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"K-effective of the World" and Other Concerns for Monte Carlo Eigenvalue Calculations

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"K_{eff} of the World" & Other Concerns for Monte Carlo Eigenvalue Calculations

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Abstract

"K_{eff} of the World" & Other Concerns for Monte Carlo Eigenvalue Calculations

Forrest Brown, XCP-3, LANL

Monte Carlo methods have been used to compute k_{eff} and the fundamental mode eigenfunction of critical systems since the 1950s. Despite the sophistication of today's Monte Carlo codes for representing realistic geometry and physics interactions, correct results can be obtained in criticality problems only if users pay attention to source convergence in the Monte Carlo iterations and to running a sufficient number of neutron histories to adequately sample all significant regions of the problem. Recommended best practices for criticality calculations are reviewed and applied to several practical problems for nuclear reactors and criticality safety, including the "K-effective of the World" problem. Numerical results illustrate the concerns about convergence and bias. The general conclusion of is that with today's high-performance computers, improved understanding of the theory, new tools for diagnosing convergence (e.g., Shannon entropy of the fission distribution), and clear practical guidance for performing calculations, practitioners will have a greater degree of confidence than ever of obtaining correct results for Monte Carlo criticality calculations.

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)

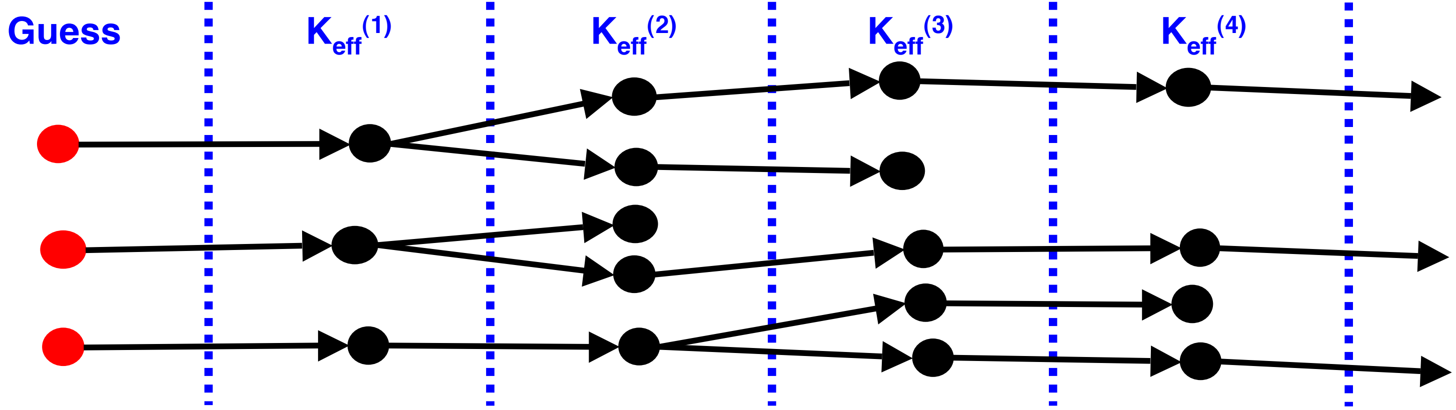
- These problems are well-understood & can be readily avoided, if some simple "best practices" guidelines are followed

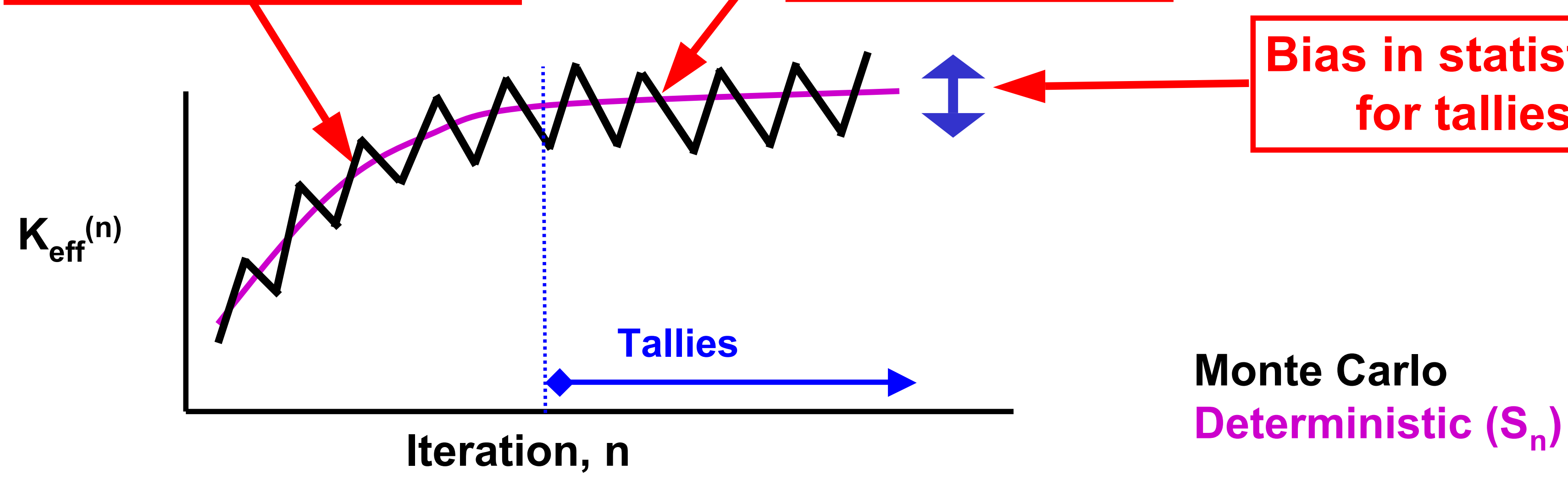
- Previous discussion of details:
  - 2008 - PHYSOR - Monte Carlo workshop
  - 2009 - M&C - Monte Carlo workshop
  - 2009 - NCSD - ‘Best Practices’ paper
  - 2010 - PHYSOR - Monte Carlo workshop

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 $\mathbf{M_0 / M_1}$
  - Dividing by stochastic quantity ($\mathbf{M_1}$) introduces bias in K_{eff} & tallies
- **Bias in Keff, due to renormalization**

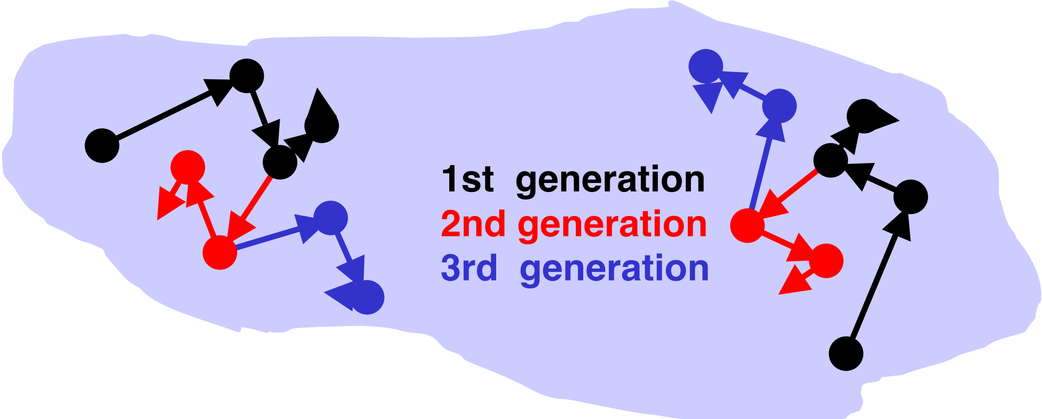
$$\text{Bias in } K_{eff} \propto \frac{1}{M}$$

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 <u>spatially correlated</u> with tallies in successive generations**
  - **The correlation is <u>positive</u>**
  - **MCNP & other MC codes ignore this correlation, so computed statistics are <u>smaller</u> 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 <u>not</u> reduce the underprediction bias in statistics**
  - **(True σ^2) > (computed σ^2), since correlations are <u>positive</u>**



$$\frac{\text{True } \sigma_{\bar{x}}^2}{\text{Computed } \sigma_{\bar{x}}^2} = \frac{\sigma_{\bar{x}}^2}{\tilde{\sigma}_{\bar{x}}^2} \approx 1 + 2\cdot\begin{pmatrix}\text{sum of lag-i correlation} \\ \text{coeff's between tallies}\end{pmatrix}$$

Numerical Results

-

K_{eff} of the World Problem

Introduction

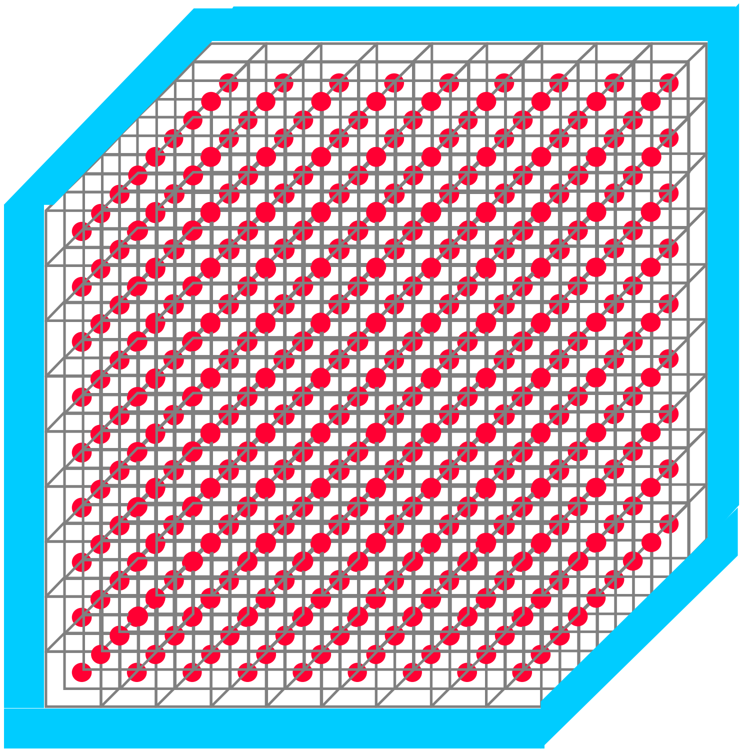
Elliot Whitesides, 1971:

> *… 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

- 739 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:

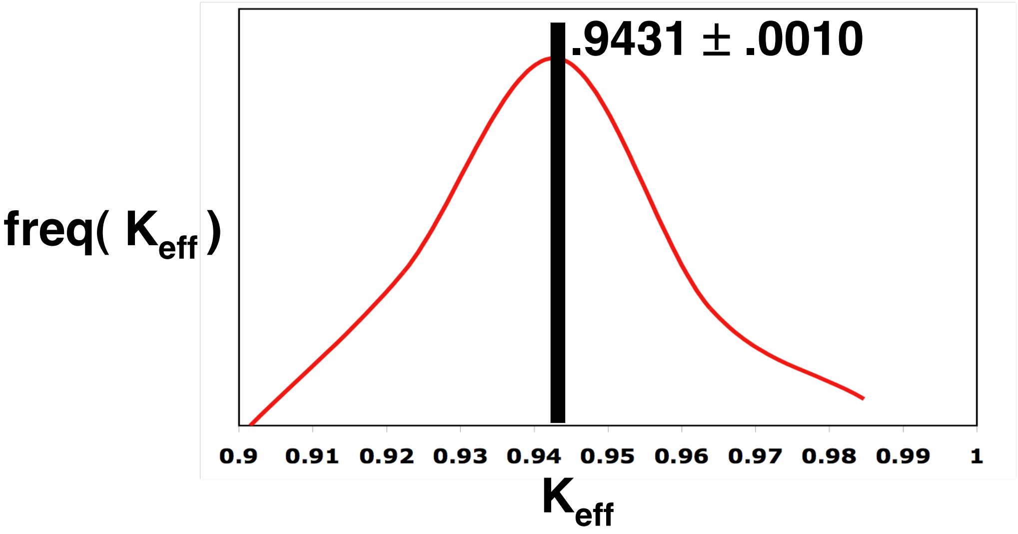
  Replace center sphere of array by larger (critical) sphere

Should be supercritical - is it ?

Whitesides' Problem, circa 1971

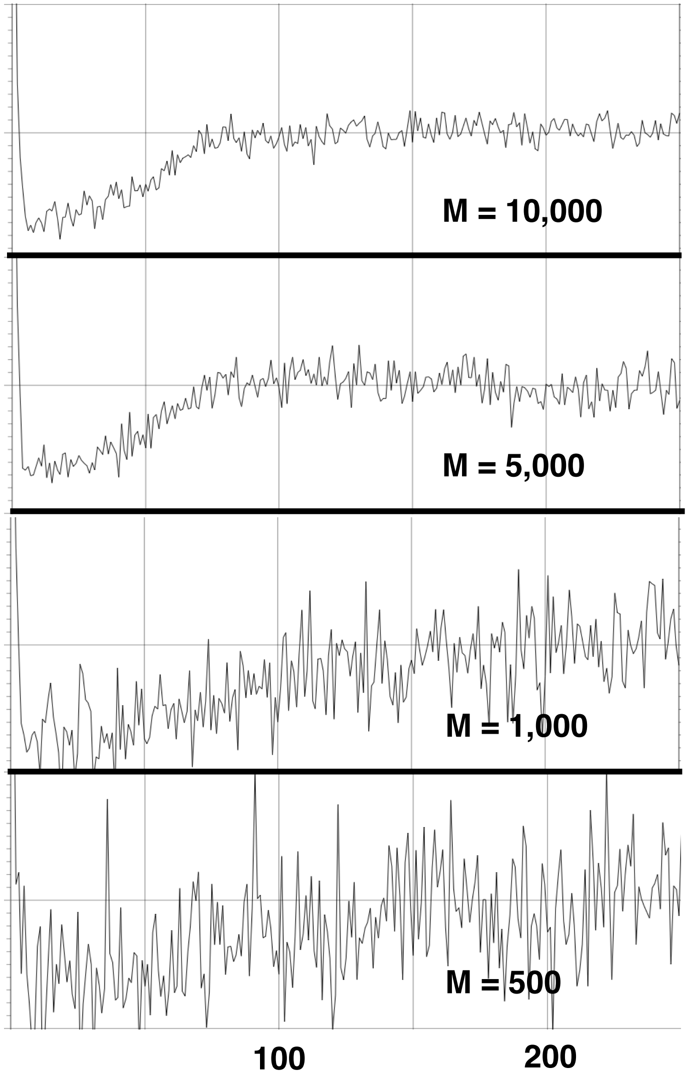
- **Due to severe computer limitations ~1971, KENO defaults were:**
  - 300 neutrons/cycle
  - Discard first 3 cycles
  - Run 100 more cycles

- **If MCNP5 is run using the 1971 KENO defaults, 200 independent replica calculations give:**
  - Average of 200 replicas: **K_{eff} = .9431 ± .0010**
  - <u>None</u> of the 200 calculations produced $K_{eff} > 1$
  - Distribution of replica results:

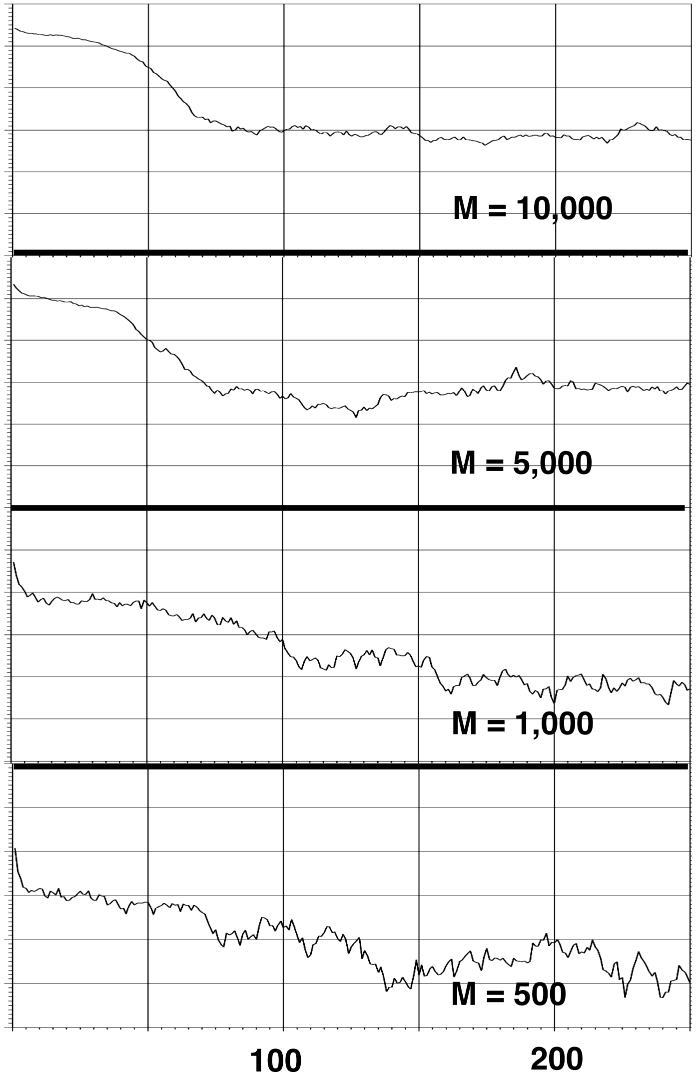


Convergence

K_{eff} vs cycle, various M
M = neutrons/cycle



H_{src} vs cycle, various M
M = neutrons/cycle



K_{eff} converges in 75-100 cycles

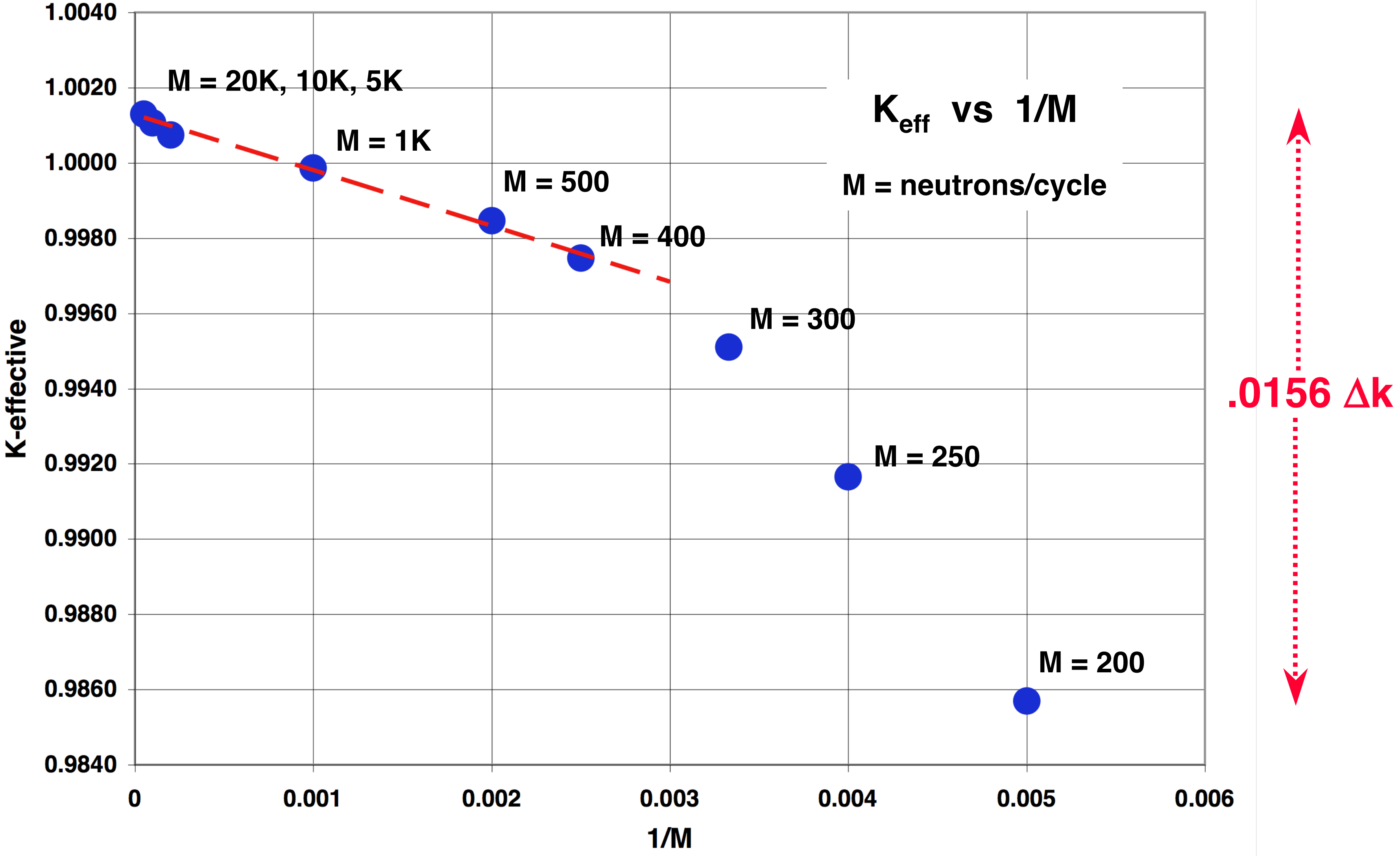
H_{src} converges in 100-150 cycles

Must discard 150 or more initial cycles

Convergence depends on the dominance ratio & source guess, NOT on neutrons/cycle

Initial source guess = uniform sampling of points at sphere centers

K_{eff} Bias



Historical note:

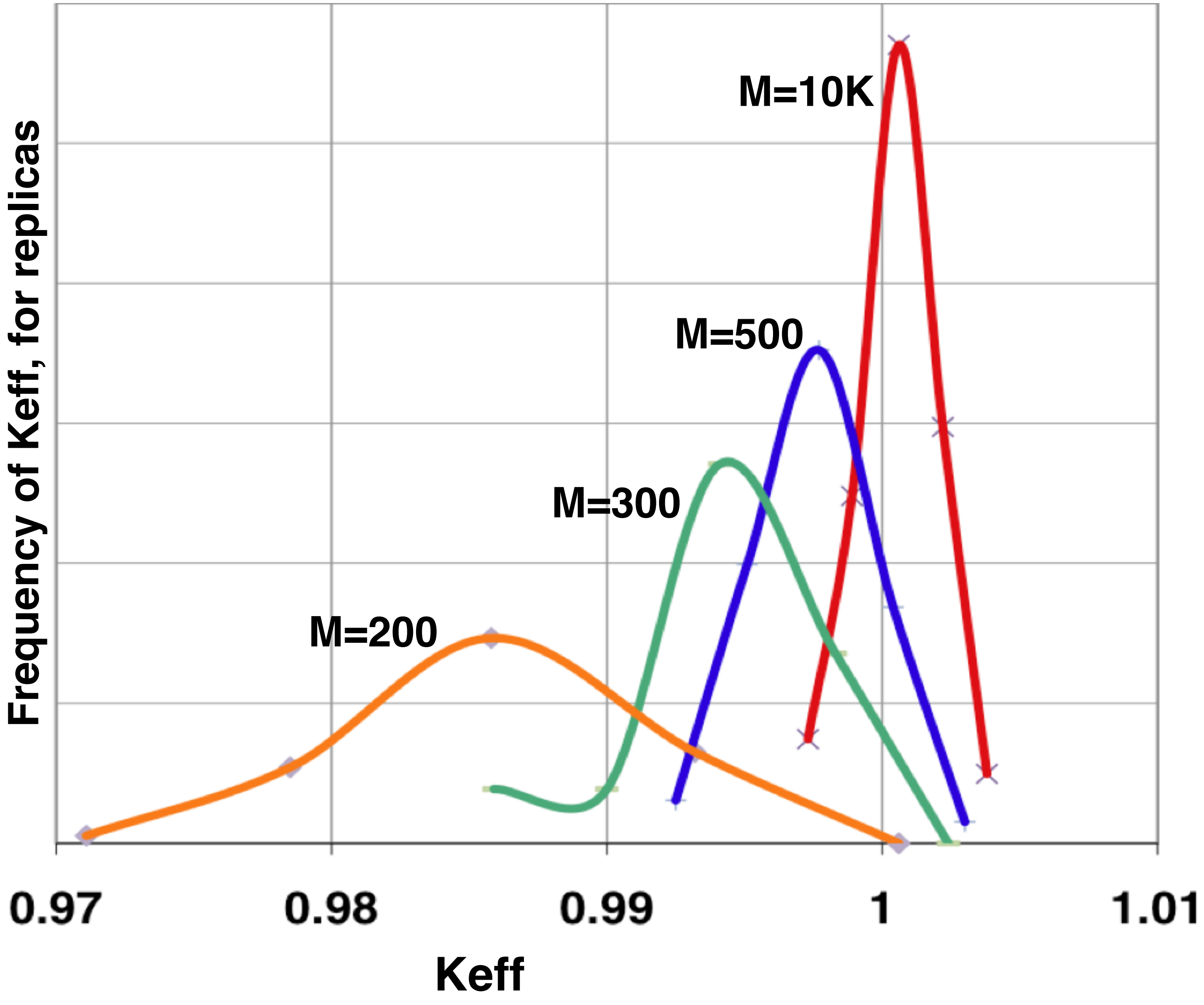
When this problem was first proposed in 1971,
the default batch size for KENO was 300 neutrons/cycle

Notes:

- All cases discarded the first 150 cycles
- All cases used 10M neutrons in active cycles
- All cases: $\sigma \sim .00025$, smaller than plot markers

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 (739 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

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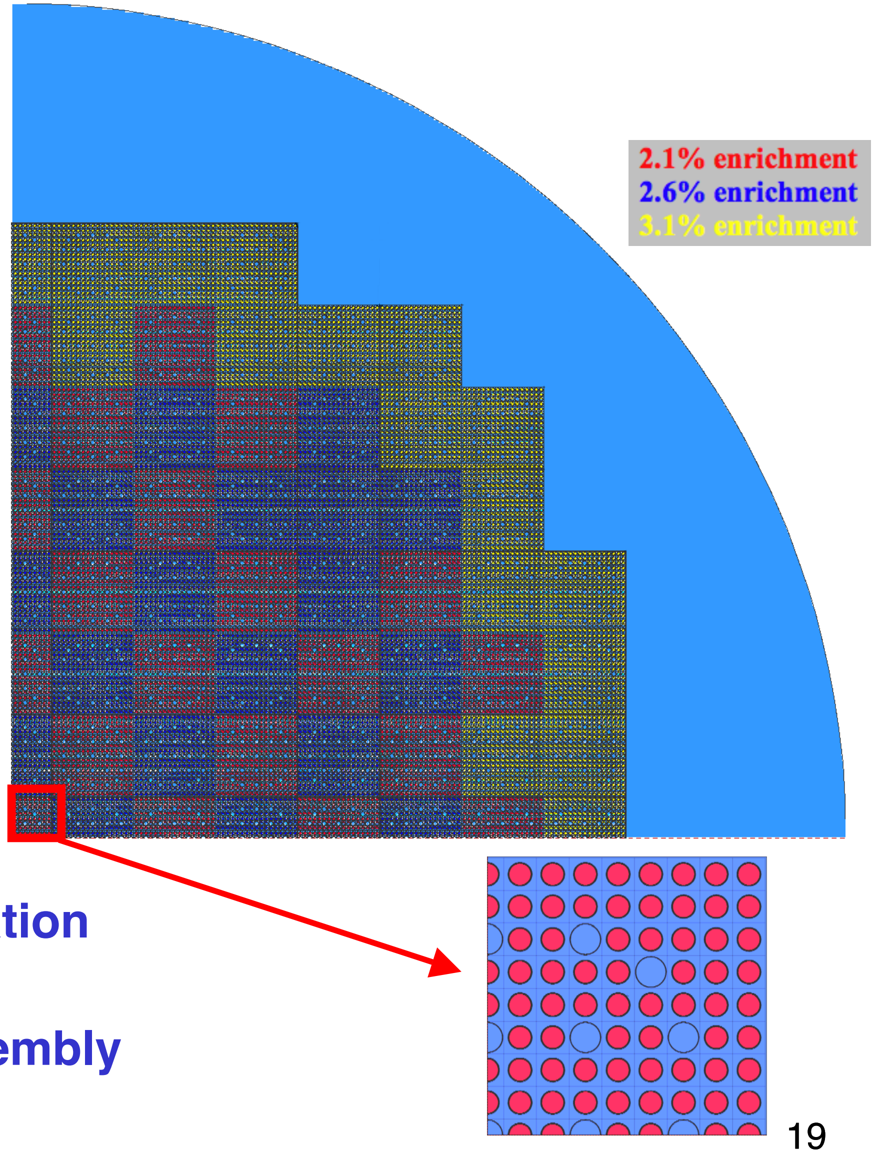
1/4-Core PWR

Example Problem - Reactor

2D quarter-core PWR

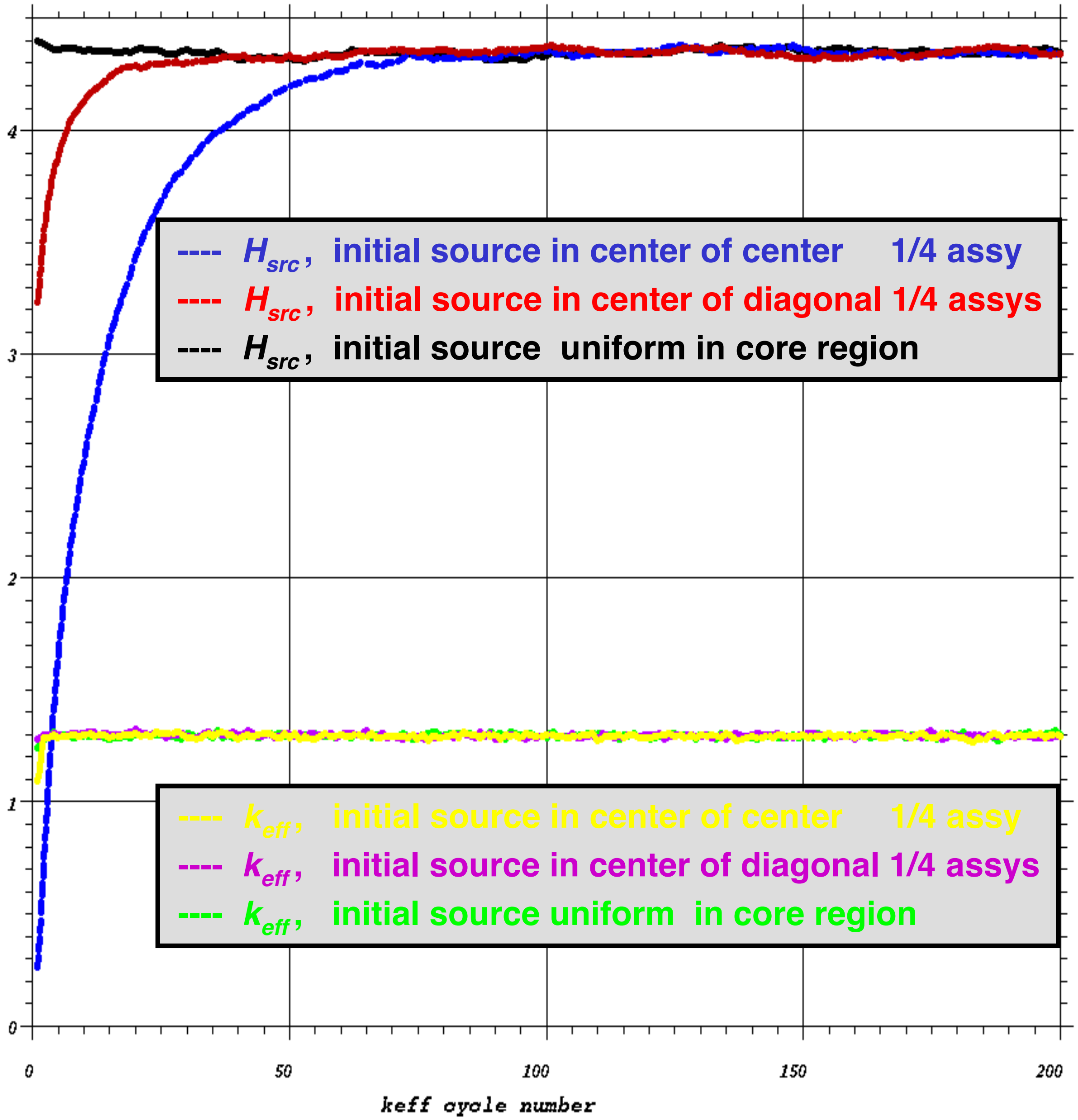
(Nakagawa & Mori model)

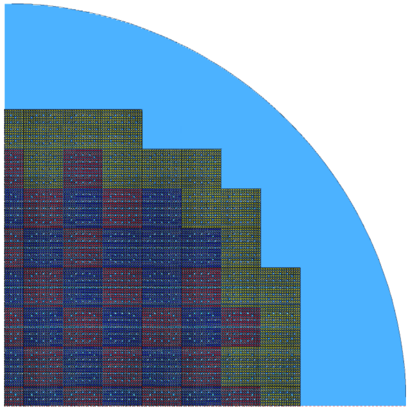


- **48 1/4 fuel assemblies:**
  - 12,738 fuel pins with cladding
  - 1206 1/4 water tubes for control rods or detectors
- **Each assembly:**
  - Explicit fuel pins & rod channels
  - 17x17 lattice
  - Enrichments: 2.1%, 2.6%, 3.1%
- **Dominance ratio ~ .96**

- **125 M active neutrons for each calculation**
- **ENDF/B-VII data, continuous-energy**
- **Tally fission rates in each quarter-assembly**

Convergence



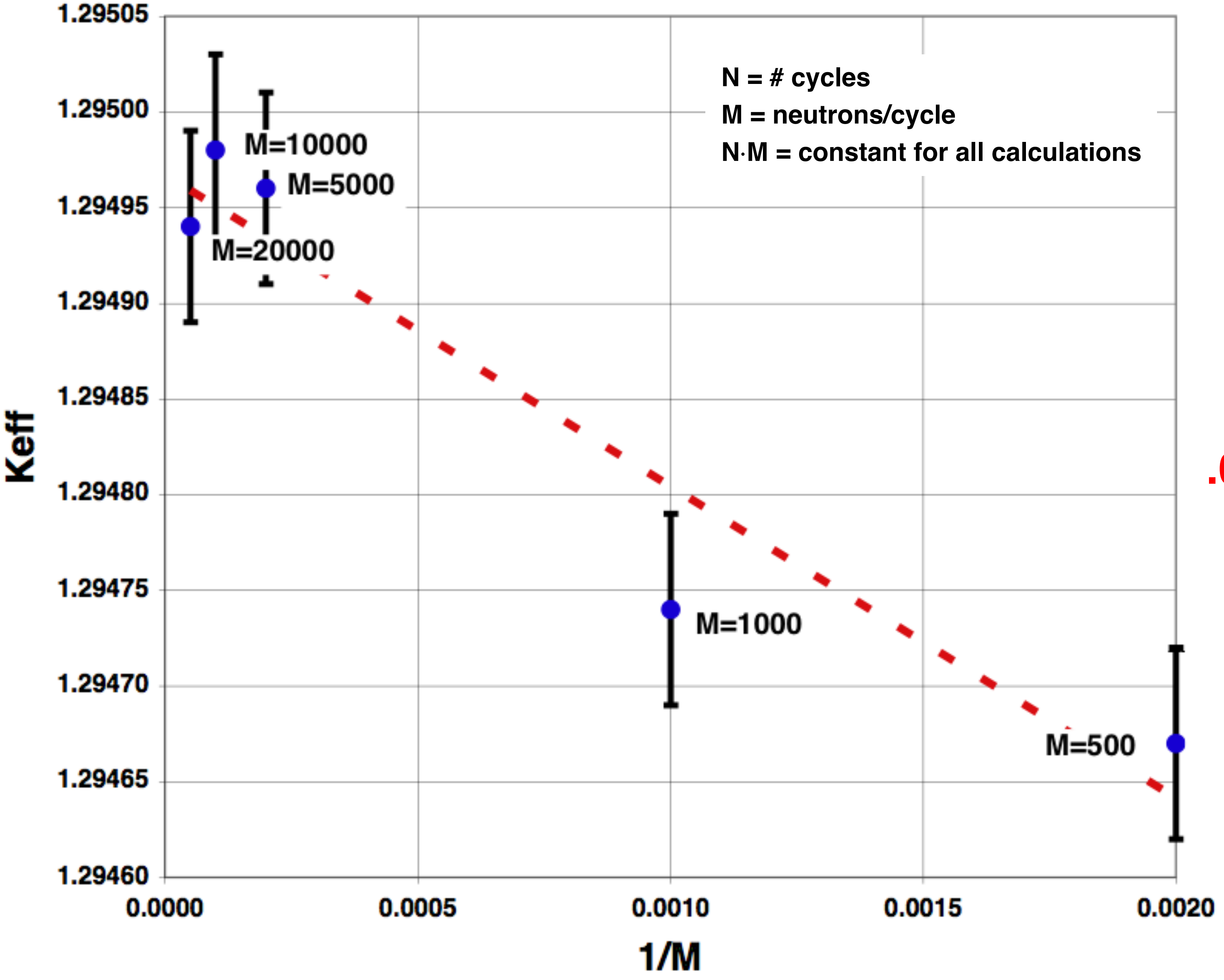


K_{eff} converges sooner than the fission distribution

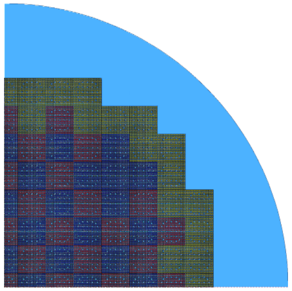
H_{src} =

- **Shannon entropy of fission source distribution**
- **A metric for assessing convergence of the distribution**
- **Computed/plotted by MCNP**

Bias in K_{eff}



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



.0003 Δk

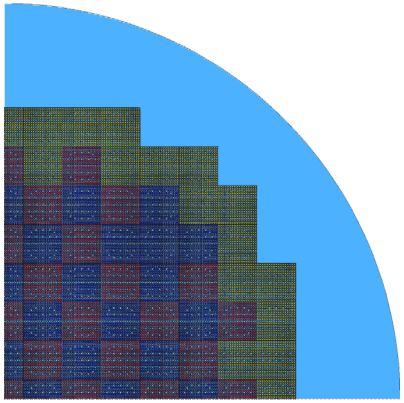
Bias in Tallies

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

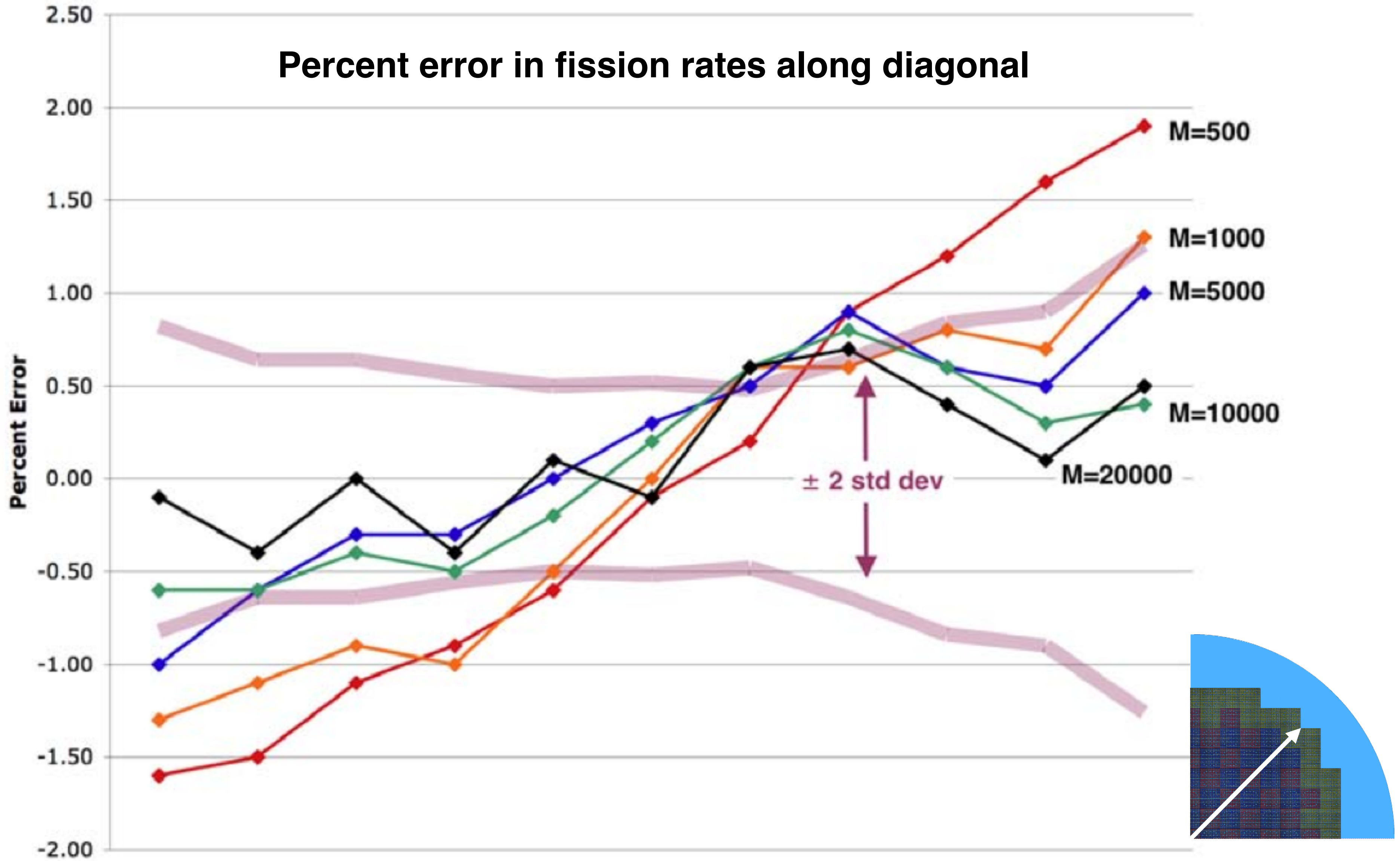
Errors of -1.7% to +3.2%

Statistics ~ .1% to .3%



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

Bias in Tallies



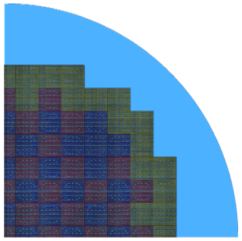
Bias in σ's

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



Numerical Results

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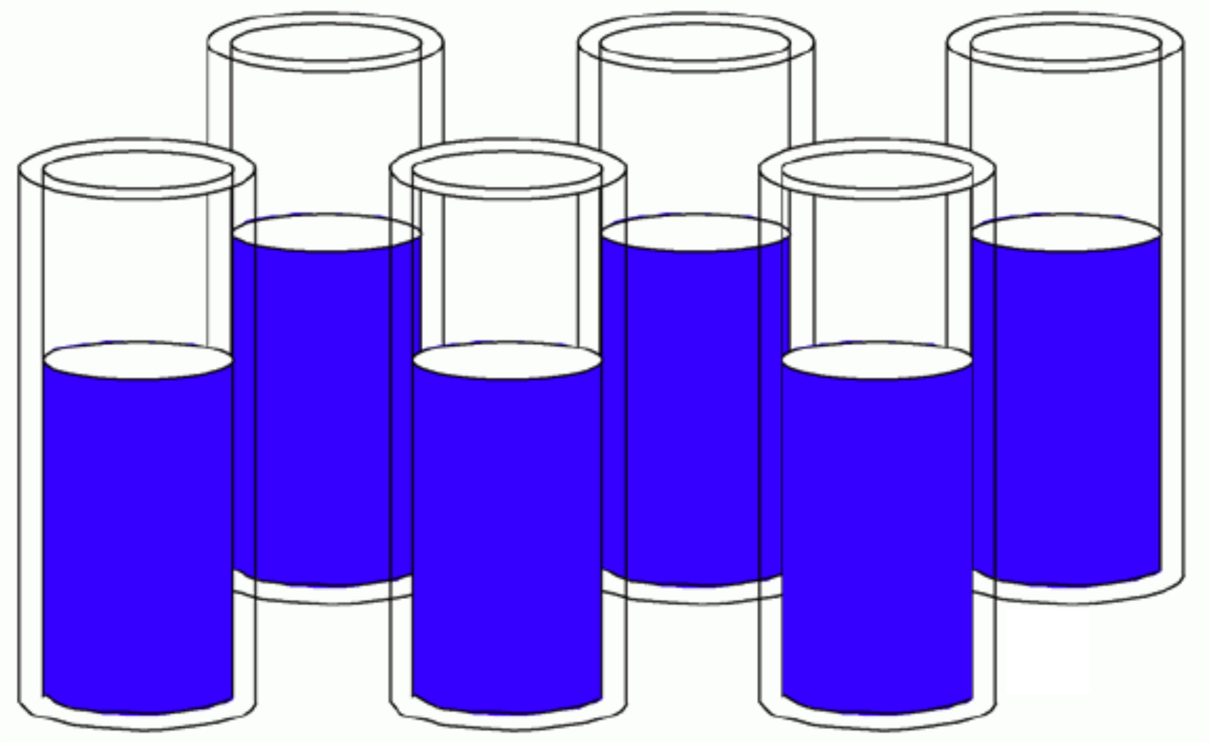
Crit-Safety Problem

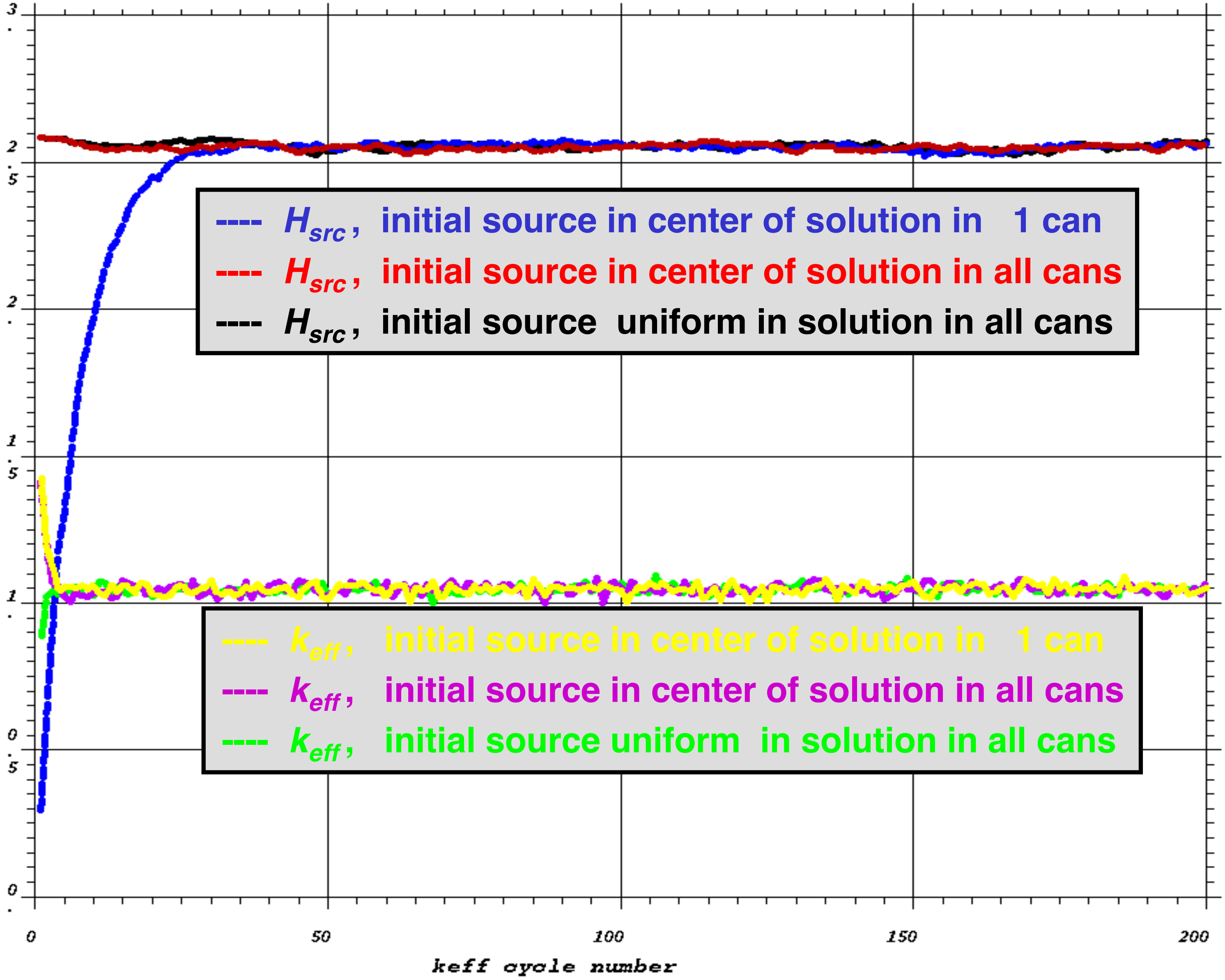
Example Problem - Criticality Safety

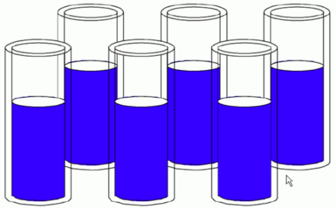
2 x 3 array of steel cans containing plutonium nitrate solution



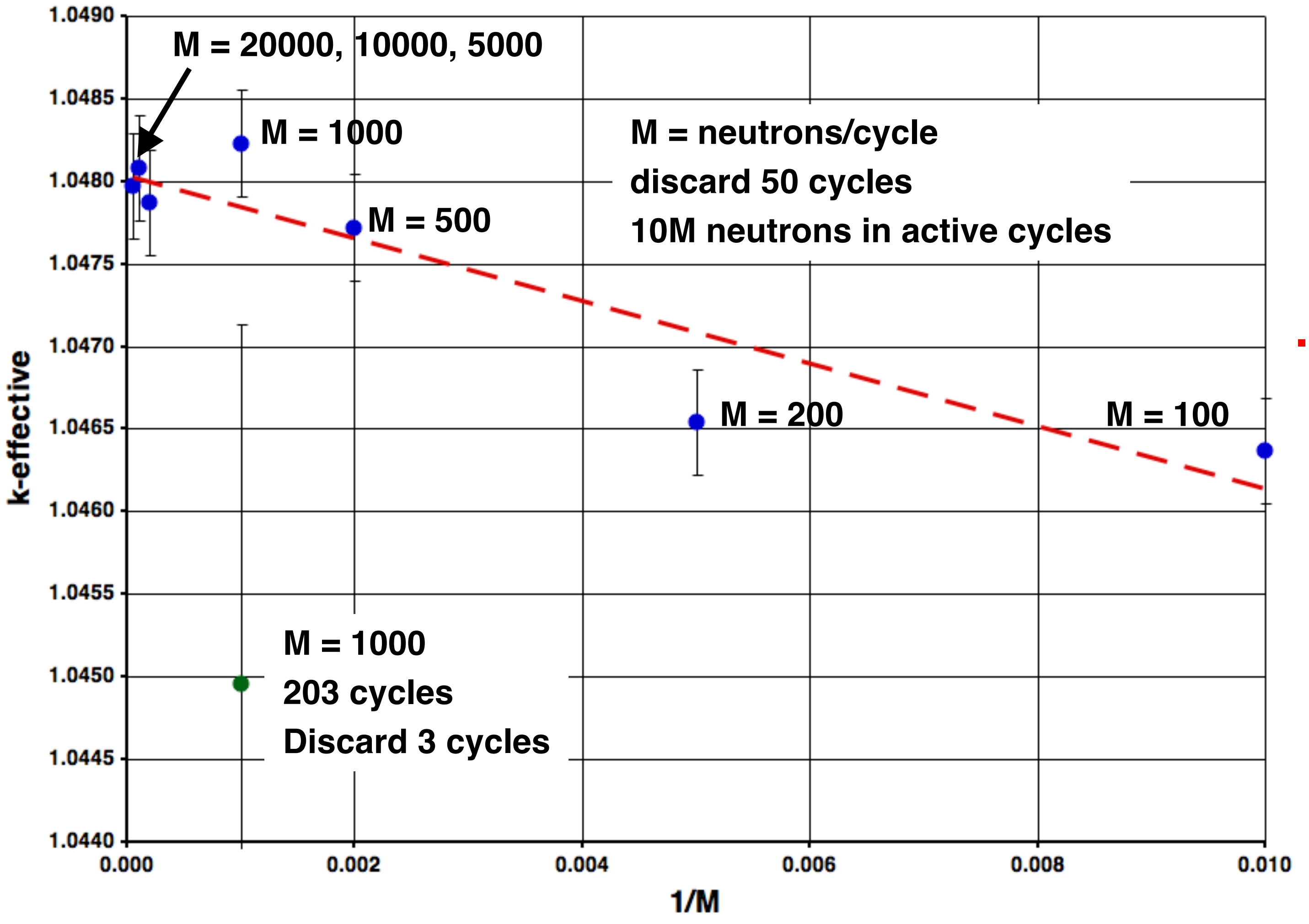
From MCNP Criticality Primer (chap 5) & MCNP Criticality Classes

Convergence

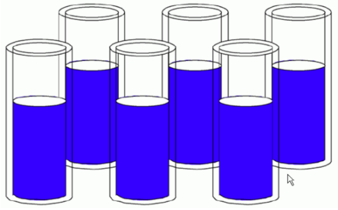




Bias in K_{eff}



.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

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 <u>always negative</u> (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 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 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 <u>underestimated</u>, often by 2-5x;
  possibly make multiple independent runs

References

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- F.B. BROWN, ET AL. "MCNP5-1.51 Release Notes", LA-UR-09-00384, Los Alamos National Laboratory (2009).

- **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**

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