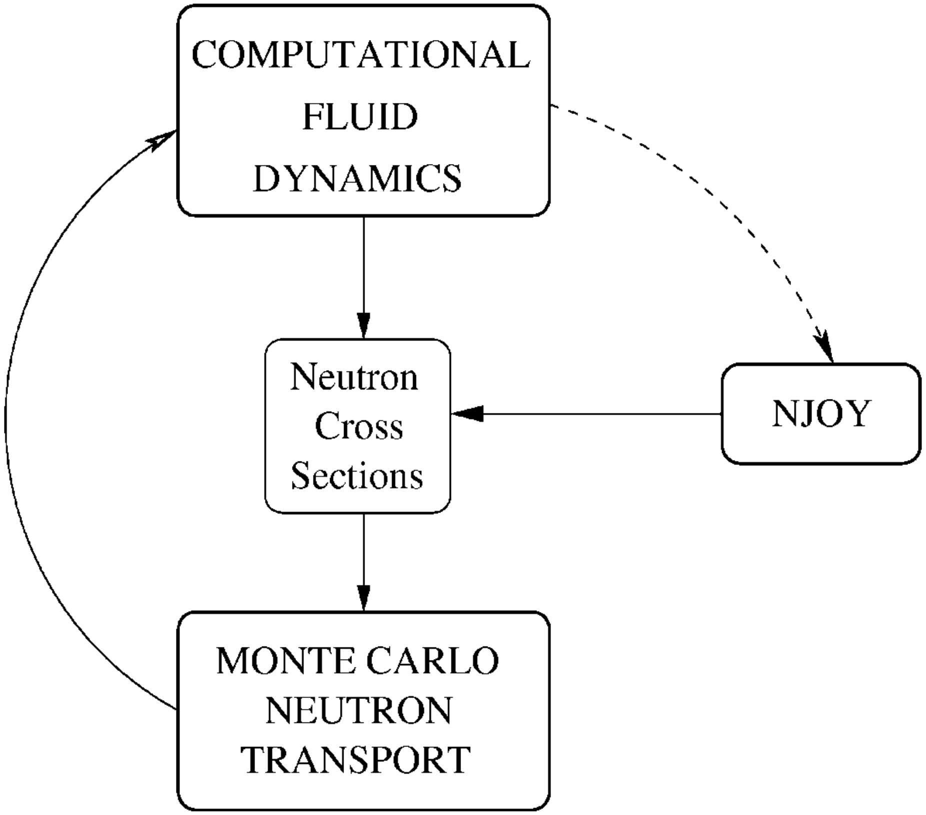
- **Pregenerated NJOY libraries** is a reasonable approach
  - Used to couple STAR-CD and MCNP
  - NJOY was run at 5K temperature increments over the temperature range. (Temperature increments of 1-2 K cause memory problems with MCNP.)
  - A Perl script was used to manage the NTH iterations.
  - The 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**

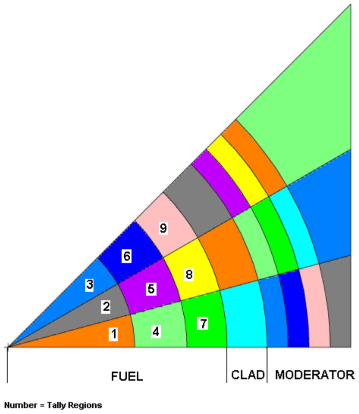
- **Computational Fluid Dynamics : STAR-CD**

- **Cross Sections: NJOY**

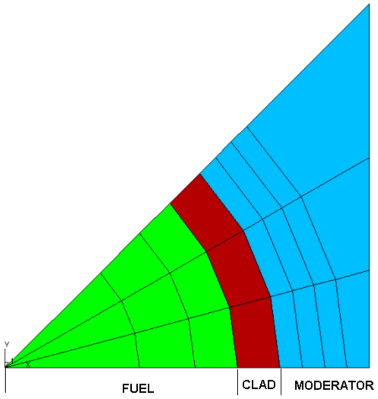


Results: coupled STAR-CD and MCNP results

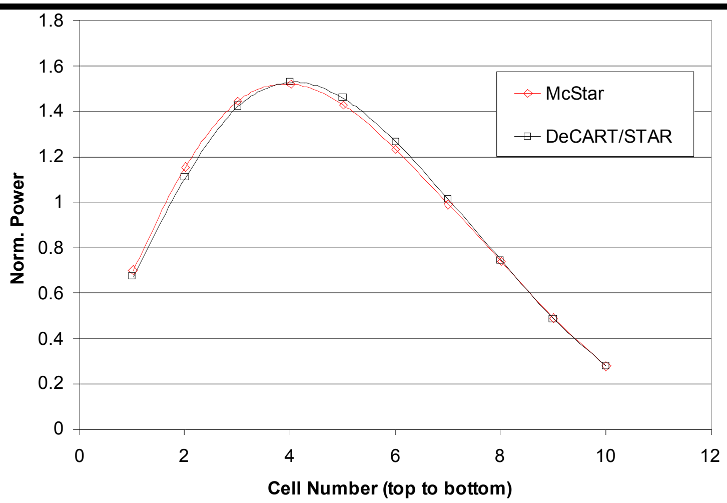
1/8 pin cell



MCNP MODEL

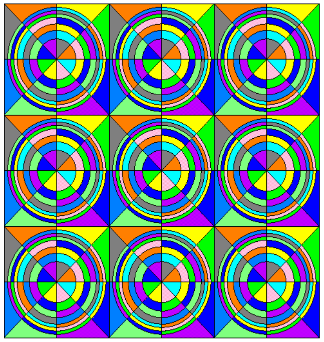


STAR-CD MODEL

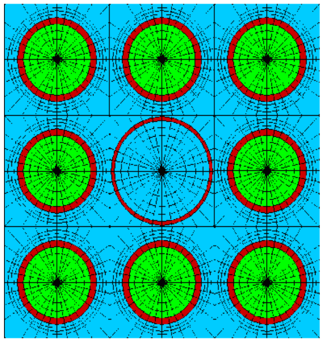


keff agrees within 52 pcm with DeCart/STAR-CD

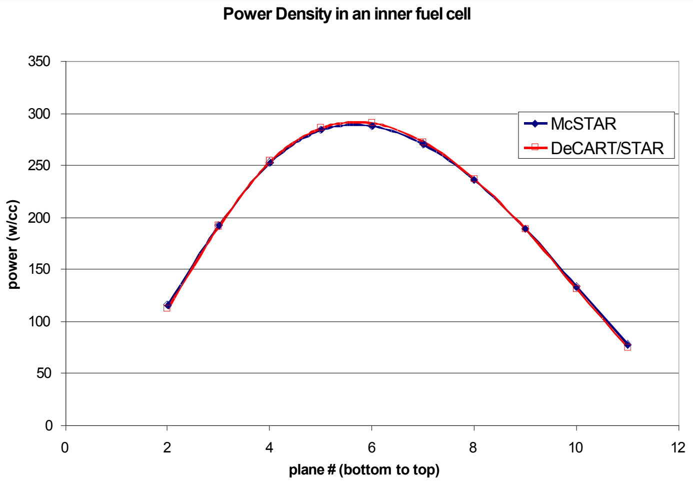
3x3 array of pin cells



•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 MCNP5/1.51 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)

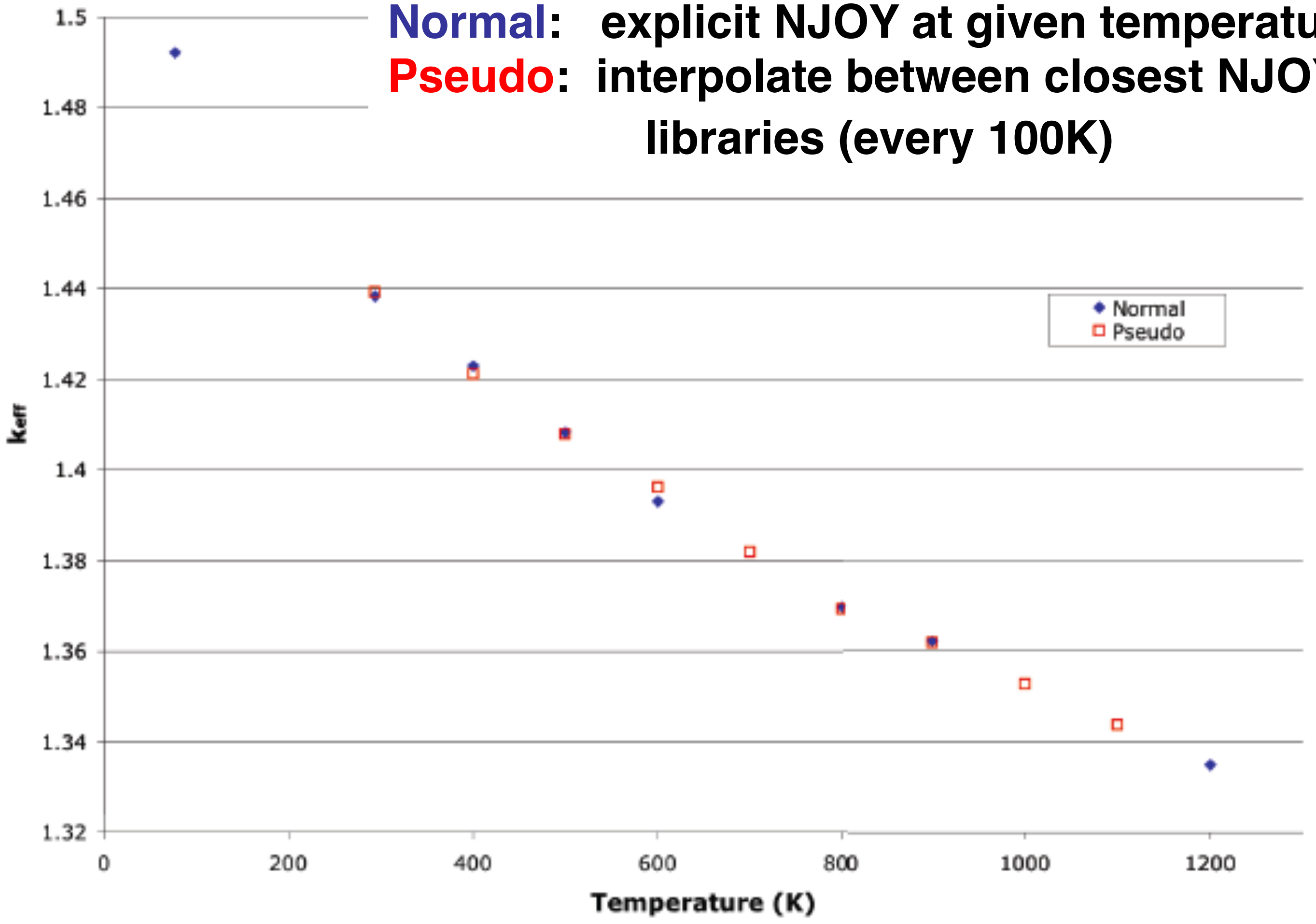


Figure 1. Comparison of k_{eff} between normal and pseudo materials with the VHTGR geometry.

*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
f in Fuel	1.37933 (± 0.0003)	1.37929 (± 0.0003)	0.00003
$s_{aF}f$	3.67362e-03 (± 0.0006)	3.67648E-03 (± 0.0006)	0.0008
$s_f f$	5.62964e-03 (± 0.0007)	5.63817E-03 (± 0.0007)	0.0010
$ns_f f$	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.

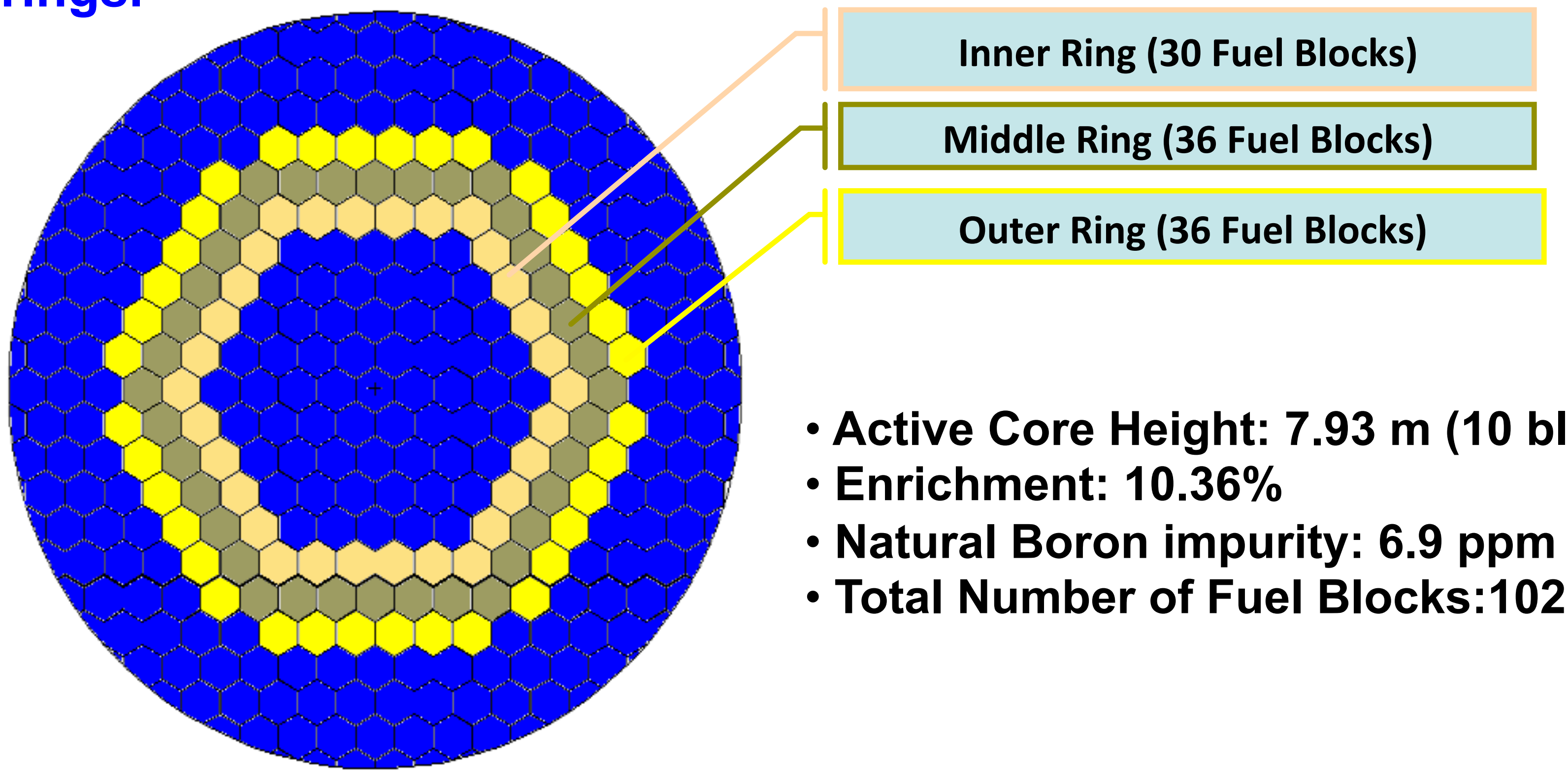
- Updated RELAP5 temperature distributions are used for the next MCNP simulation to obtain updated power fractions. MCNP5 and RELAP5 iterations were performed in a cyclic fashion until convergence in temperature and power distributions were obtained.

- 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.



Inner Ring (30 Fuel Blocks)

Middle Ring (36 Fuel Blocks)

Outer Ring (36 Fuel Blocks)

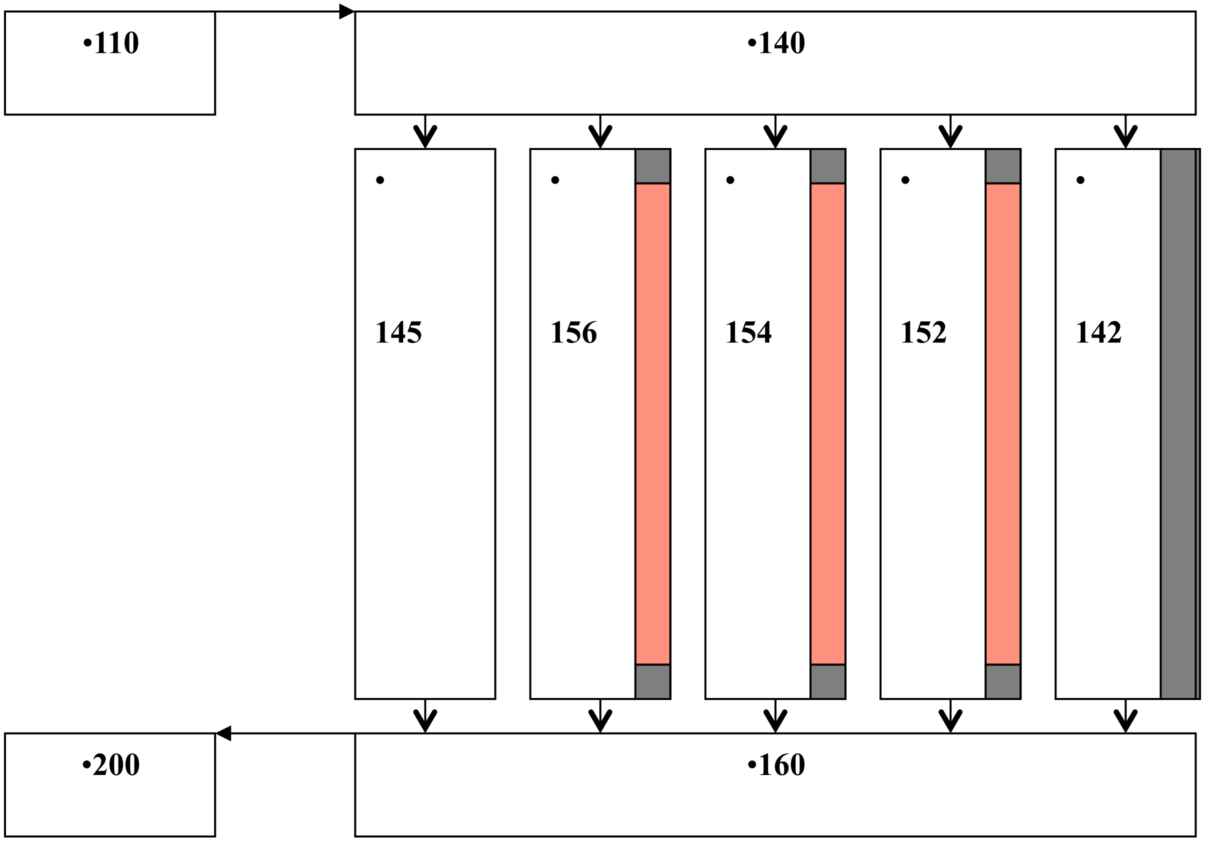
- **Active Core Height: 7.93 m (10 blocks)**
- **Enrichment: 10.36%**
- **Natural Boron impurity: 6.9 ppm**
- **Total Number of Fuel Blocks:1020**

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.

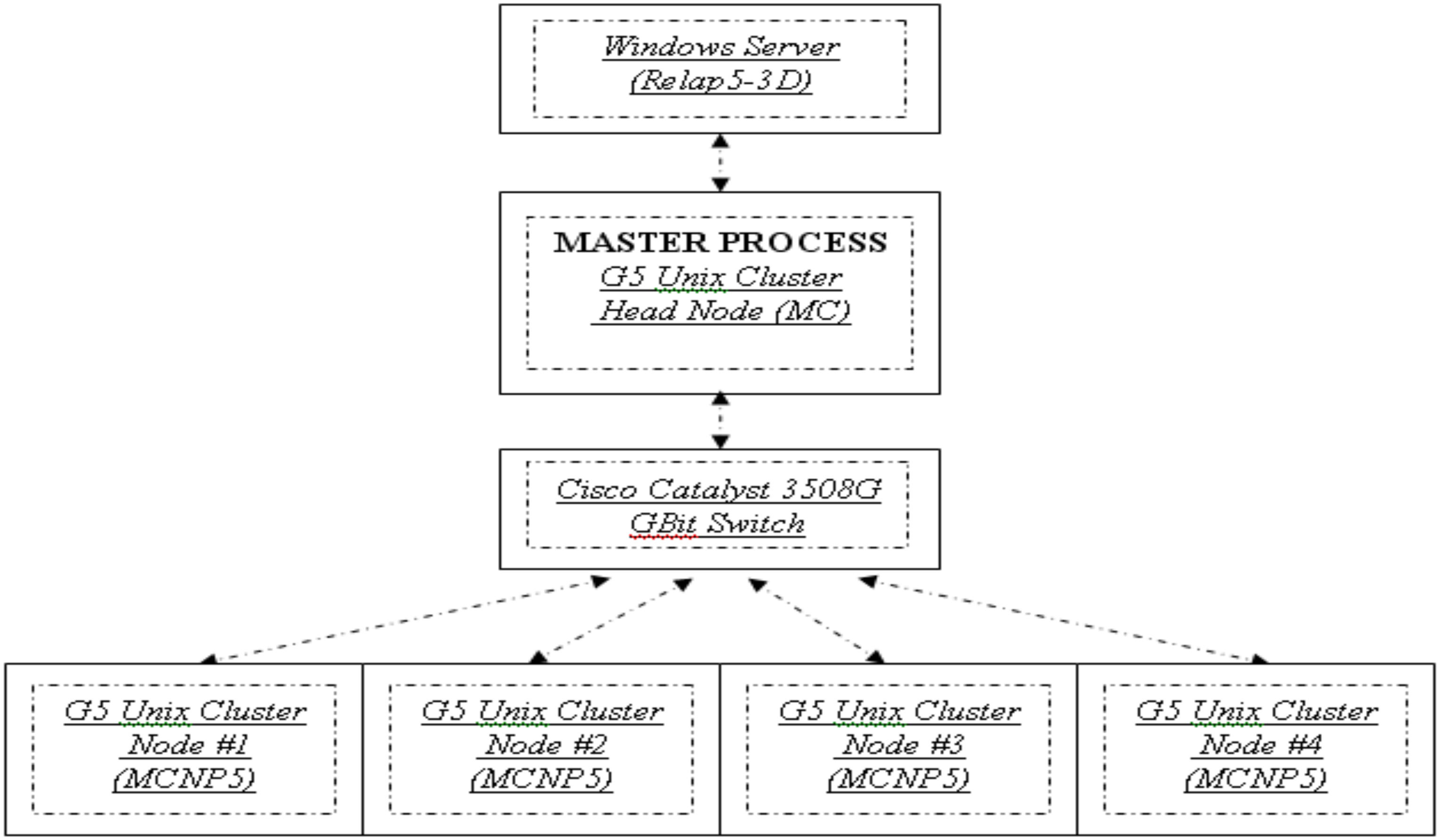
RELAP5 Methodology (cont.)

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.



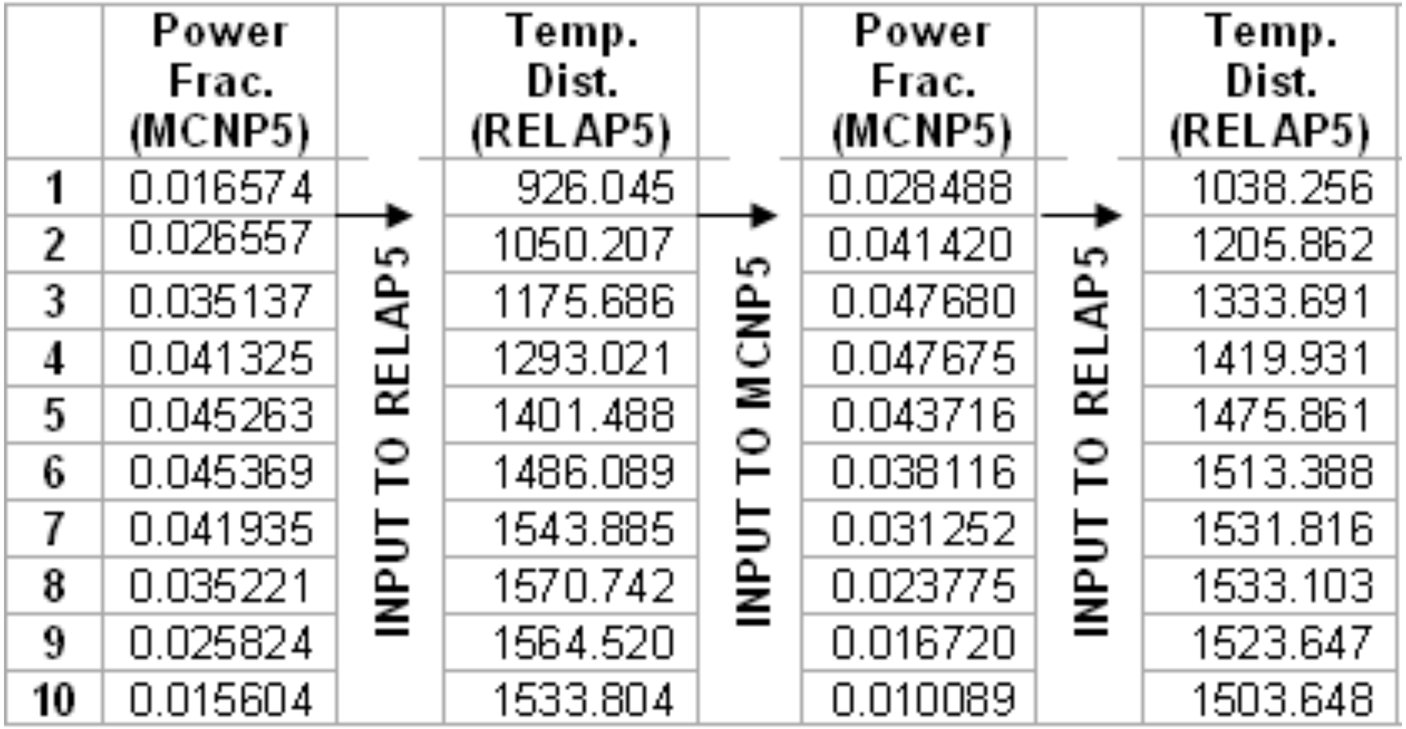
VHTR - Cross Platform NTH Architecture

- 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.



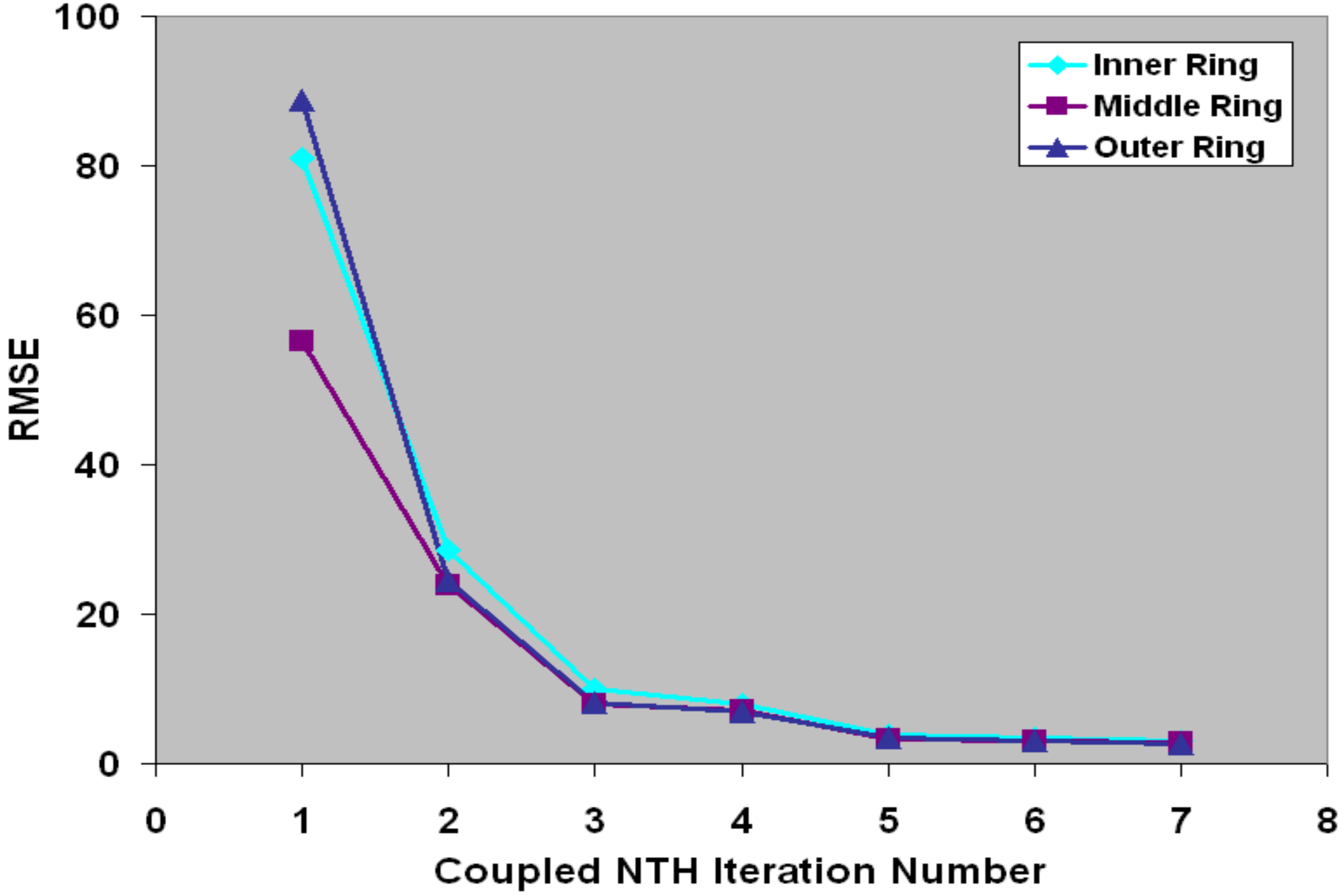
VHTR - NTH Data Communication

- **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.**

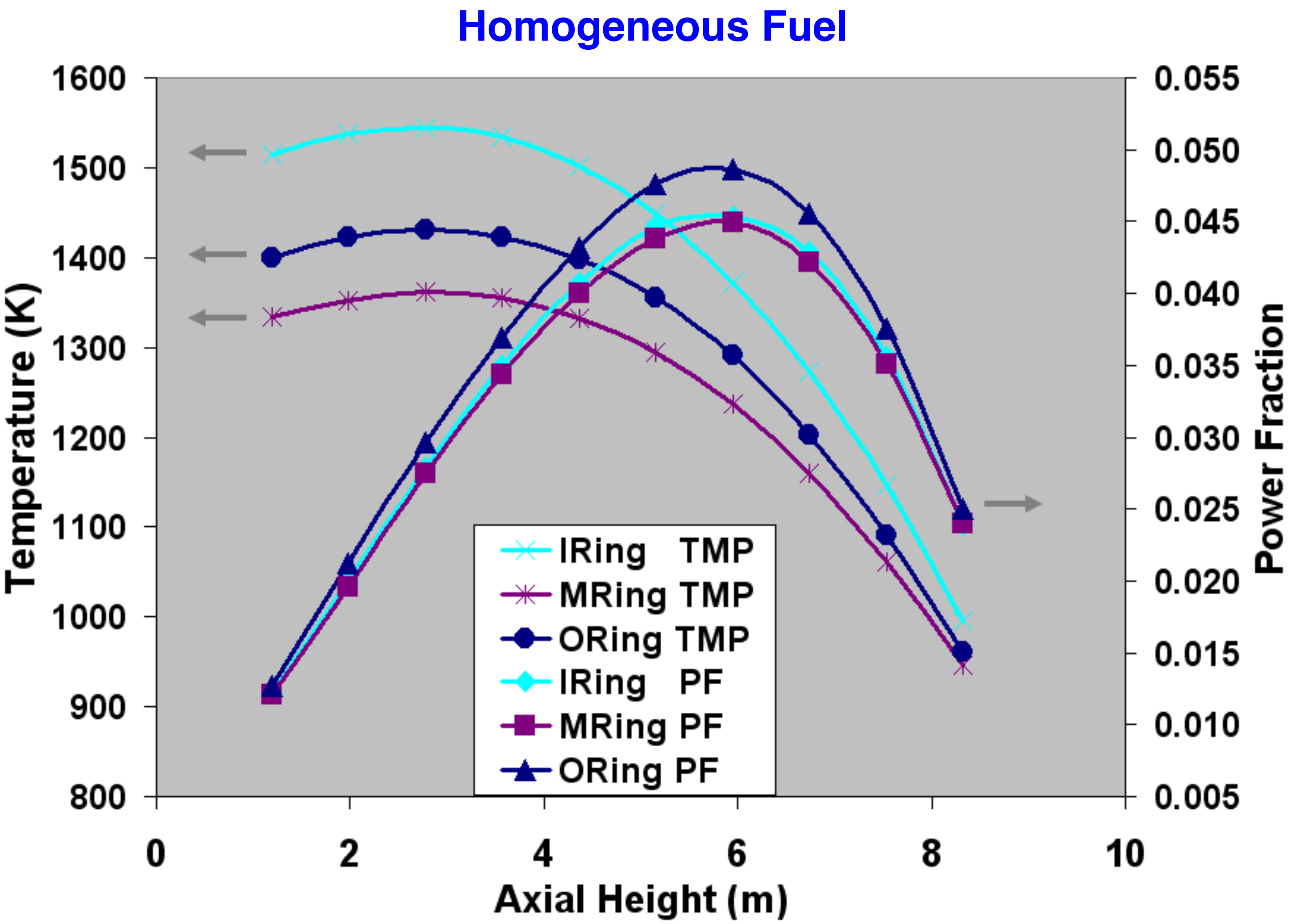


	Power Frac. (MCNP5)		Temp. Dist. (RELAP5)		Power Frac. (MCNP5)		Temp. Dist. (RELAP5)
1	0.016574	→ INPUT TO RELAP5	926.045	→ INPUT TO MCNP5	0.028488	→ INPUT TO RELAP5	1038.256
2	0.026557		1050.207		0.041420		1205.862
3	0.035137		1175.686		0.047680		1333.691
4	0.041325		1293.021		0.047675		1419.931
5	0.045263		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

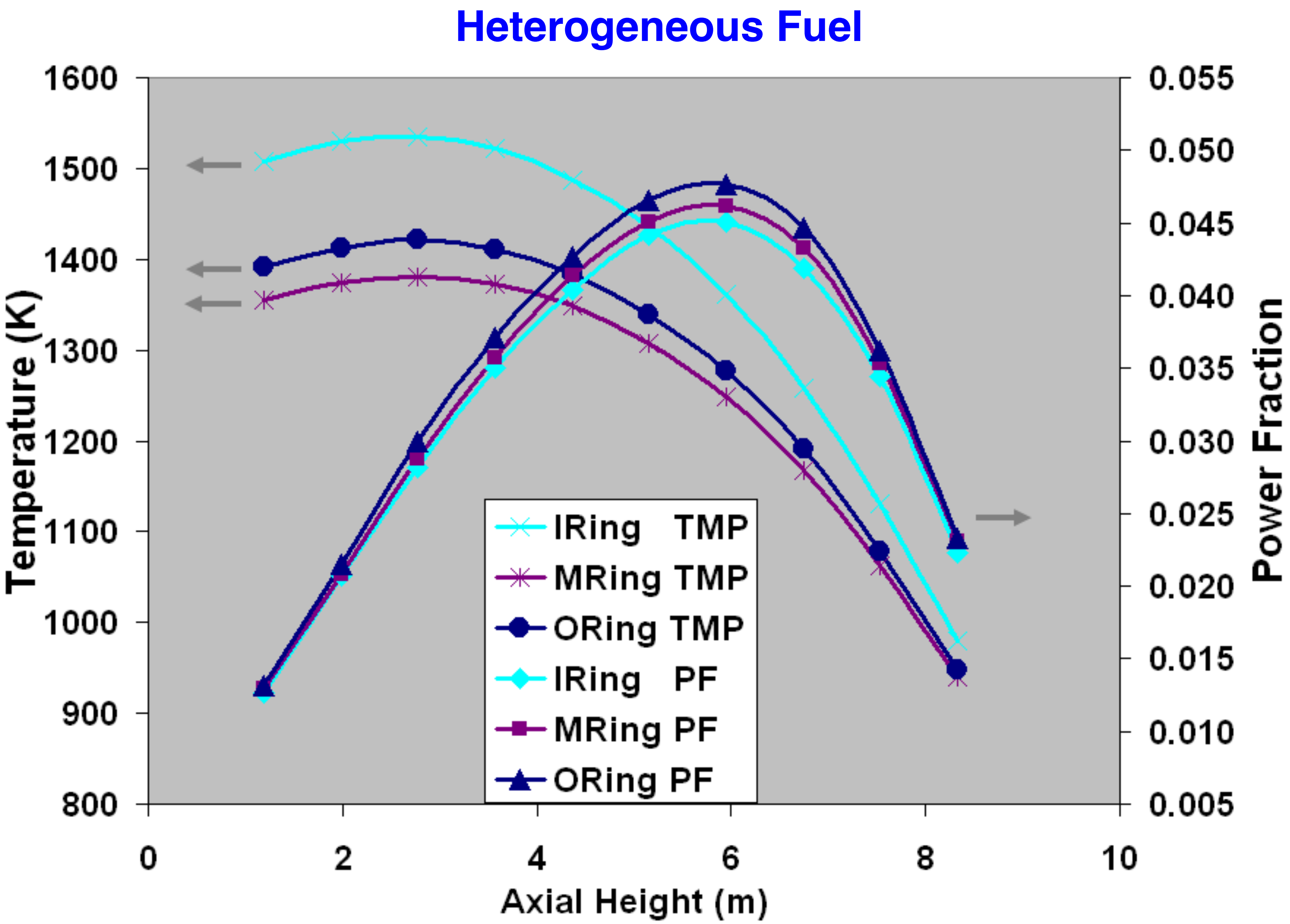
RMS Error in Temperature vs. NTH Iteration



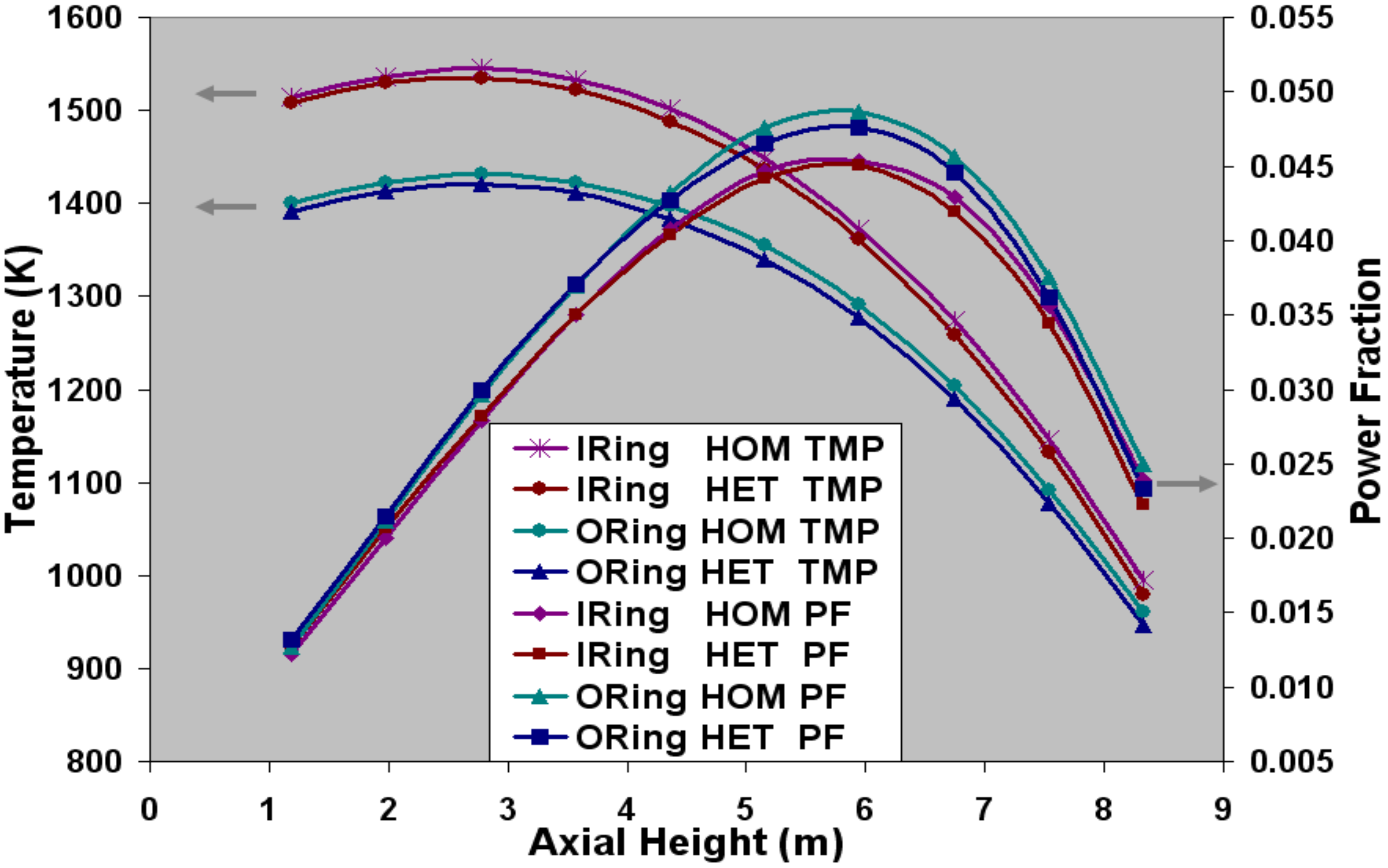
Converged Temperature/Power Distributions



Converged Temperature/Power Distributions



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

From: FB Brown, WR Martin, RD Mosteller, "Monte Carlo - Advances and Challenges",
PHYSOR'08 Monte Carlo Workshop, LA-UR-08-03328 (2008)

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

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- Other contributors, all from the Department of Nuclear Engineering and Radiological Sciences at the University of Michigan, include:
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  - 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 $H(\underline{r})$, where $H(\underline{r})dr$ = amount of energy/s deposited in $d\underline{r}$ about $\underline{r}$ 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 $H(\underline{r})$

- Run multiple MCNP runs to get all contributions to the overall fission energy deposition.

– Prompt gammas (H_{gp}):	F6:p tally with PIKMT card.
– Capture gammas (H_{gc}):	F6:p tally with PIKMT card.
– Delayed gammas (H_{gd}):	Scale H_{gp} by Q_{gd}/Q_{gp}.
– Fission products + neutrons (H_{fn}):	regular F6:n tally.
– Betas (H_b):	Scale regular F7:n tally by Q_b/Q_{F7}, where Q_{F7} = 180.88 MeV for U-235 fuel.

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

$$H(\underline{r}) = H_{fn} + H_{gp} + H_{gc} + H_{gd} + H_b$$

- Scale $H(\underline{r})$ to get correct total power P.

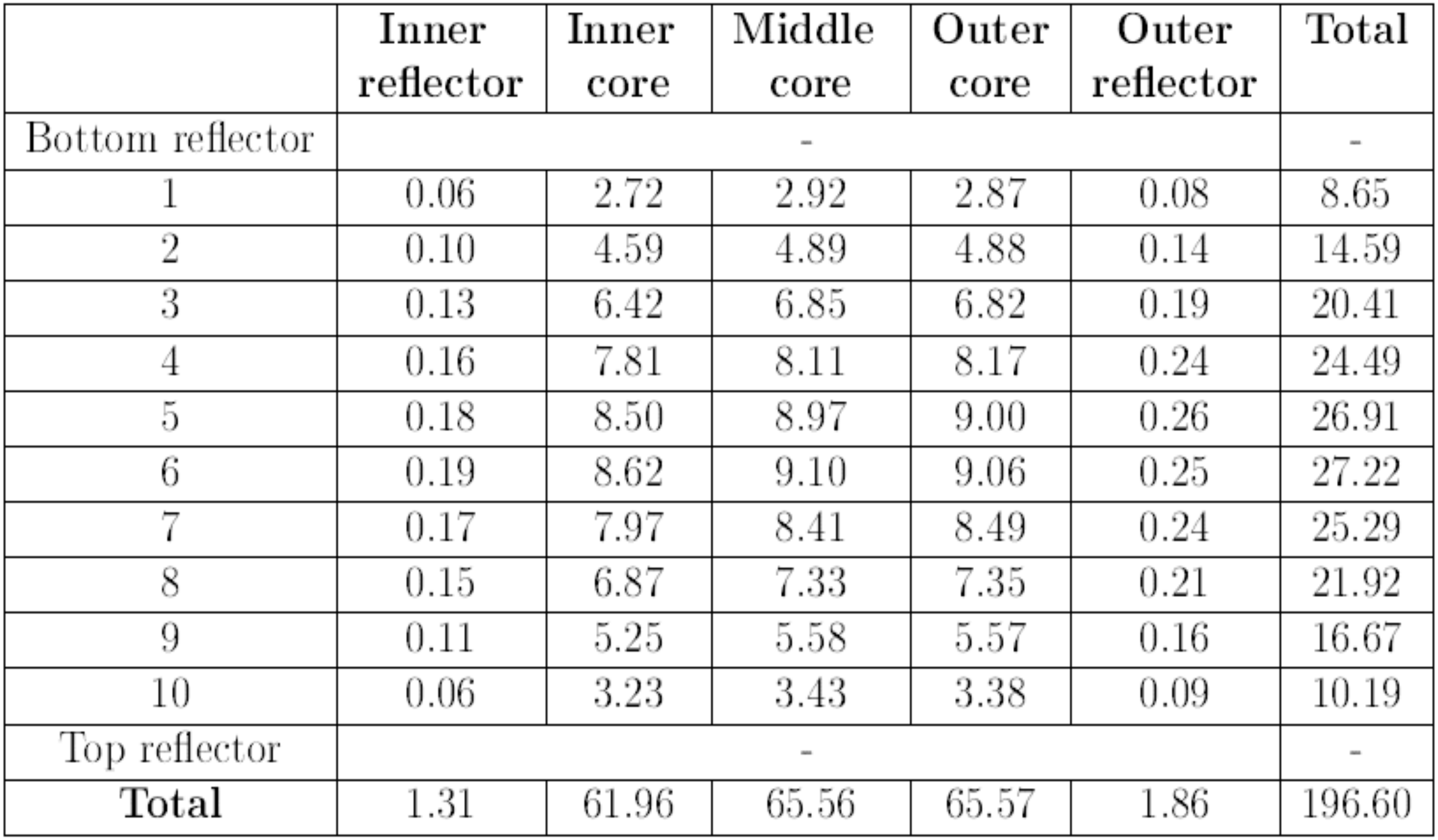
Summary of overall methodology

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)



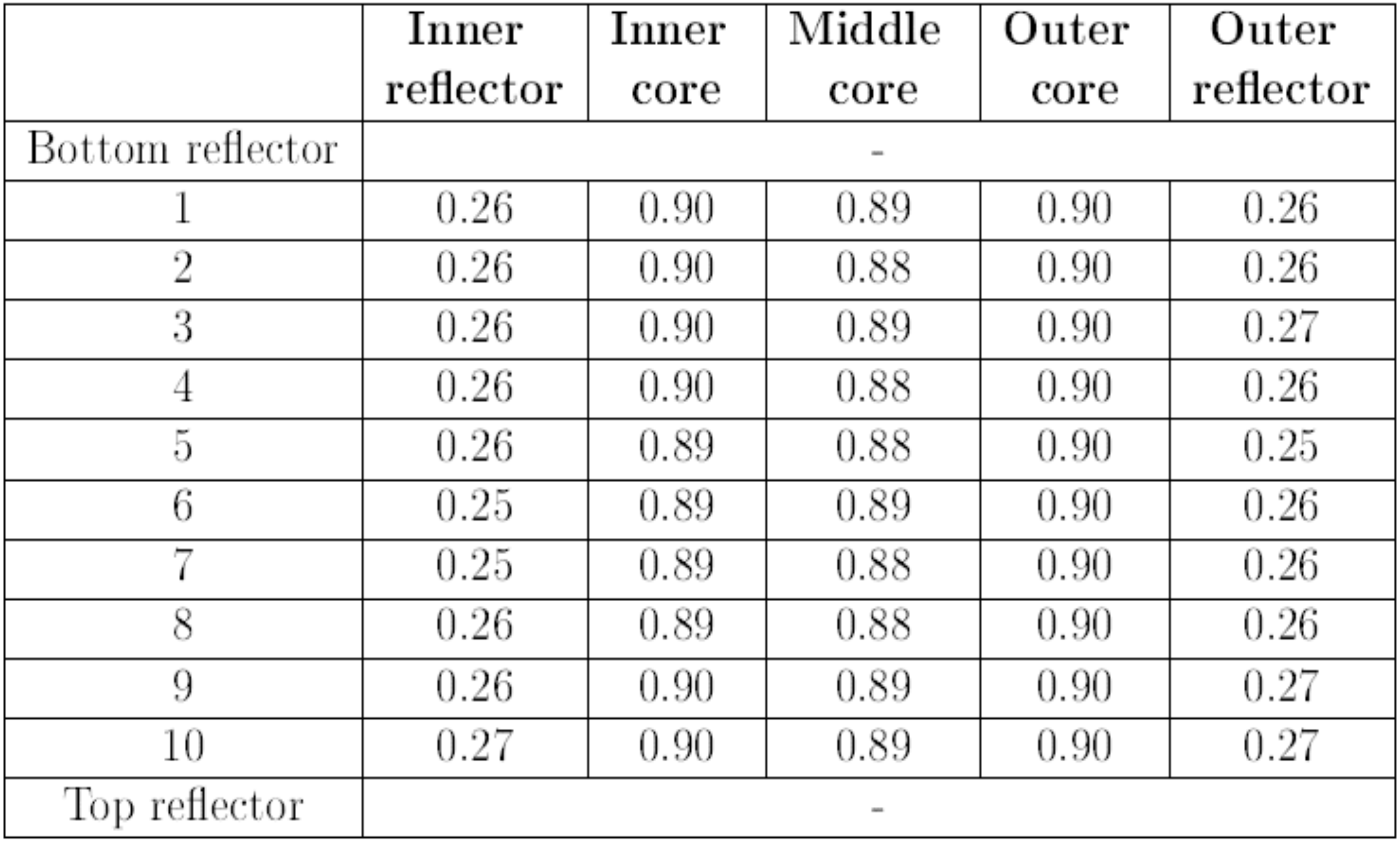
	Inner reflector	Inner core	Middle core	Outer core	Outer reflector	Total
Bottom reflector	-					-
1	0.06	2.72	2.92	2.87	0.08	8.65
2	0.10	4.59	4.89	4.88	0.14	14.59
3	0.13	6.42	6.85	6.82	0.19	20.41
4	0.16	7.81	8.11	8.17	0.24	24.49
5	0.18	8.50	8.97	9.00	0.26	26.91
6	0.19	8.62	9.10	9.06	0.25	27.22
7	0.17	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.