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Title: A Review of Best Practices for Monte Carlo Criticality Calculations

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A Review of Best Practices for Monte Carlo Criticality Calculations

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Monte Carlo Codes, X-3-MCC

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Abstract

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A Review of Best Practices for Monte Carlo Criticality Calculations

Forrest Brown (LANL)

Monte Carlo criticality calculations are performed routinely on large, complex models for reactor physics and criticality safety applications. This talk provides a review of the theory & practice of Monte Carlo criticality calculations, including best practices for assuring convergence, avoiding bias in Keff and tallies, and assessing bias in confidence intervals. Numerous practical examples with MCNP5 are included. It should benefit both Monte Carlo practitioners and developers.

- **Several fundamental problems with the MC solution of k-eigenvalue problems were identified in the 1960s - 1980s:**
  - Convergence of Keff & source distribution
  - Bias in Keff & tallies
  - Underprediction bias in confidence intervals

(see Lieberoth, Gelbard & Prael, Gast & Candelore, Brissenden & Garlick)

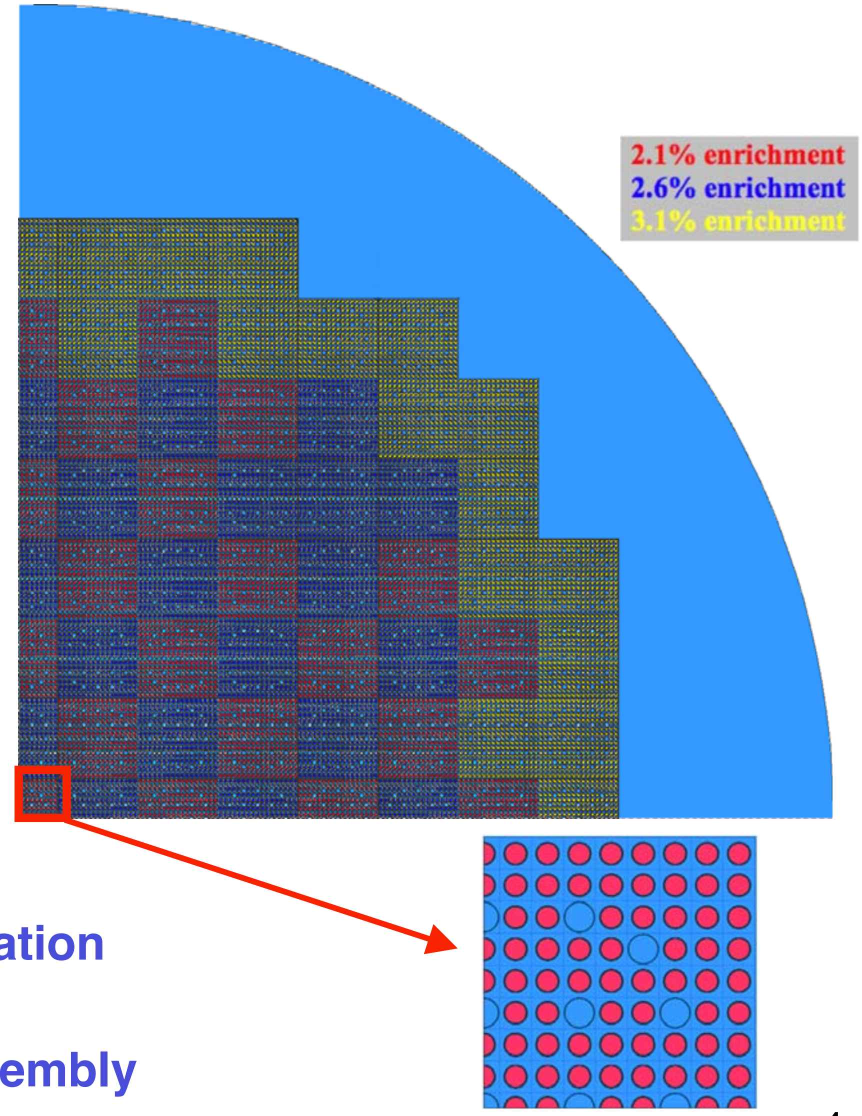
- **Prior to now, all examples were toy problems that gave no guidance to MC practitioners**

- **This talk:**
  - Brief description & explanation for each concern
  - Illustrate magnitude using
    1. Reactor: **realistic PWR quarter-core**
    2. Criticality Safety: **array of Pu-nitrate solution tanks**
  - Discuss practical approaches to avoid the problems

Example Problem - Reactor

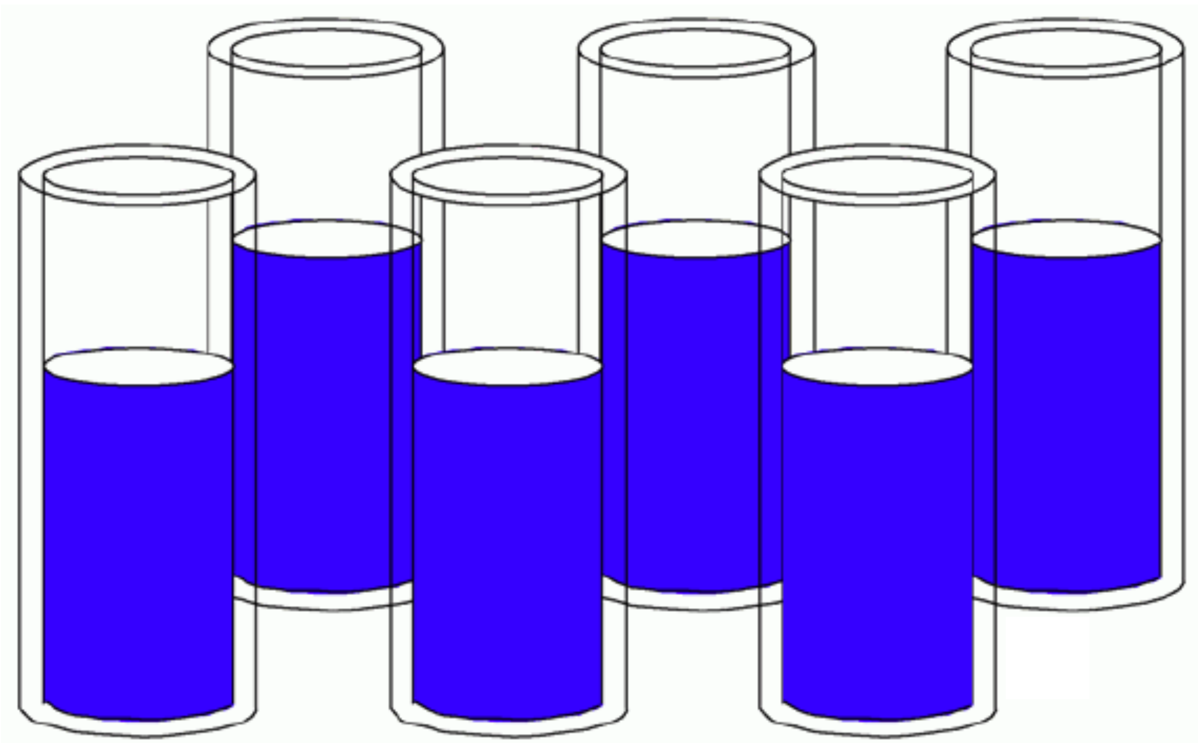
2D quarter-core PWR (Nakagawa & Mori model)

- **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**

2 x 3 array of steel cans containing plutonium nitrate solution



K-eigenvalue equation

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

where

L = leakage operator

T = collision operator

S = scatter-in operator

M = fission multiplication operator

➜ This eigenvalue equation is solved by <u>power iteration</u>

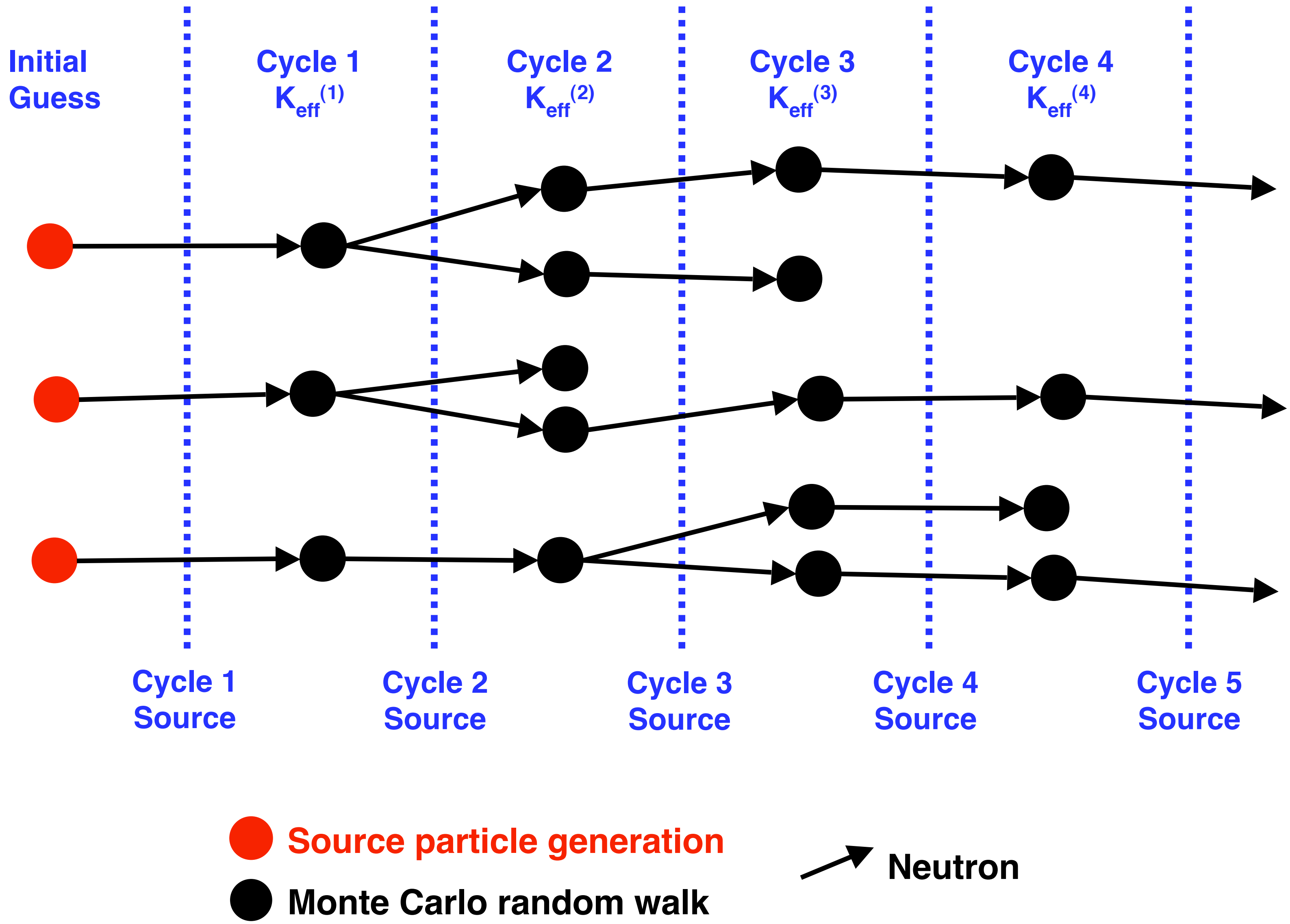
$$(L + T - S)\Psi^{(n+1)} = \frac{1}{K_{eff}^{(n)}} M\Psi^{(n)}$$

run MC histories to get $\Psi^{(n+1)}$ & $K_{eff}^{(n+1)}$

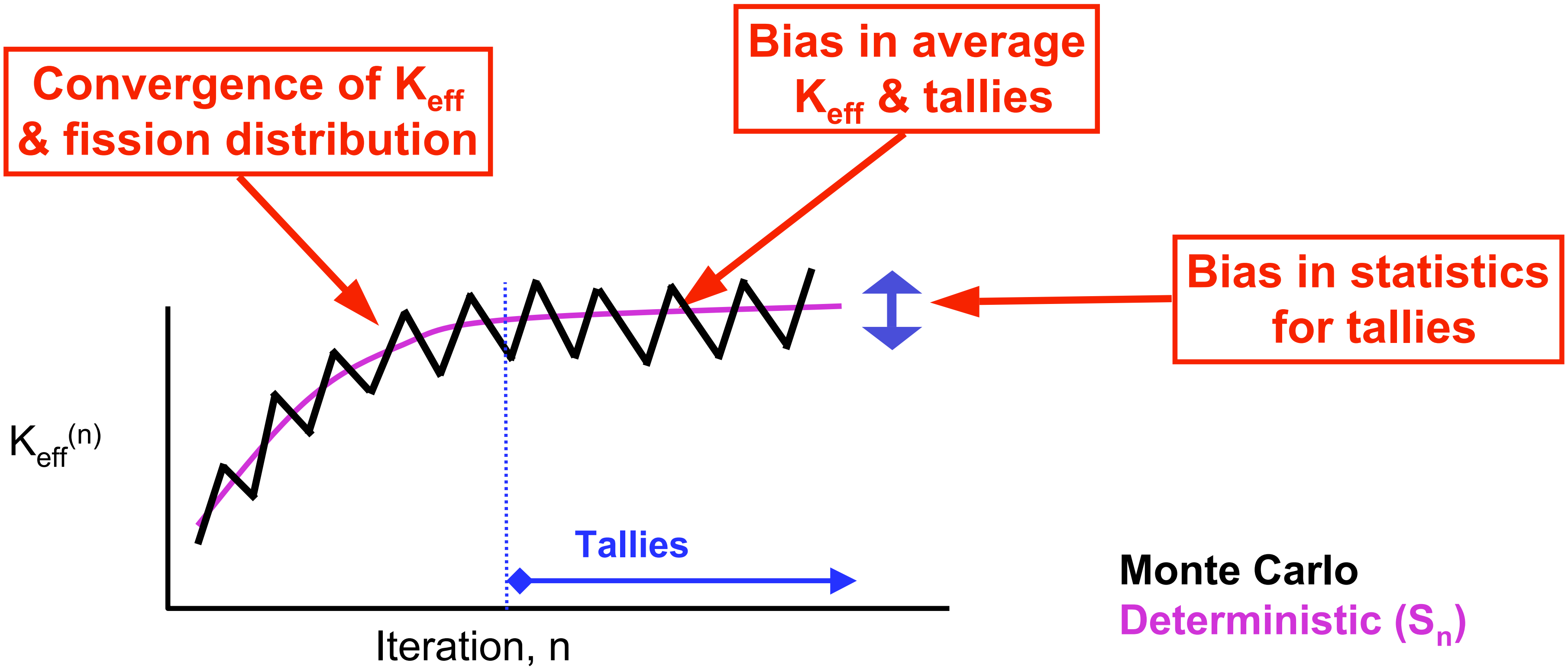
fixed source from cycle (n)

Power Iteration for MC Criticality Calculations

cycle ≡ iteration ≡ batch ≡ generation



Concerns



This talk:

- Brief description & explanation for each concern
- Illustrate magnitude using **realistic PWR quarter-core**
- Discuss practical approaches to avoid the problems

Convergence of Source Distribution

Introduction

- 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

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

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

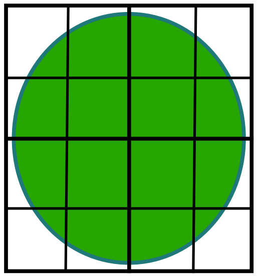
  - First-harmonic source errors die out as ρ^n, $\rho = k_1 / k_0 < 1$
  - First-harmonic K_{eff} errors die out as $\rho^{n-1}(1-\rho)$
  - Source converges slower than K_{eff}

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

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

K_{eff} Calculations - Convergence Diagnostics

- Divide the fissionable regions of the problem into N_S **spatial bins**



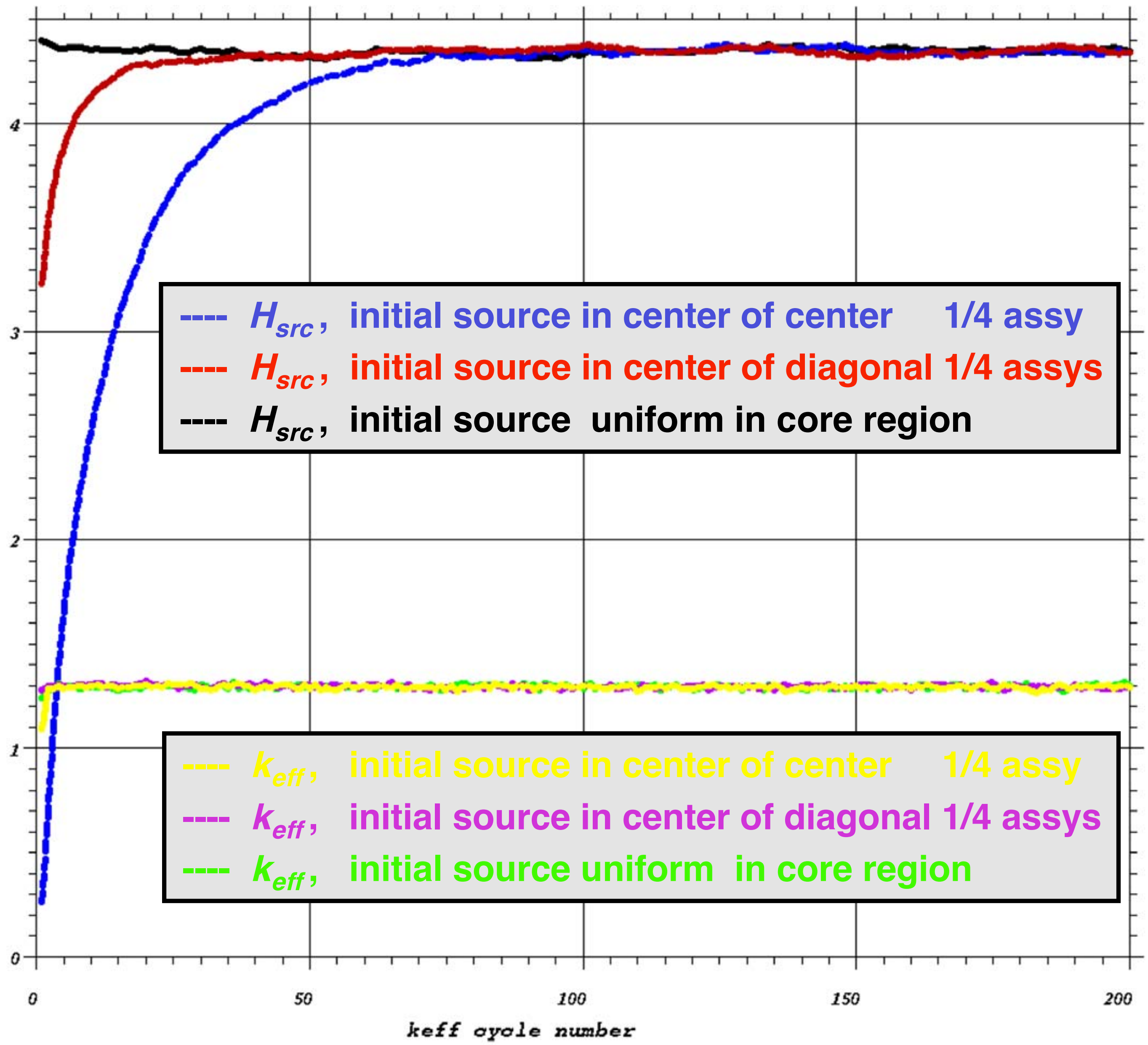
- **Shannon entropy of the source distribution**

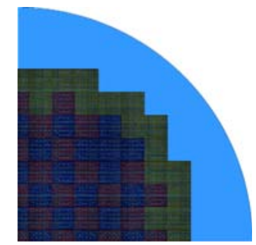
$$H(S) = -\sum_{J=1}^{N_S} p_J \cdot \ln_2(p_J), \quad \text{where} \quad p_J = \frac{(\text{\# source particles in bin J})}{(\text{total \# source particles in all bins})}$$

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

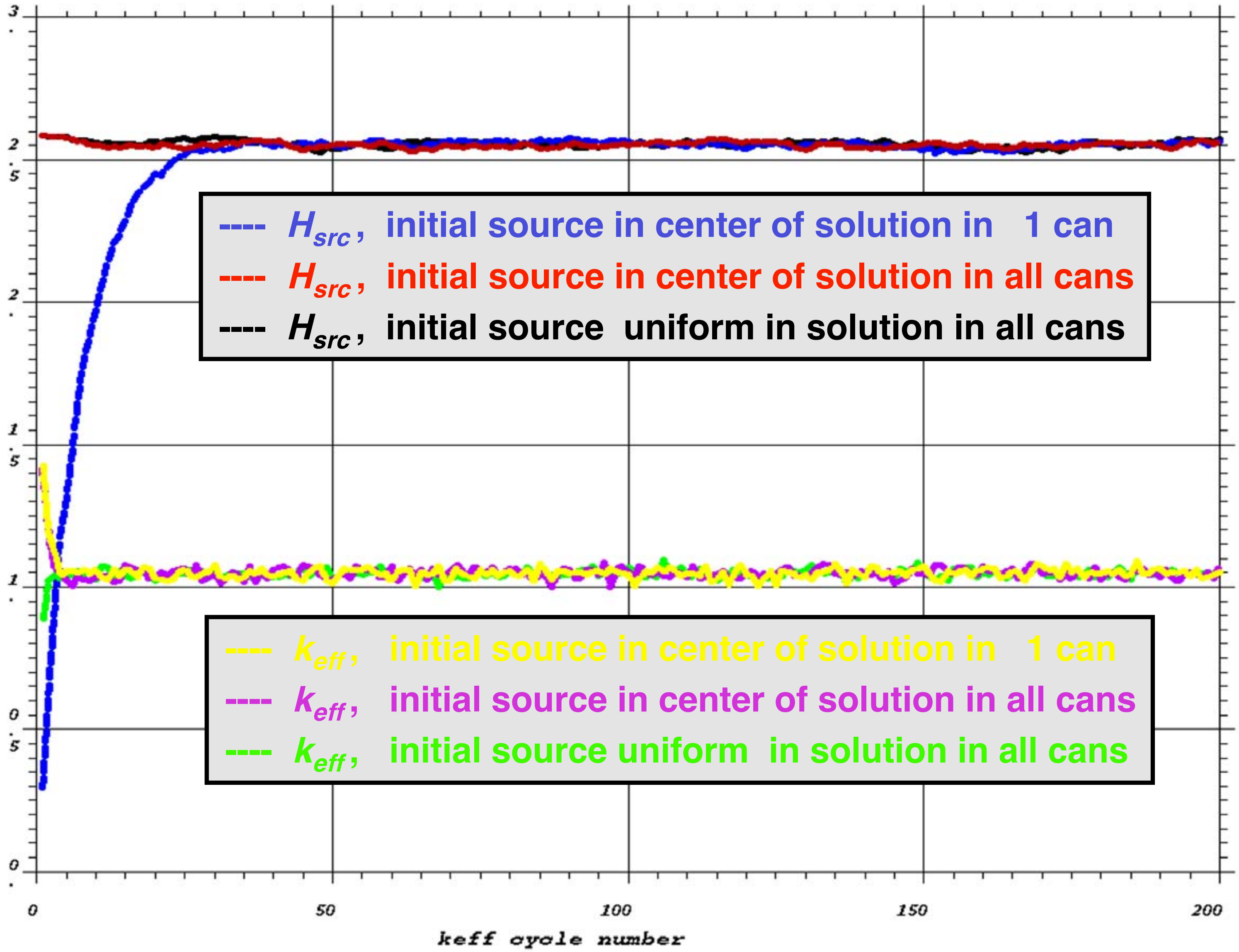
⇒ As the source distribution converges in 3D space, a line plot of $H(S^{(n)})$ vs. n (the iteration number) converge

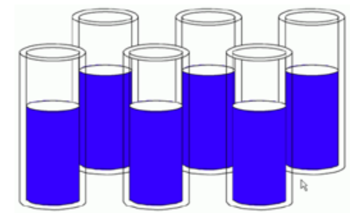
Reactor - Convergence for Different Source Guesses





Crit. Safety - Convergence for Different Source Guesses





Keff & Fission Source Convergence

- Use K_{eff} vs cycle & H_{src} vs cycle to assess convergence of both K_{eff} and the fission distribution
- The number of cycles to converge is determined by:
  - **Dominance ratio** $\rho = k_1 / k_0$
  - Closeness of **initial source guess** to converged distribution
- Note that convergence does <u>not</u> depend on the number of neutrons/cycle (M)

- **Dominance ratio determines the rate of convergence**

  $\rho > .9 \Rightarrow$ many cycles to converge

- **To reduce the dominance ratio**
  - Take advantage of problem symmetry & reflecting boundary, to eliminate some higher modes

PWR reactor example:

full core	$\rho \sim .98$
1/2 core	$\rho \sim .97$
1/4 core	$\rho \sim .96$
1/8 core	$\rho \sim .94$

- **Smaller dominance ratio $\Rightarrow$ fewer cycles to converge**

Keff & Fission Source Convergence

- **Better initial source guess ⇒ fewer cycles to converge**

- **Typical**

  – Point at center - terrible guess

  – Reactor: uniform in core region - good guess

  – Criticality Safety: points in each fissionable region, or
  uniform in each fissionable region - good guess

Conclusions - Convergence

- **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

- **Use problem symmetry, if possible**

- **Better initial source guess ⇒ fewer cycles to converge**
  - Reactor: uniform in core region
  - Criticality Safety: points in each fissionable region, or uniform in each fissionable region

Bias in Keff & Tallies

Bias in Keff

- **Power iteration is used for Monte Carlo Keff calculations**
  - For one cycle (iteration):
    - $\mathbf{M_0}$ neutrons start
    - $\mathbf{M_1}$ neutrons produced, $E[\,\mathbf{M_1}\,] = \text{Keff} \cdot \mathbf{M_0}$
  - At end of each cycle, must **renormalize** by factor $\mathbf{M_0 / M_1}$
  - Dividing by stochastic quantity ($\mathbf{M_1}$) introduces bias

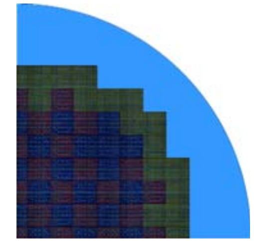
- **Bias in Keff, due to renormalization**

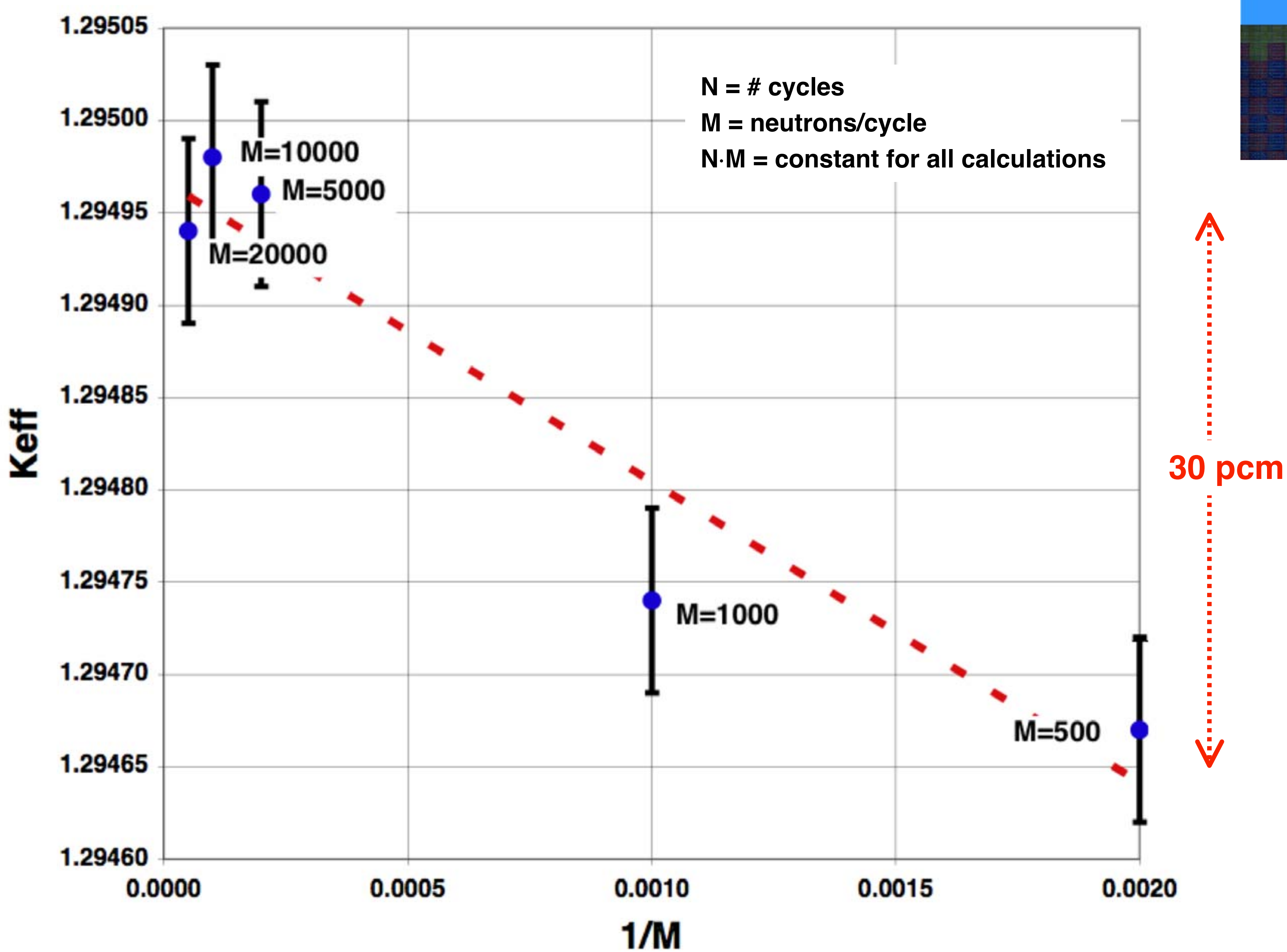
$$\text{bias in } K_{eff} \;=\; -\frac{\sigma_k^2}{K_{eff}} \cdot \left(\begin{array}{c} \text{sum of lag-i correlation} \\ \text{coeff's between batch K's} \end{array} \right) \;\propto\; \frac{1}{M_0}$$

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

- **Run the reactor problem with different M (neutrons/cycle)**
  500, 1000, 5000, 10000, 20000

Reactor - Bias in Keff





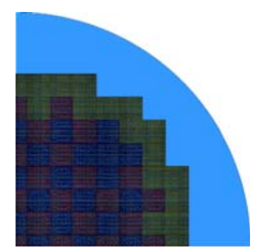
Reactor - Bias in Fission Tallies

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%

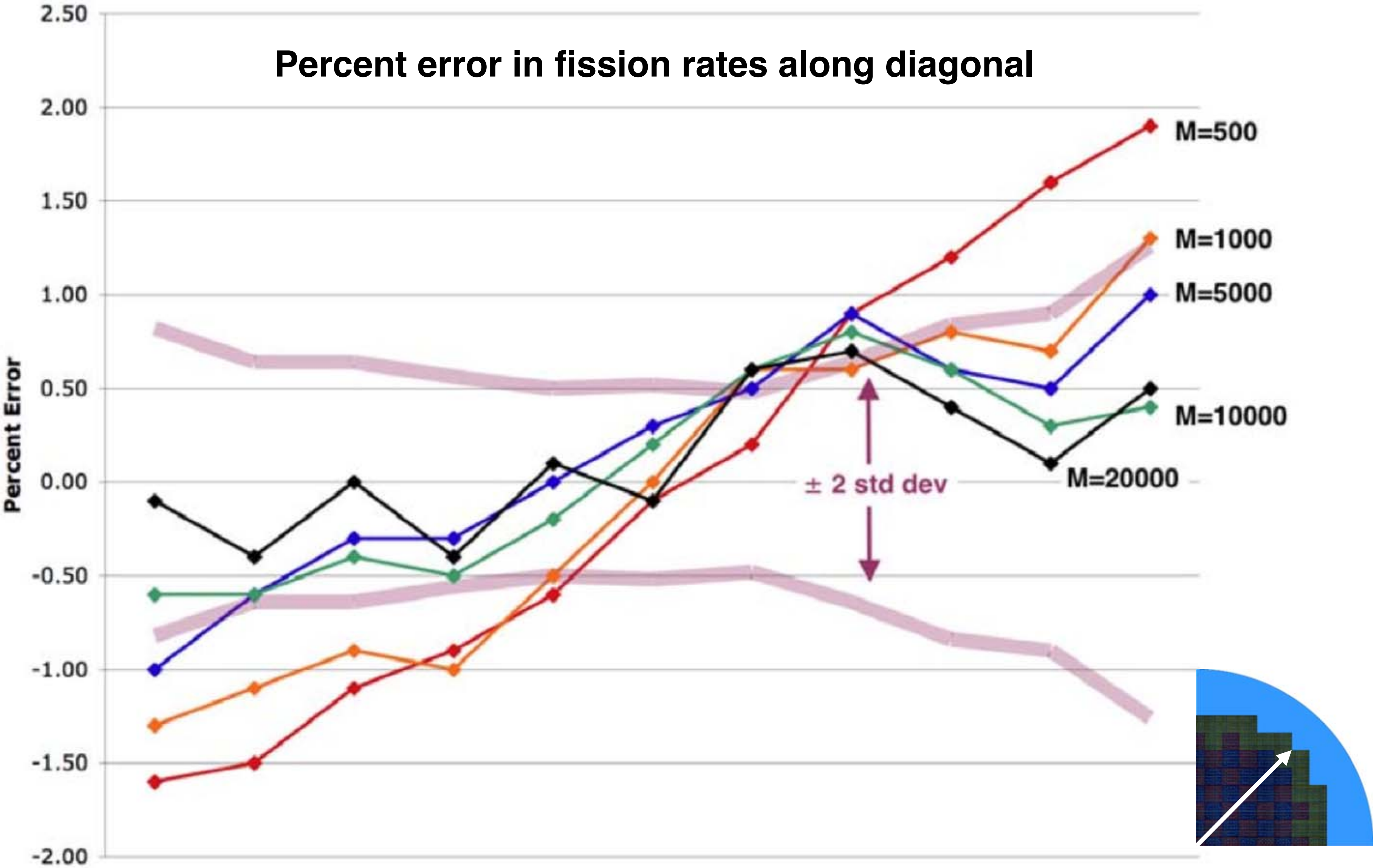
Statistics ~ .1% to .3%



Reference: ensemble-average of 25 independent calculations, with 25 M neutrons each & 20K neutrons/cycle

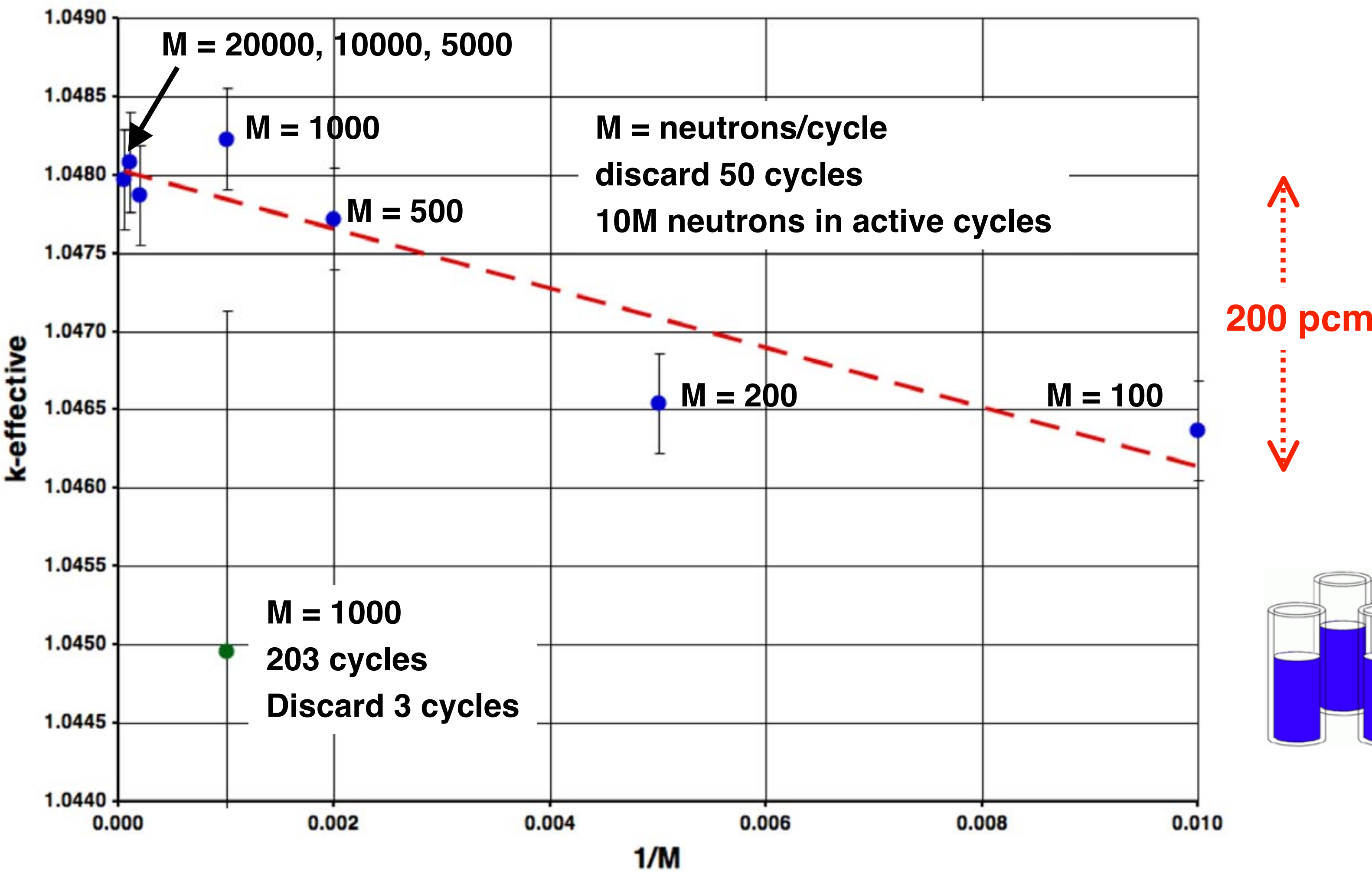
Reactor - Bias in Fission Tallies

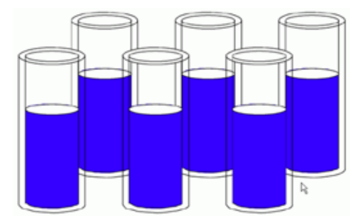
Monte Carlo Codes
X-3-MCC, LANL



Criticality Safety - Bias in Keff

Monte Carlo Codes
X-3-MCC, LANL





Note: Bias in green point is a <u>convergence</u> problem due to using Keno <u>default</u> - discard 3 cycles, 203 cycles total

Bias in Keff & Tallies - Comments

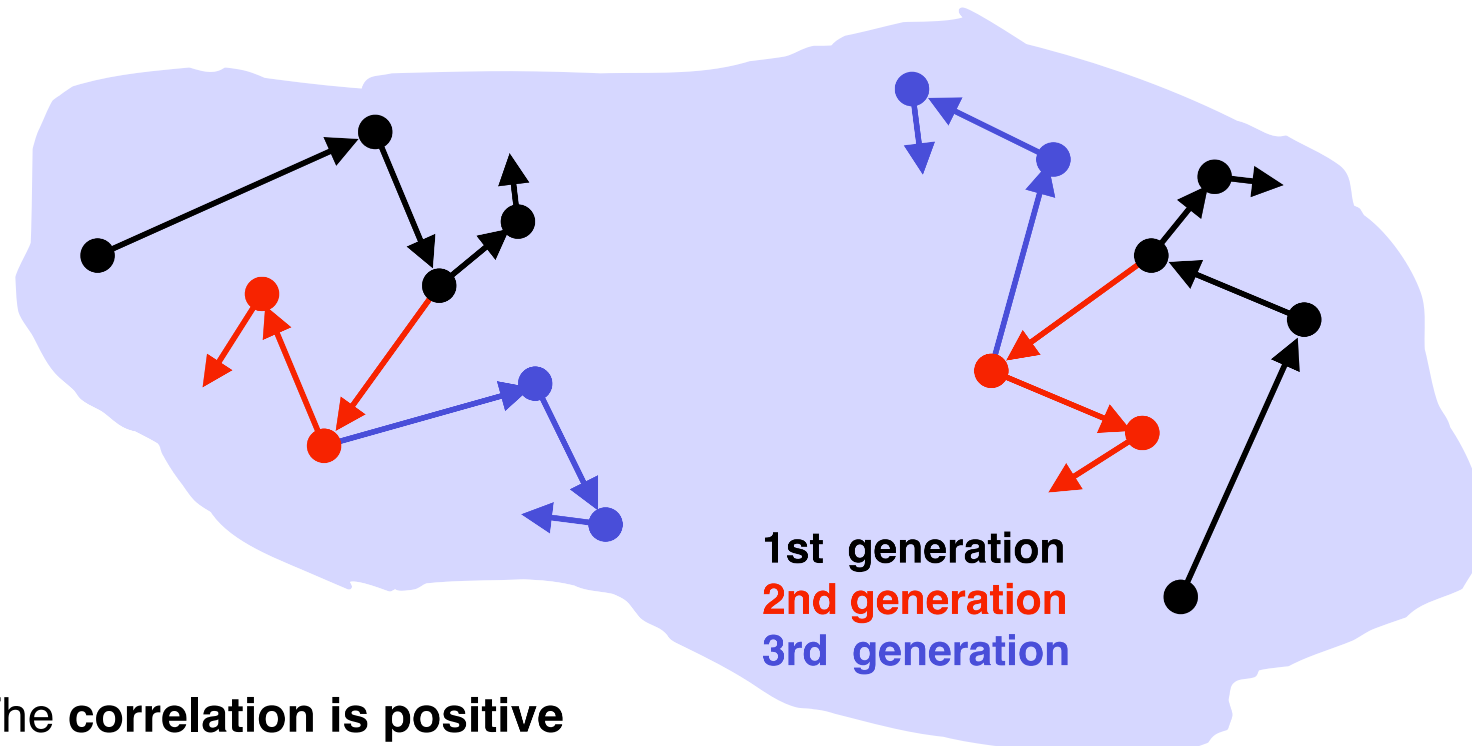
- **For reactor problem with 500 neutrons/cycle**
  - Bias in Keff is ~ 30 pcm
  - Bias in the power distribution shows a significant tilt
  - Errors of -1.7 % to +3.2 % in power fractions
  - The bias is much larger than the MC uncertainties
- **Bias in Keff & the fission distribution is smaller with 1000 neutrons per cycle, and smaller still with 5,000 or 10,000 neutrons per cycle**
- **Practical solution - use large M (neutrons/cycle)**
  - For M ~ 10K or more ⇒ bias negligible
  - Large M gives more efficient parallel calculations

Underprediction Bias in Confidence Intervals

in Monte Carlo Keff Calculations

Tallies & Correlation

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



  - The **correlation is positive**

Bias in σ^2

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

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

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

$$\sigma_{\bar{X}}^2 \approx \tilde{\sigma}_{\bar{X}}^2 + \tilde{\sigma}_{\bar{X}}^2 \cdot 2 \cdot \sum_{i=1}^{\infty} r_i \quad = \quad \text{True variance, including correlations}$$

$r_i =$ lag-i correlation coef. between X_n's

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

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

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

Bias in Uncertainties

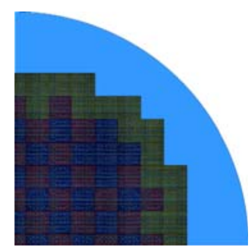
mcnp Monte Carlo Codes
X-3-MCC, LANL

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

True relative errors in 1/4-assembly fission rates, as multiples of calculated relative errors, $\sigma_{TRUE} / \sigma_{MCNP}$

Calculated uncertainties are 1.7 to 4.7 times smaller than true uncertainties



Bias in Uncertainties - Comments

- Uncertainties computed by MC codes exhibit a bias due to inter-cycle correlation effects that are neglected in tallies
- 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 per cycle does not 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 Keff & tally distributions, use 10K or more neutrons/cycle
- Always check convergence of both Keff & Hsrc
- Take advantage of problem symmetry, if possible
- Use a good initial source guess, uniform in fissionable regions
- Run at least a few hundred active cycles to allow codes adequate information to compute statistics
- Be aware that statistics on tallies from codes are underestimated, possibly make multiple independent runs