LA-UR-09-02377

Approved for public release; distribution is unlimited.

Title: A Review of Monte Carlo Criticality Calculations - Convergence, Bias, Statistics

Author(s): Forrest B. Brown

Intended for: American Nuclear Society
Mathematics & Computation Topical Meeting
Saratoga, NY
May 3-7, 2009

LA-UR-09-02377

M&C 2009
Saratoga Springs, NY
May 3-7, 2009

A Review of Monte Carlo Criticality Calculations - Convergence, Bias, Statistics

Forrest B. Brown

Los Alamos National Laboratory, Los Alamos, NM, USA

Los Alamos NATIONAL LABORATORY EST. 1943

Acknowledgment

The author & LANL greatly appreciate the inspiration & support from:

Ely Gelbard, who devoted much of his career to the theory & practice of Monte Carlo criticality calculations

Enrico Sartori, for his long-time support of Monte Carlo & various international expert study groups through the OECD / NEA Data Bank

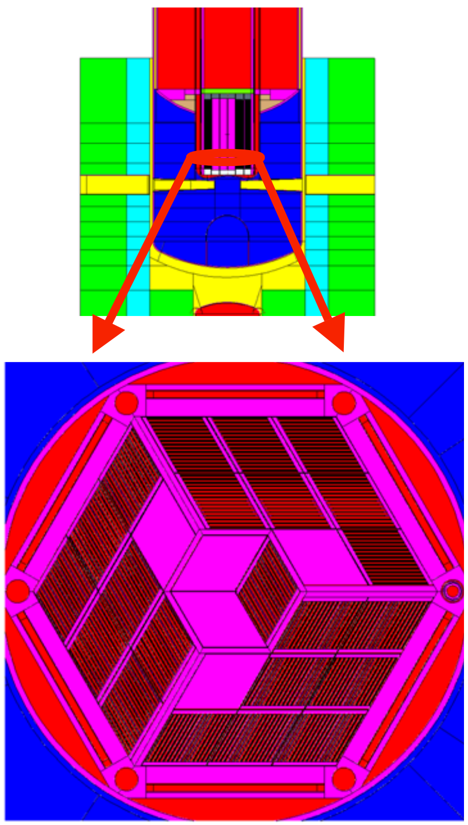
US DOE Nuclear Criticality Safety Program

This review and related R&D work on Monte Carlo criticality calculations would not have been possible without them.

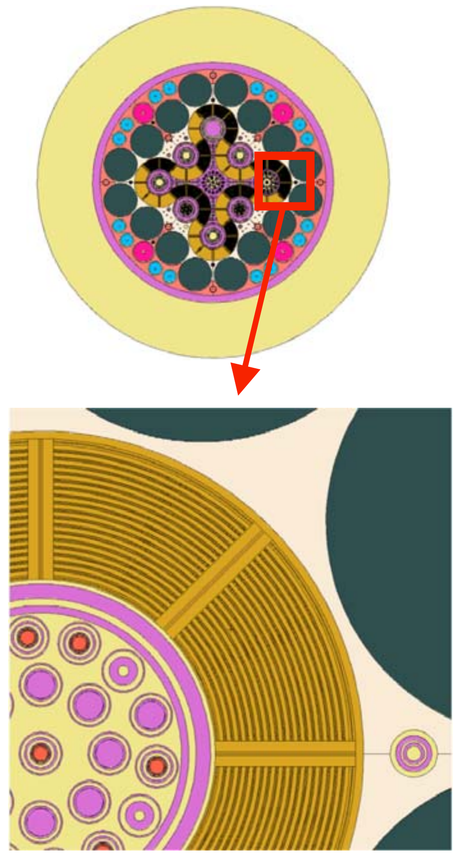
- Introduction
- Power method for MC
- Convergence of Keff & fission source
- Bias in Keff & tallies
- Bias in confidence intervals
- Conclusions

Examples - Reactor Analysis with Monte Carlo

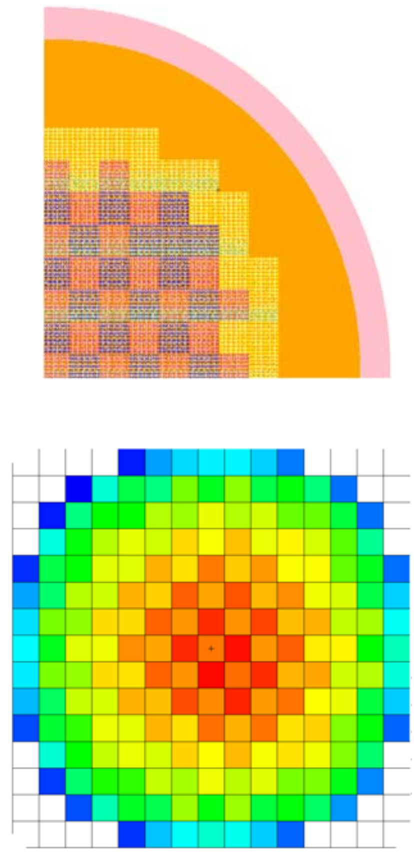
MIT
research reactor



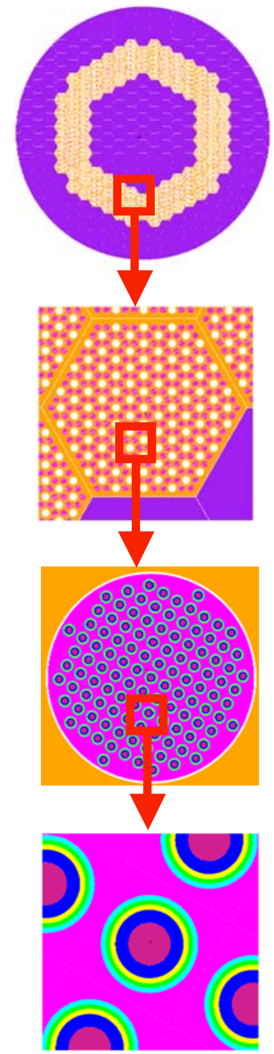
ATR



PWR
(1/4 of geometry)



VHTR
with TRISO fuel



Pictures from
mcnp plotter

Accurate & explicit modeling at multiple levels

Perspective

- Bigger, faster computers ➜ more Monte Carlo calculations
  ➜ better local statistics
- Principal uses of Monte Carlo have evolved:

  1960s: K-effective

  Today: K-effective, detailed 3D whole-core, depletion, reactor design parameters, …

➜ More important now than ever to address the fundamental theory & best practices for Monte Carlo criticality calculations

Longstanding problems with the fundamental theory:

- Convergence of K_{eff} & source distribution
- Bias in K_{eff} & tallies
- Bias in statistics on tallies

Power Method for Monte Carlo Criticality Calculations

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

Initial guess: $Keff^{(0)}$, $\Psi^{(0)}$

Outer iterations (n)

- Inner iterations to solve for $\Psi^{(n+1)}$

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

- Solve linear equations or sweep through space/angle mesh

- Compute new Keff

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

- Renormalize $\Psi^{(n+1)}$
- If converged ➜ stop

.....

Monte Carlo

Initial guess: $Keff^{(0)}$, $\Psi^{(0)}$

Outer iterations (n)

- Follow histories to solve for $\Psi^{(n+1)}$

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

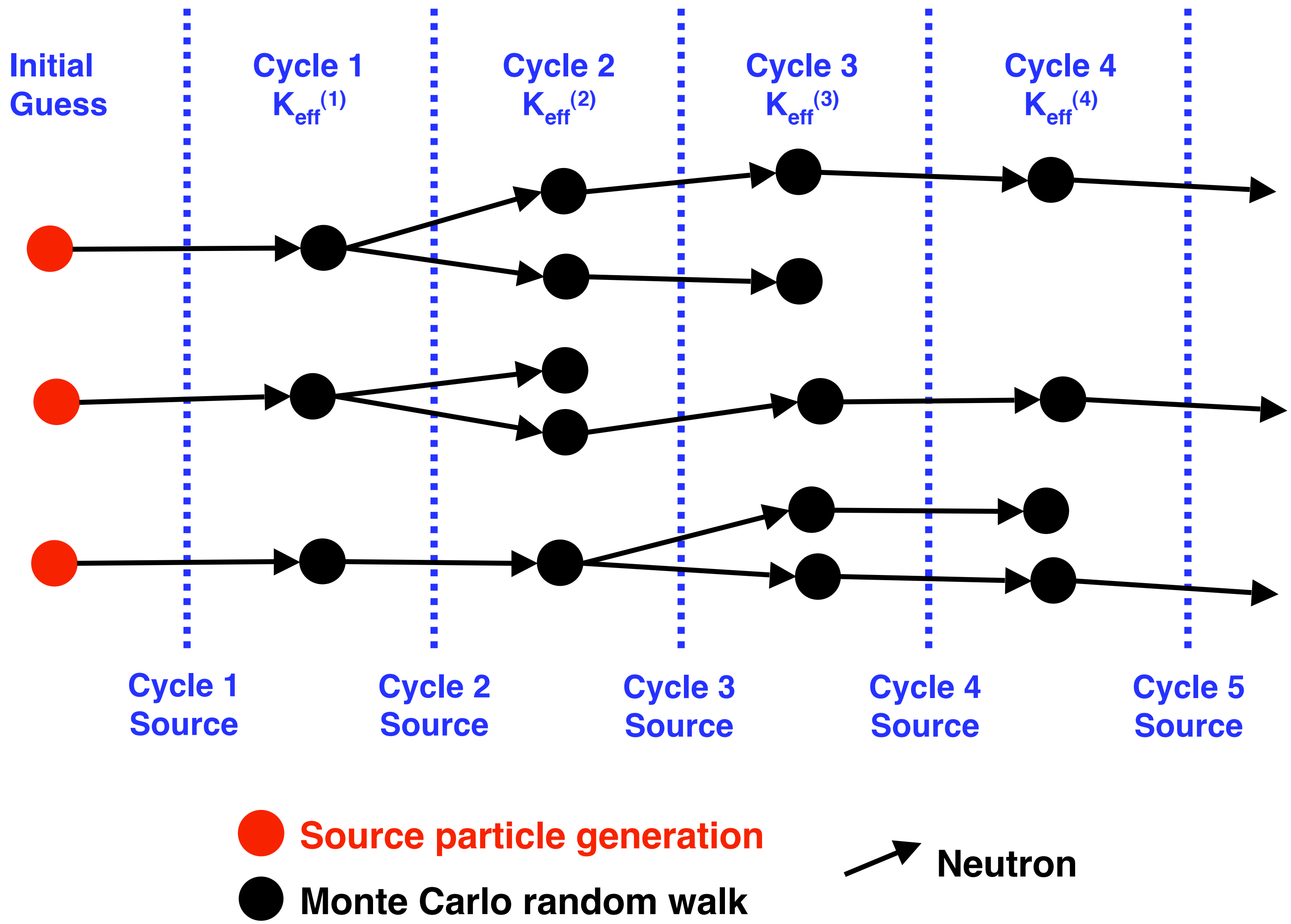
- During histories, save fission sites to use for source in next iteration

- Compute new Keff
  - Tally $Keff^{(n+1)}$ during histories

- Renormalize $\Psi^{(n+1)}$
- If converged ➜ turn on tallies
- If statistics small enough ➜ stop

.....

- Power iteration for Monte Carlo k-effective calculation



Concerns

- **Assessing convergence of Keff & fission distribution**
  - Keff and fission distribution converge differently
  - Both should be converged before beginning tallies
- **Bias in Keff & tallies**
  - Power iteration requires renormalization every cycle
  - MC renormalization involves dividing by a stochastic quantity, which introduces bias in Keff & tallies
- **Bias in uncertainties on tallies**
  - MC codes ignore cycle-to-cycle correlation when computing statistics
  - MC codes give statistics that are <u>too small</u>

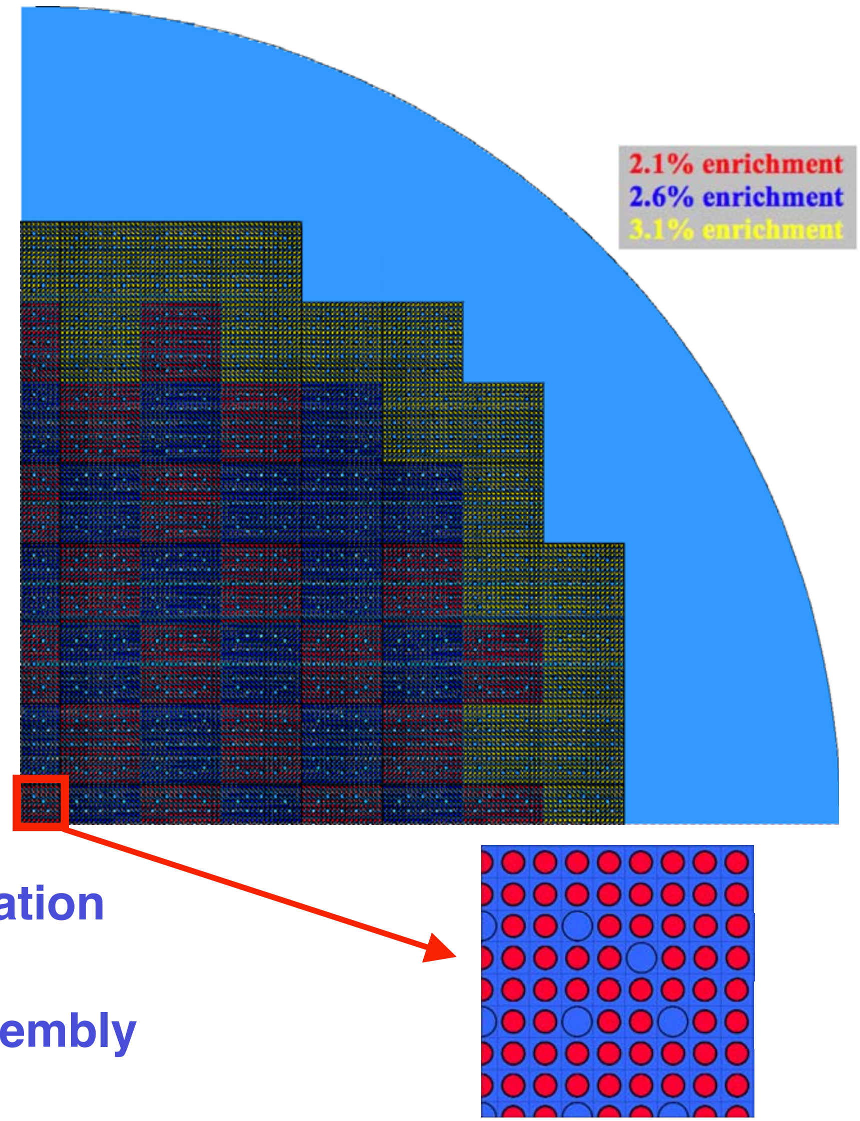
This talk:

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

Example Problem

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 of Source Distribution

Power Iteration Convergence

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

  n = cycle number, k_0,u_0 - fundamental, k_1,u_1 - 1st higher mode

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

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

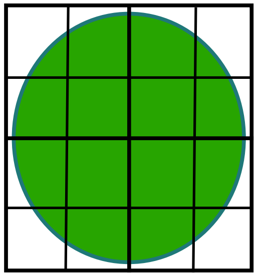
  - **First-harmonic source errors die out as ρ^n, $\rho = k_1 / k_0 < 1$**
  - **First-harmonic K_{eff} errors die out as $\rho^{n-1}(1-\rho)$**
  - **<u>Source converges slower than K_{eff}</u>**

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

- **MCNP5 also gives Shannon entropy of the source distribution, H_{src}**

Source Convergence Diagnostic - H_{src}

- 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) converges

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

Source Convergence - Dominance Ratio

Monte Carlo Codes
X-3-MCC, LANL

- **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	$\rho \sim .94$

  – **Use Wielandt method** (when available) to increase the average number of generations per cycle, L

  PWR 1/4 core example:

	L = 1	$\rho \sim .96$
	L = 5	$\rho \sim .83$
	L = 10	$\rho \sim .72$
	L = 20	$\rho \sim .57$

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

Source Convergence - Initial Guess

- Better initial source guess $\Rightarrow$ fewer cycles to converge

- Typical

  – Point at center - terrible guess

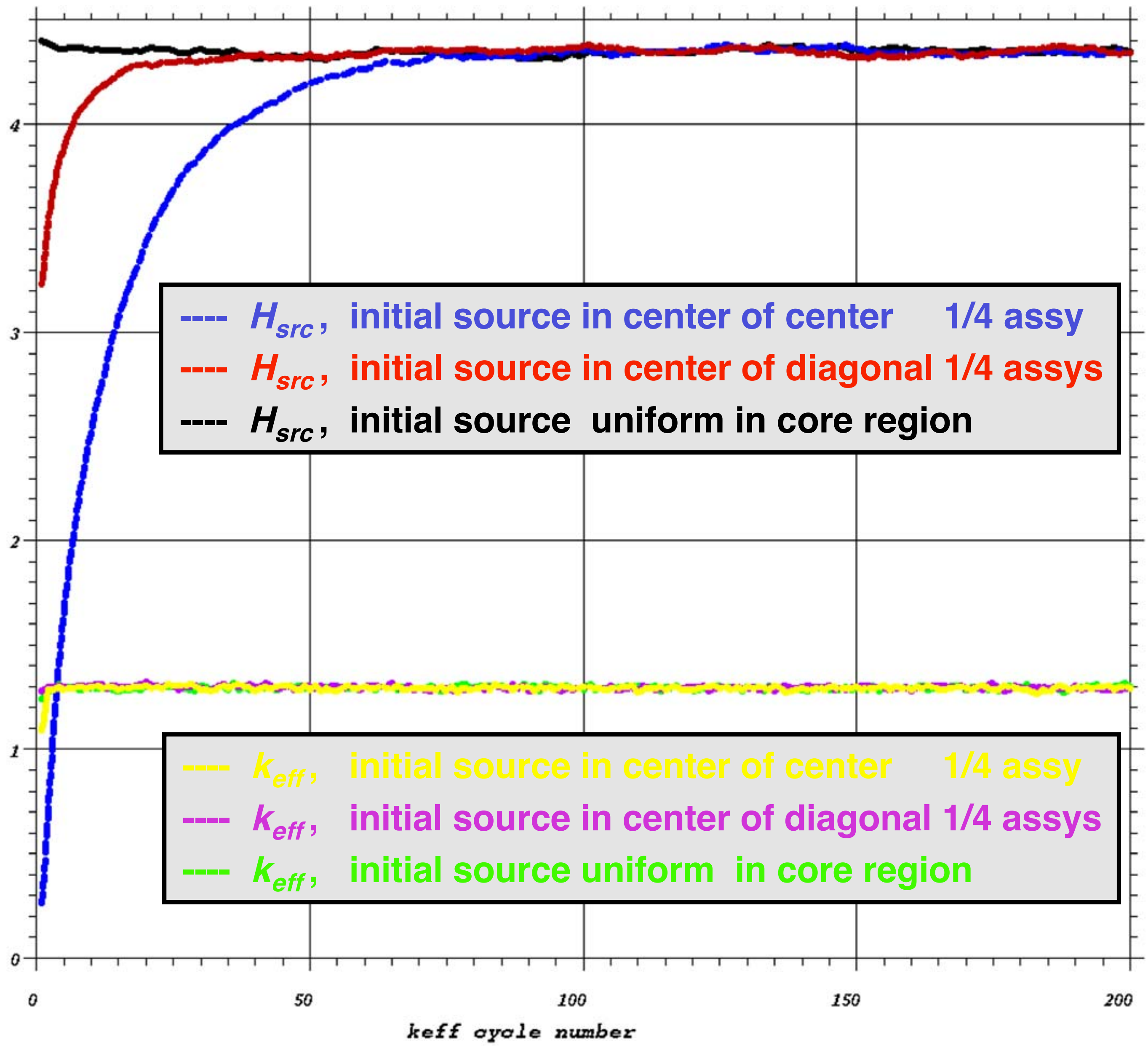
  – Reactor:

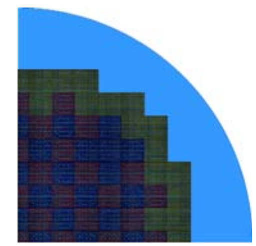
    uniform in core region - good guess

  – Criticality Safety:

    points in each fissionable region, or
    uniform in each fissionable region - good guess

Convergence for Different Source Guesses





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**
- **Use Wielandt method, when available**
- **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

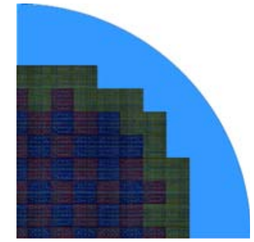
- **Bias in Keff, due to renormalization**

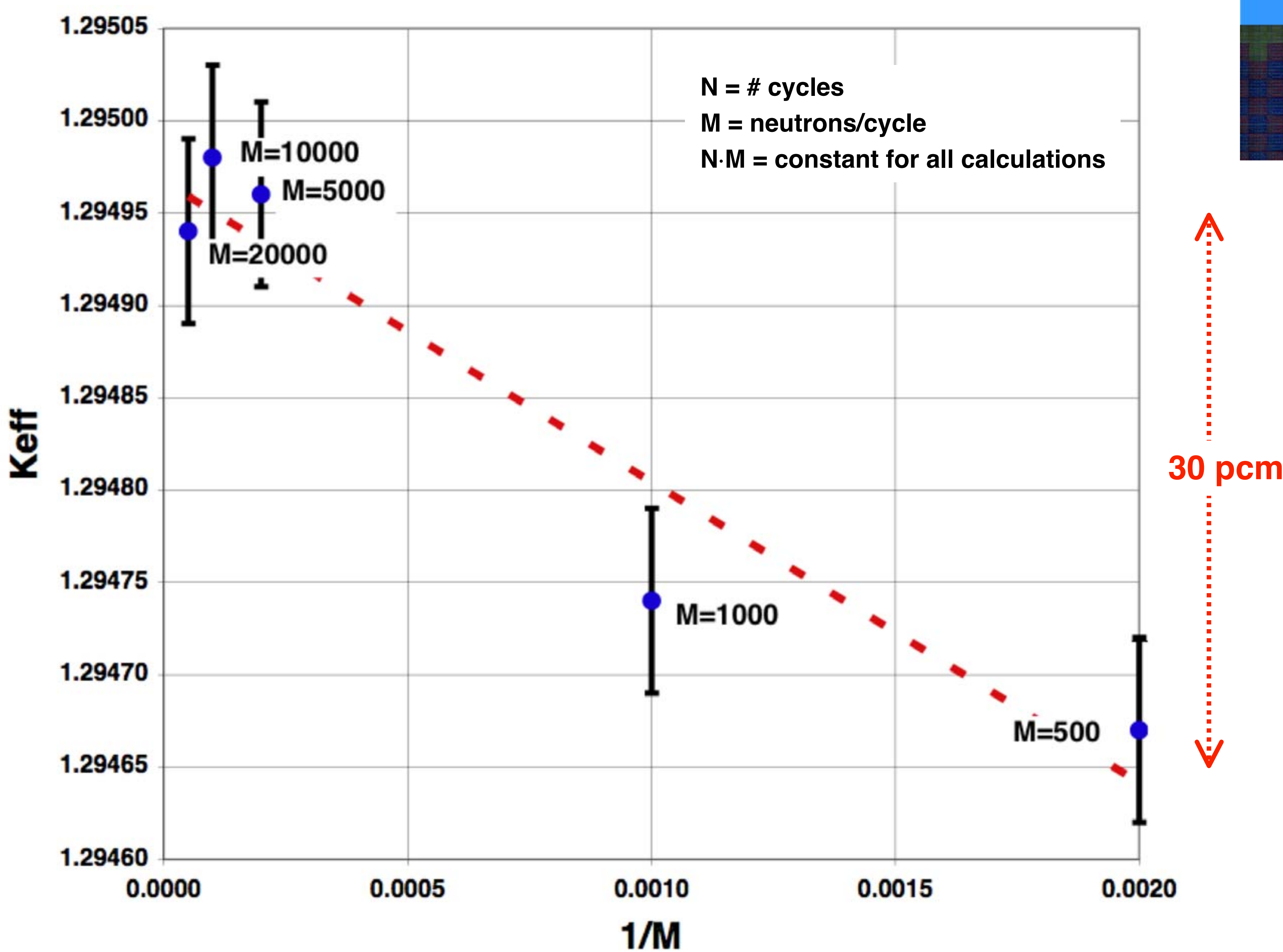
$$\text{bias in } K_{eff} = -\frac{\sigma_k^2}{K_{eff}} \cdot \left(\begin{matrix} \text{sum of lag-i correlation} \\ \text{coeff's between batch K's} \end{matrix} \right) \propto \frac{1}{M_0}$$

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

Bias in Keff




Keff
1.29505
1.29500
1.29495
1.29490
1.29485
1.29480
1.29475
1.29470
1.29465
1.29460
0.0000
0.0005
0.0010
0.0015
0.0020
1/M
N = # cycles
M = neutrons/cycle
N·M = constant for all calculations
M=10000
M=5000
M=20000
M=1000
M=500
30 pcm

Bias in Fission Tallies

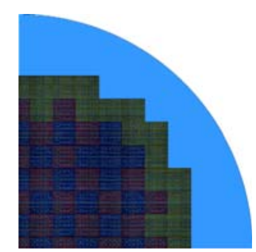
mcnp Monte Carlo Codes X-3-MCC, LANL

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%

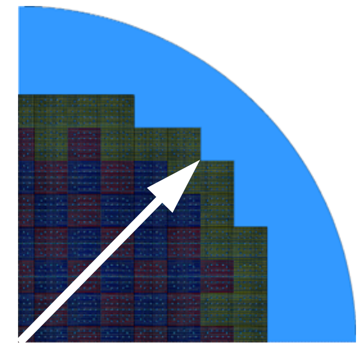
Statistics ~ .1% to .3%



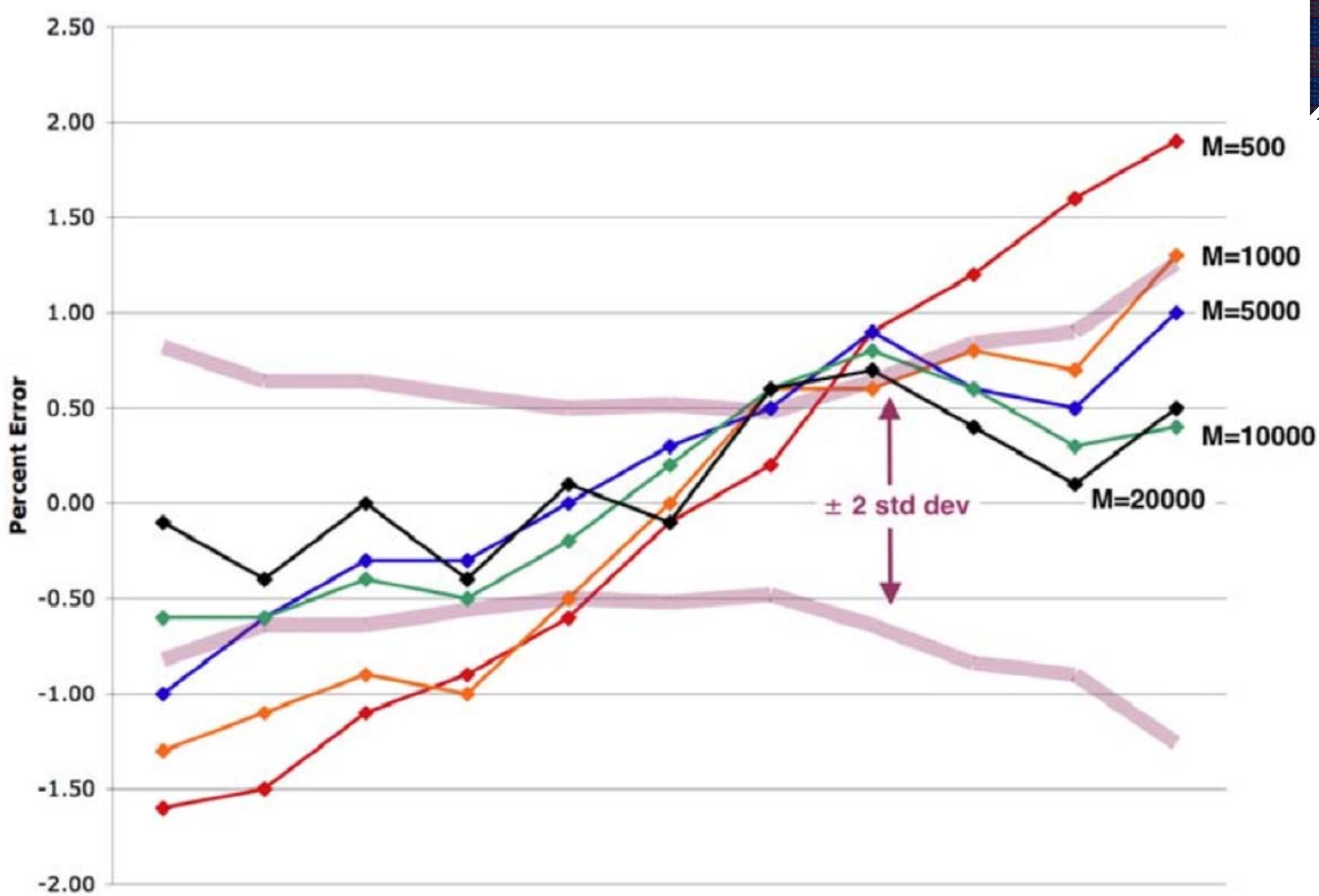
RMS error = 1.1 %
MCNP std deviations: .1% - .3%
True std deviations: .3% - .8%

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

Bias in Fission Tallies



Percent error in fission rates along diagonal



Bias in Keff & Tallies

- **Past work - eliminating bias**
  - **MacMillan**
    - Weight the tallies for each cycle **n** by

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

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

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 negligible with 10,000 or more neutrons per cycle**

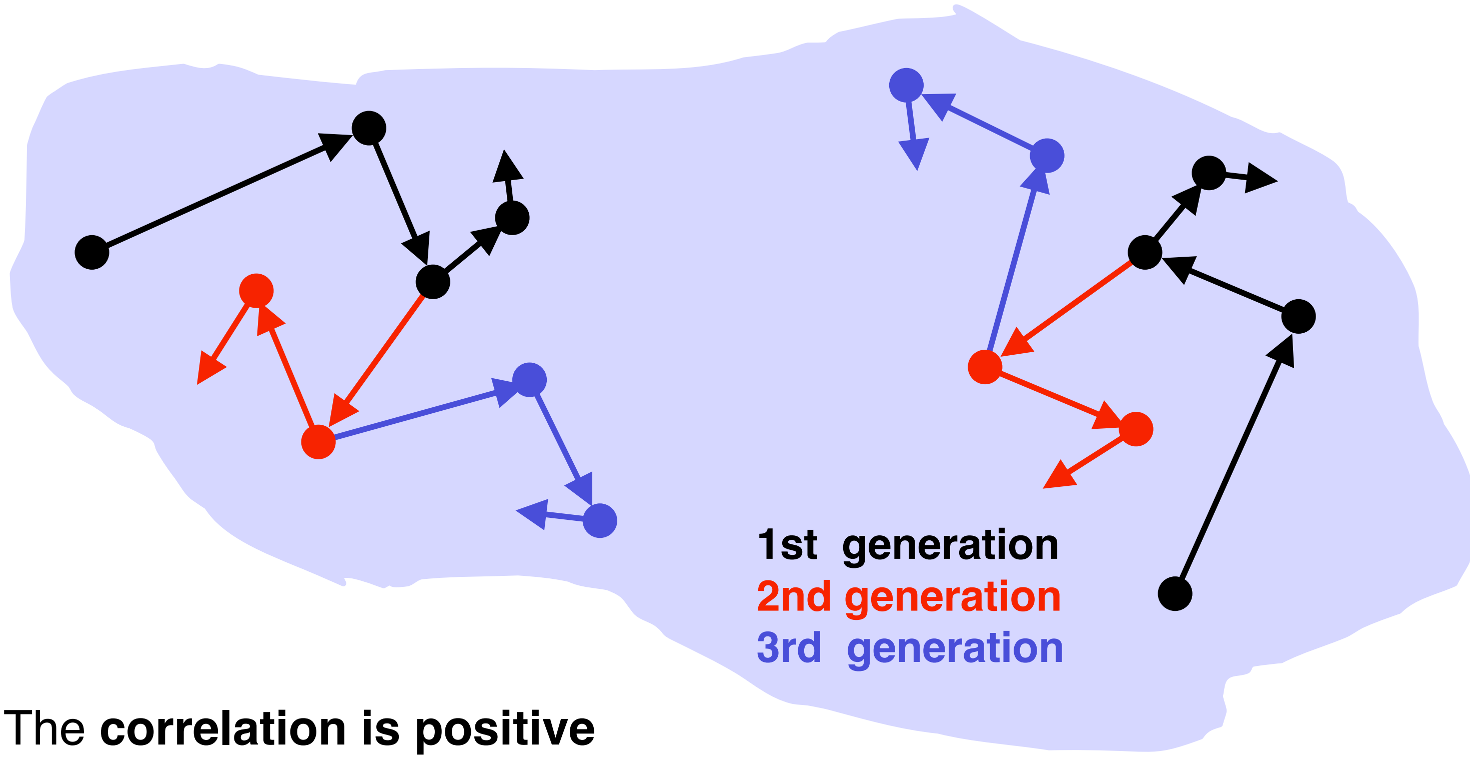
- **Practical solution - use large M (neutrons/cycle)**
  - For M ~ 10K or more ⇒ bias negligible
  - Large M gives more efficient parallel calculations

- **Wielandt's method also reduces bias**
  - Reduces frequency of renormalizations, reduces correlation

Underprediction Bias in Confidence Intervals

in Monte Carlo Keff Calculations

- **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)**

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

$$\tilde{\sigma}_{\bar{X}}^2 = \frac{1}{N} \cdot \left(\frac{\sum_{n=1}^{N} X_n^2}{N-1} - \bar{X}^2 \right) \quad =$$

variance computed by codes, assuming independence of X_n's

$$\sigma_{\bar{X}}^2 \approx \tilde{\sigma}_{\bar{X}}^2 + \tilde{\sigma}_{\bar{X}}^2 \cdot 2 \cdot \sum_{i=1}^{\infty} r_i \quad =$$

True variance, including correlations
r_i = lag-i correlation coef. between X_n's

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

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

Variance underprediction bias is independent of N and M

Correlation vs Tallies

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

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

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

MCNP:	generation tallies for Keff, **history** tallies for everything else	Larger
VIM, KENO, RACER, RCP, …:	**generation** tallies	Correlation & Bias
MCNP+Wielandt, MONK:	**several generations**	↓
Repeated MC runs, averaged:	**all generations** from each run	None

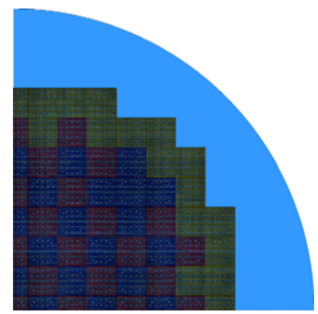
Bias in Uncertainties

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



Past Work - Bias in Uncertainties

$$\frac{\text{True } \sigma_{\bar{x}}^2}{\text{Computed } \sigma_{\bar{x}}^2} = 1 + 2 \cdot \sum_{k=1}^{\infty} r_k$$

- MacMillan (1973) [similar approach by Gast in 1974]
  - **Calculate r_1** for each tally (lag-1 inter-cycle correlation coefficient)
  - **Assume dominance ratio ρ is known**
  - **Assume $r_k \le r_1 \cdot \rho^k$** for k=2,3,….
  - Then,

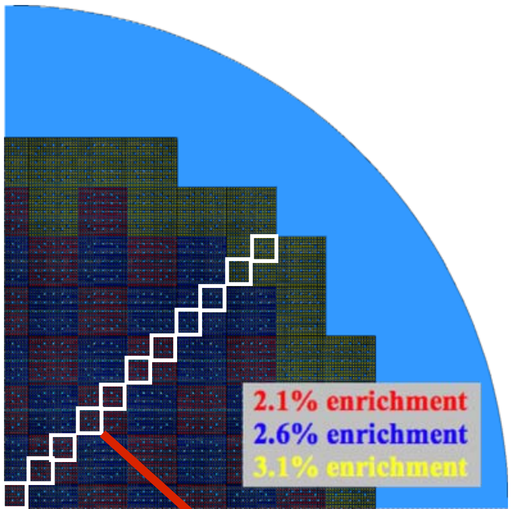
$$\frac{\text{True } \sigma_{\bar{x}}^2}{\text{Computed } \sigma_{\bar{x}}^2} \le 1 + \frac{2 \cdot r_1}{1-\rho}$$

  - This factor can then be used to correct the computed σ for the tally
  - **Difficulties:**
    - Only gives a conservative upper bound
    - Useless if ρ near 1.0
    - Requires extra storage for each tally
    - **Notoriously sensitive to noise ….**
    - **Assumption for higher r_k's may often be incorrect**
    - **Dominance ratio is usually not known**

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** (see next slide)

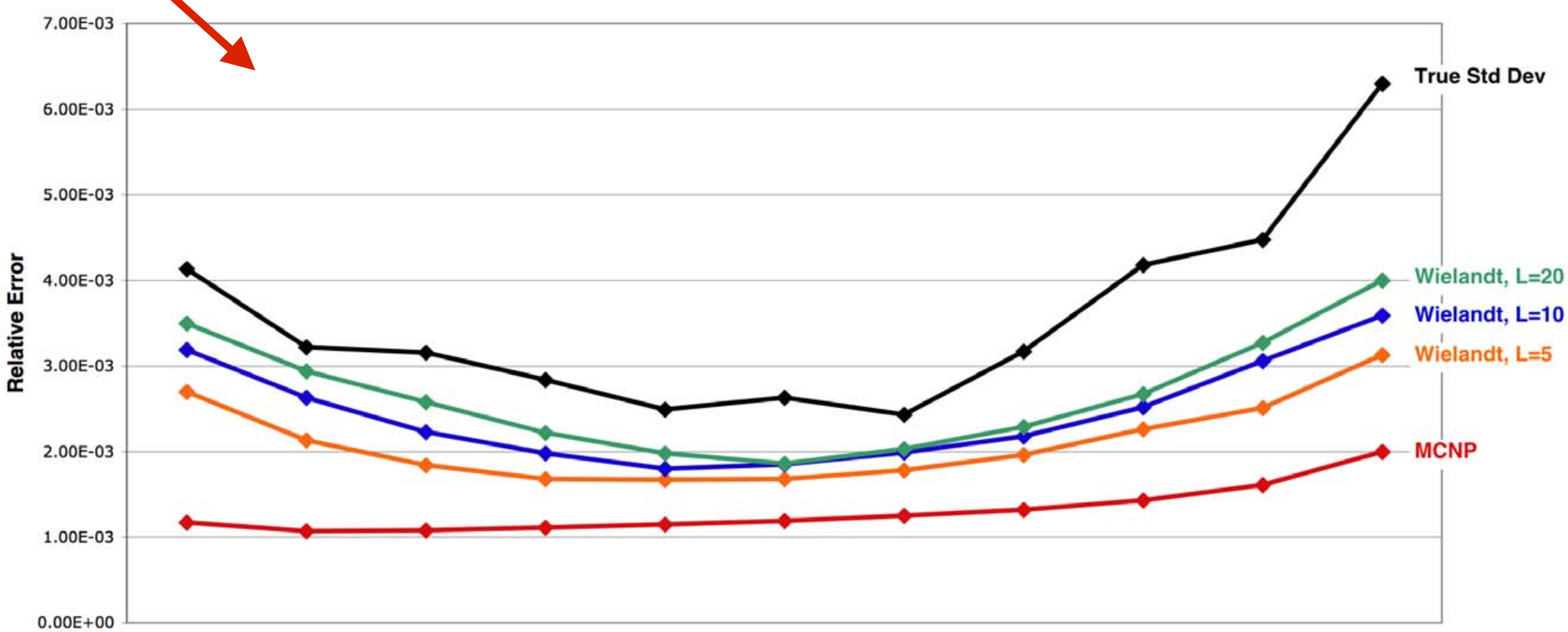
Reduced Uncertainty Bias, using Wielandt



Wielandt's method increases the fission chain-length in each cycle, and reduces inter-cycle correlations

Run the problem using different amounts of Wielandt acceleration (different shift parameters) to get average chain-lengths of 5, 10, 20 generations per cycle

Plot relative error in quarter-assemblies along diagonal



Conclusions

New features for MCNP5 (soon)
+ Wielandt method
+ Dominance ratio calculation

Final remarks

Wielandt Method - Basics

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

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

- Modify the transport equation & solve by power iteration

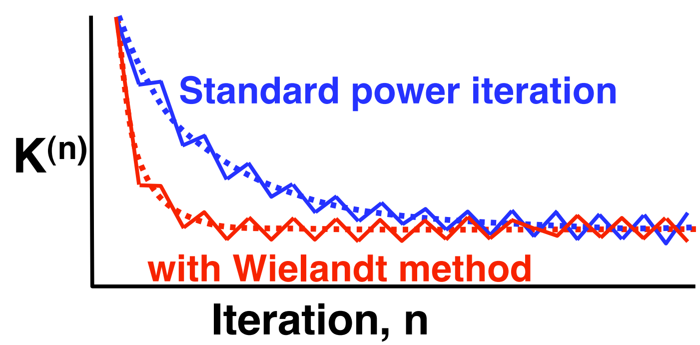
$$(L + T - S - \tfrac{1}{k_e} M)\Psi^{(n)} = (\tfrac{1}{K_{eff}^{(n-1)}} - \tfrac{1}{k_e})M\Psi^{(n-1)}$$

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

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

⇒ Wielandt method will converge in fewer iterations

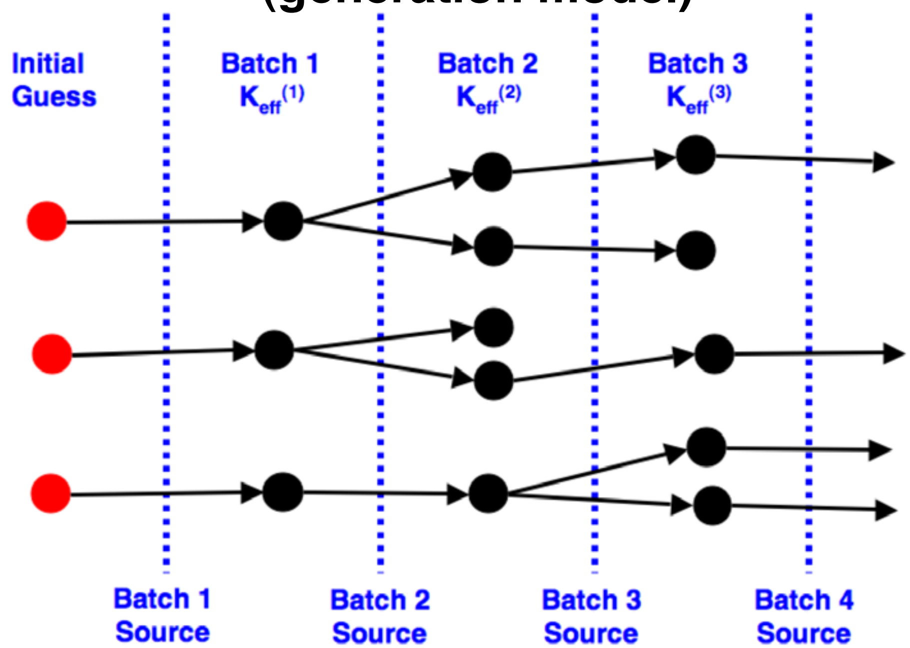
⇒ Reduces inter-cycle correlation, hence improves statistics



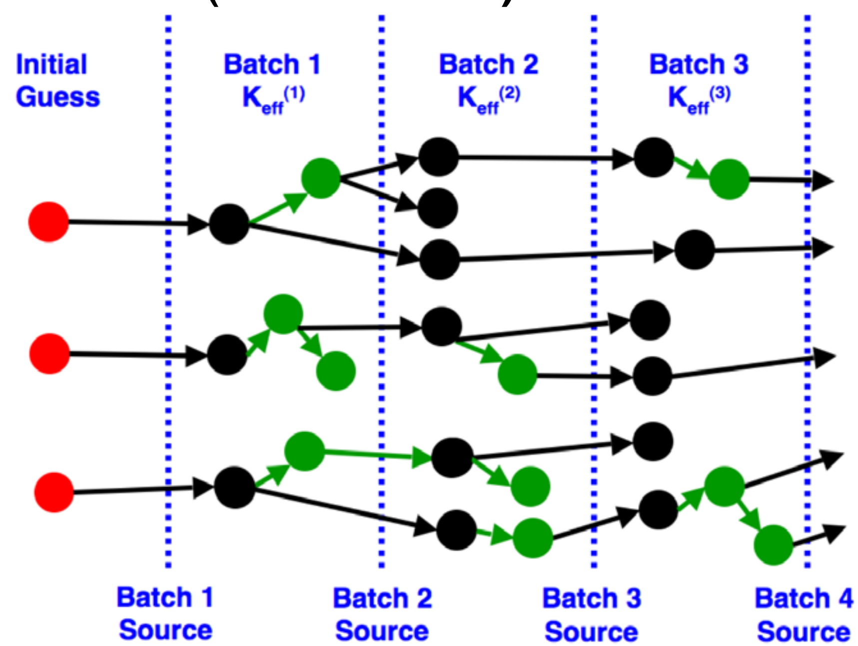
Wielandt Method - Generations vs Iterations

- **Power method:** one neutron generation per iteration
- **Wielandt method:** multiple neutron generations per iteration, <u>varies</u> 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

$k_e = k_0 + \Delta$

Average chain length,
$L = 1 + k_0/\Delta$

Dominance Ratio Calculation in MCNP5

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

Best Practices - Summary

- To avoid bias in K_{eff} & tally distributions, use 10K or more neutrons/cycle
- Always check convergence of both K_{eff} & H_{src}
- 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

References

- **Monte Carlo Methods**
  - F. B. Brown, "Fundamentals of Monte Carlo Particle Transport," LA-UR-05-4983, available at http://mcnp.lanl.gov/publications (2005).
- **Monte Carlo k-effective Calculations**
  - J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," Nukleonik 11,213 (1968).
  - M. R. Mendelson, "Monte Carlo Criticality Calculations for Thermal Reactors," Nucl. Sci Eng. 32, 319-331 (1968).
  - H. Rief and H. Kschwendt, "Reactor Analysis by Monte Carlo," Nucl. Sci. Eng., 30, 395 (1967).
  - W. Goad and R. Johnston, "A Monte Carlo Method for Criticality Problems," Nucl. Sci. Eng. 5, 371-375 (1959).
  - J Yang & Y. Naito, "The Sandwich Method for Determining Source Convergence in Monte Carlo Calculations", Proc. 7th Int. Conf. Nuclear Criticality Safety, ICNC2003, Tokai-mura, Iburaki, Japan, Oct 20-24, 2003, JAERI-Conf 2003-019, 352 (2003).
- **Superhistory Method**
  - R.J. Brissenden and A.R. Garlick, "Biases in the Estimation of Keff and Its Error by Monte Carlo Methods," Ann. Nucl. Energy, Vol 13, No. 2, 63-83 (1986).
- **Wielandt Method**
  - F.B. Brown, “Wielandt Acceleration for MCNP5 Monte Carlo Eigenvalue Calculations”, M&C+SNA-2007, LA-UR-07-1194 (2007)
  - T Yamamoto & Y Miyoshi, "Reliable Method for Fission Source Convergence of Monte Carlo Criticality Calculation with Wielandt's Method", J. Nuc. Sci. Tech., 41, No. 2, 99-107 (Feb 2004).
  - S Nakamura, Computational Methods in Engineering and Science, R. E. Krieger Pub. Company, Malabar, FL (1986).
- **Shannon entropy & convergence**
  - T. Ueki & F.B. Brown, “Stationarity and Source Convergence in Monte Carlo Criticality Calculations”, ANS Topical Meeting on Mathematics & Computation, Gatlinburg, TN April 6-11, (2003).
  - T. Ueki & F.B. Brown, “Stationarity Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations”, Nucl. Sci. Eng. 149, 38-50 (2005)
  - F.B. Brown, “On the Use of Shannon Entropy of the Fission Distribution for Assessing Convergence of Monte Carlo Critiicality Calculations”, proceedings PHYSOR-2006, Vancouver, British Columbia, Canada (Sept 2006).

References

- **Bias, correlation, & statistics**

  - E.M. Gelbard and R.E. Prael, "Monte carlo Work at Argonne National Laboratory", in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).
  - R. C. Gast and N. R. Candelore, "Monte Carlo Eigenfunction Strategies and Uncertainties," in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).
  - R. J. Brissenden & A. R. Garlick, “Biases in the Estimation of Keff and Its Error by Monte Carlo Methods,” Ann. Nucl. Energy, 13, 2, 63-83 (1986)
  - D. B. MacMillan, “Monte Carlo Confidence Limits for Iterated-Source Calculations,” Nucl. Sci. Eng., 50, 73 (1973).
  - E. M. Gelbard and R. E. Prael, “Computation of Standard Deviations in Eigenvalue Calculations,” Prog. Nucl. Energy, 24, 237 (1990).
  - T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations", Nucl. Sci. Eng. 141, 101-110 (2002)
  - L.V. Maiorov, "Estimates of the Bias in the Results of Monte Carlo Calculations of Reactors and Storage Sites for Nuclear Fuel", Atomic Energy, Vol 99, No 4, 681-693 (2005).
  - T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations", Nucl. Sci. Eng. 141, 101-110 (2002)
  - T. Ueki and F. B. Brown, “Autoregressive Fitting for Monte Carlo K-effective Confidence Intervals,” Trans. Am. Nucl. Soc., 86, 210 (2002).
  - T. Ueki, “Time Series Modeling and MacMillan’s Formula for Monte Carlo Iterated-Source Methods,” Trans. Am. Nucl. Soc., 90, 449 (2004).
  - T. Ueki & B. R. Nease, "Times Series Analysis of Monte Carlo Fission Sources - II: Confidence Interval Estimation", Nucl. Sci. Eng., 153, 184-191 (2006).
  - O. Jacquet et al., “Eigenvalue Uncertainty Evaluation in MC Calculation, Using Time Series Methodologies,” Proc. Int. Conf. Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications (Monte Carlo 2000), Lisbon, Portugal, October 23–26, 2000. A. KLING et al., Eds., Springer-Verlag, Berlin, Heidelberg (2001).

Abstract

LA-UR-09-02377

A Review of Monte Carlo Criticality Calculations - Convergence, Bias, Statistics

Forrest B. Brown (LANL)

Monte Carlo criticality calculations have been performed for over 50 years for reactor physics and criticality safety applications. With today's faster computers, these calculations are being carried out to greater precision (smaller uncertainties) in keff, and detailed distributions of power and reaction rates are being computed routinely. This paper provides a review of the fundamental theory of Monte Carlo criticality calculations, with guidance on practical methods for: (1) assuring convergence of both keff and the source distribution, (2) minimizing the bias in keff and reaction rate distributions, and (3) dealing with the underprediction bias in uncertainties for keff and reaction rate distributions.

Introduction

Perspective

- Bigger, faster computers ➜ more Monte Carlo calculations
  ➜ better localized statistics

- Principal uses of Monte Carlo have evolved:

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

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

➜ More important now than ever to address the fundamental theory & best practices for Monte Carlo criticality calculations

Current Monte Carlo codes can model almost any geometry, with continuous-energy cross-sections & collision physics

But …..

Longstanding problems with the fundamental theory:

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

Problems (1) - (4) have been addressed in the last few years.
MCNP5 features exist, or are coming this year.