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Title: FUNDAMENTALS OF MONTE CARLO PARTICLE TRANSPORT

Author(s): FORREST B. BROWN

Submitted to: Lecture notes for Monte Carlo course

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Fundamentals of Monte Carlo Particle Transport

Forrest B. Brown

Monte Carlo Group (X-3)

Los Alamos National Laboratory

Eigenvalue Calculations Part I

Forrest B. Brown
Diagnostics Applications Group (X-5)
Los Alamos National Laboratory

Time-dependent Transport

- **Time-dependent neutron transport with (prompt) fission source**

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

This equation can be solved directly by Monte Carlo

- 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, …

Overall time-behavior $\psi(r,E,\Omega,t) = \Psi(r,E,\Omega)\,e^{\alpha t}$ can be estimated by

$$\alpha \approx \frac{\ln W_2 - \ln W_1}{t_2 - t_1} \qquad \text{where } W_j = \sum_{k=1}^{N_{particles}} wgt_k(t_j)$$

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
- **If it is assumed that** $\psi(r,E,\Omega,t) = \Psi_\alpha(r,E,\Omega)\, e^{\alpha t}$, then substitution into the time-dependent transport equation yields

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

$$+ \frac{\chi(E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\,\Psi_\alpha(\vec{r},E',\vec{\Omega}')\,d\vec{\Omega}'dE'$$

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

$$\left[\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E)\right]\Psi_k(\vec{r},E,\vec{\Omega}) = \iint \Psi_k(\vec{r},E',\vec{\Omega}')\Sigma_S(\vec{r},E'\rightarrow E,\vec{\Omega}\cdot\vec{\Omega}')d\vec{\Omega}'dE'$$
$$+ \quad \frac{1}{K_{eff}}\cdot\frac{\chi(E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\Psi_k(\vec{r},E',\vec{\Omega}')d\vec{\Omega}'dE'$$

- 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. [Use α and Ψ_α instead]
- 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 & eigenfunction used for time-dependent problems
  - K_{eff} eigenvalue & 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 simulated directly using Monte Carlo methods
- α eigenvalue problems are solved by Monte Carlo indirectly using a series of K_{eff} calculations

K-Eigenvalue Calculations

- **Eigenvalue problems – reactor analysis & criticality safety**

$$\Psi(\mathbf{p}) = \int \Psi(\mathbf{p}')\mathbf{R}(\mathbf{p}' \rightarrow \mathbf{p})d\mathbf{p}' \quad + \quad \frac{1}{K_{eff}} \int \Psi(\mathbf{p}')\mathbf{F}(\mathbf{p}' \rightarrow \mathbf{p})d\mathbf{p}'$$

$$\Psi = \mathbf{R} \bullet \Psi + \frac{1}{K_{eff}} \mathbf{F} \bullet \Psi$$

Iterative solution, using power iteration method

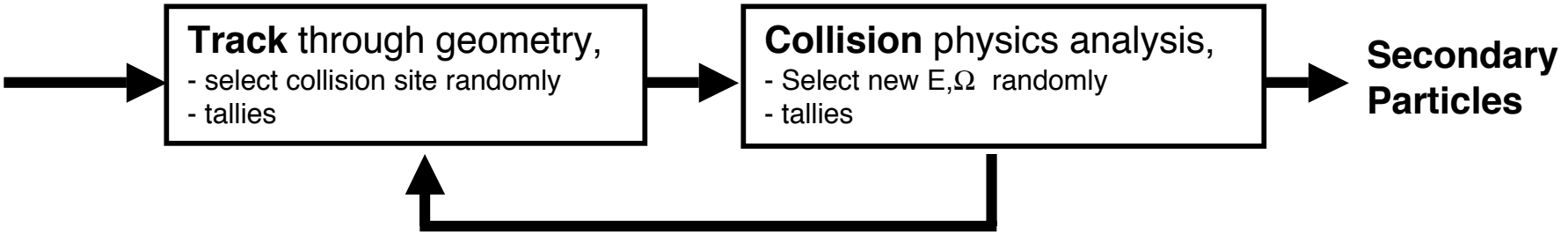
$$\Psi^{(i+1)} = \mathbf{R} \bullet \Psi^{(i+1)} + \frac{1}{K_{eff}^{(i)}} \mathbf{F} \bullet \Psi^{(i)}$$

$$\Psi^{(i+1)} = \frac{1}{K_{eff}^{(i)}} [\mathbf{I} - \mathbf{R}]^{-1} \mathbf{F} \bullet \Psi^{(i)} \qquad K_{eff}^{i} = \int \mathbf{F} \bullet \Psi^{(i)} d\mathbf{p}d\mathbf{p}'$$

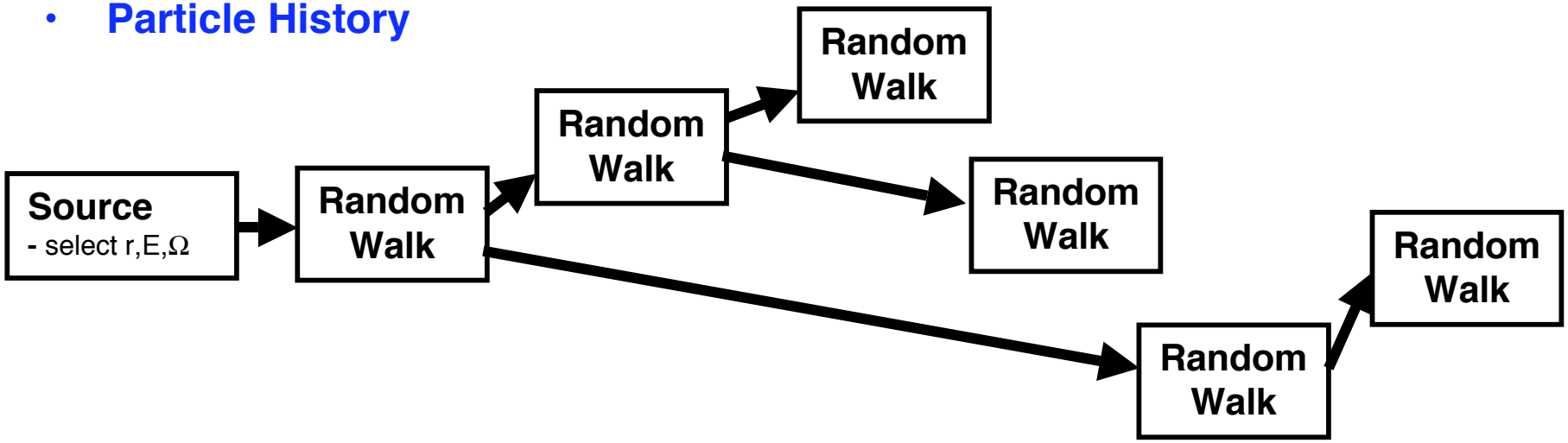
- **Monte Carlo approach:**
  - Guess $\Psi^{(0)}$, $K_{eff}^{(0)}$
  - Follow a "batch" of histories, estimate $\Psi^{(i)}$, $K_{eff}^{(i)}$
  - Repeat until converged (discard tallies)
  - After converging, begin tallies, iterate until variances small enough

Particle Histories

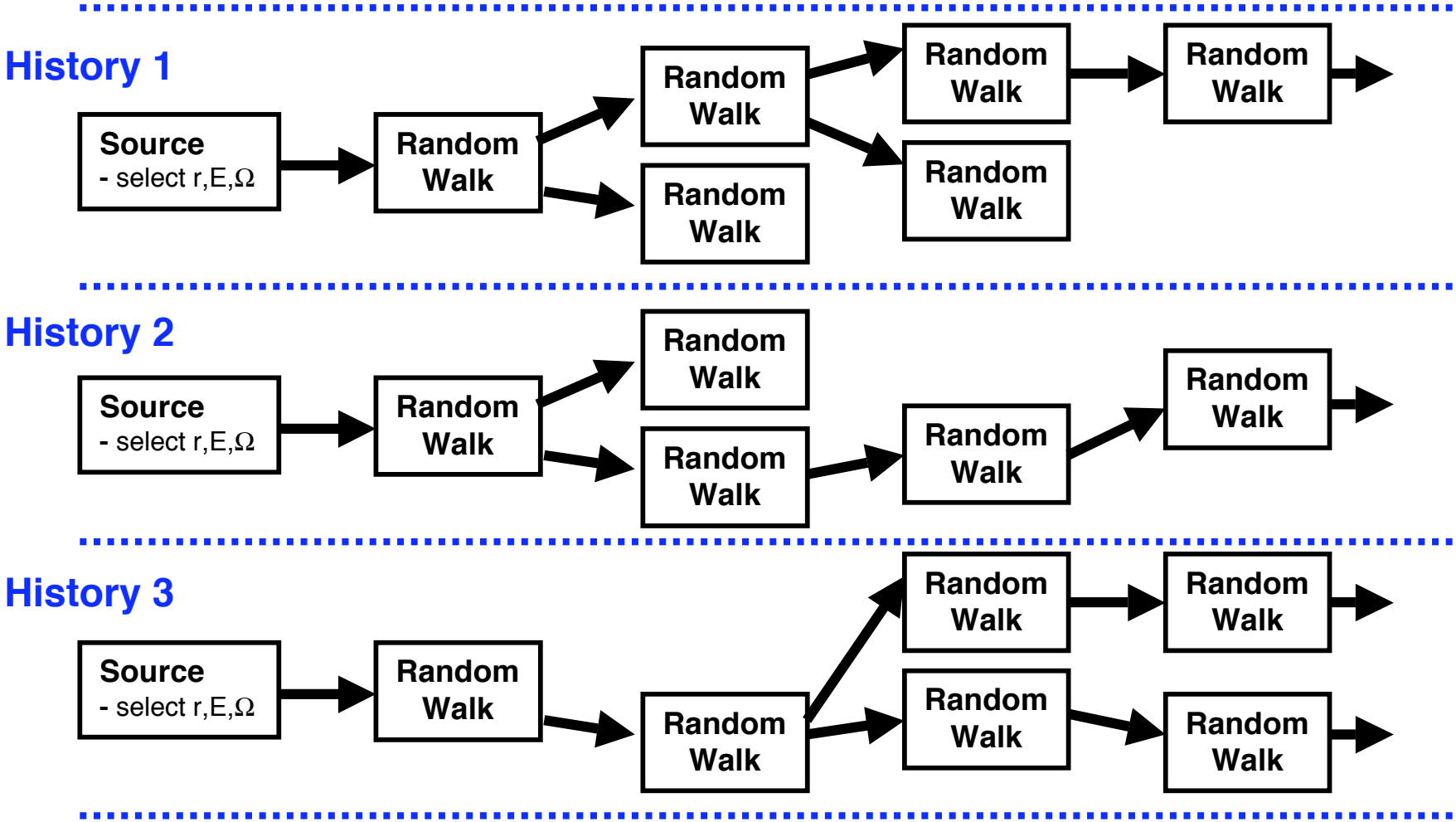
- **Random Walk for particle**



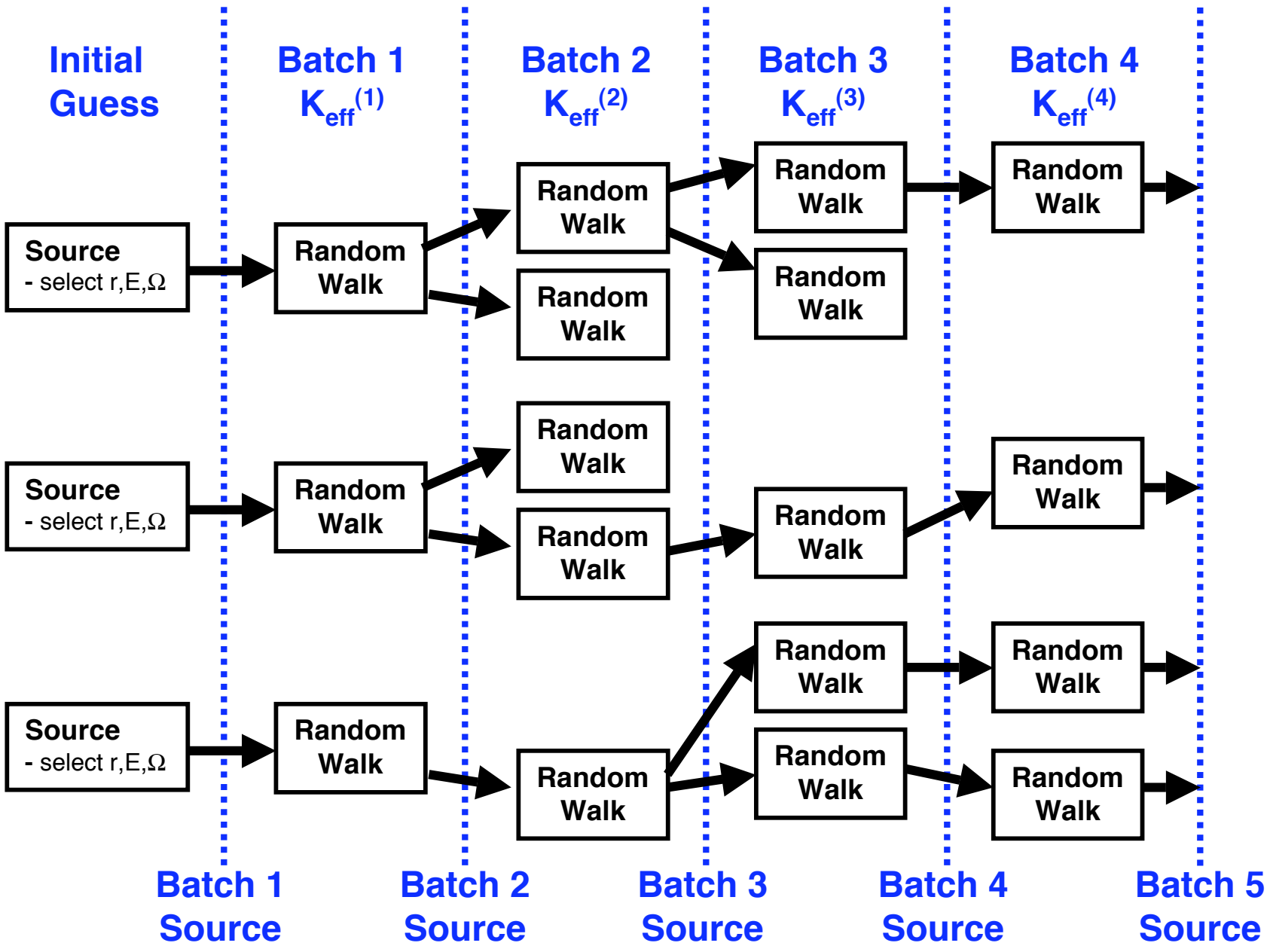
- **Particle History**



Fixed-source Monte Carlo Calculation



Monte Carlo Eigenvalue calculation

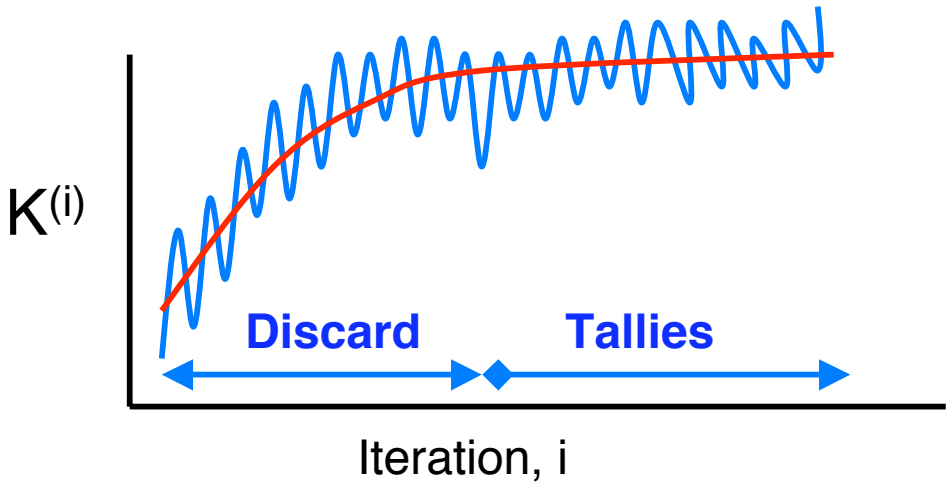


Monte Carlo Solution of K_{eff} Problems

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 … 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 $n \leq D$, discard any tallies
    - If $n > D$, accumulate tallies
  - Estimate $K_{cycle}^{(n)}$
- Compute final results & statistics using last **N** cycles

K-Calculations — Convergence



Monte Carlo

Deterministic (Sn)

- Guess an initial source distribution
- Iterate until converged (How do you know ???)
- Then
  - For Sn code: done, print the results
  - For Monte Carlo: start tallies, keep running until uncertainties small enough
- **Batch size? Convergence? Stationarity? Bias? Statistics?**

K-Calculations — Banking Fission Sites

- During a particle random walk,

$$\mathbf{wgt} \cdot \frac{\nu\Sigma_F}{\Sigma_T}$$ = expected number of fission neutrons created at collision point

- Averaged over all collisions for all histories, the expected value for $wgt \cdot \nu\Sigma_F / \Sigma_T$ 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:

$$\mathbf{R = wgt} \cdot \frac{\nu\Sigma_F}{\Sigma_T} \cdot \frac{1}{K}, \qquad n = \lfloor R \rfloor$$

If $\xi < R - n$, **store** $n+1$ **sites in bank with** $wgt' = K$

Otherwise, **store** n **sites in bank with** $wgt' = K$

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: $E[N'_J] = K_{eff} \cdot N_J$
  - (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 — Overall Keff

- The Keff estimators from each cycle (K_{path}, $K_{collision}$, $K_{absorption}$) are used to compute the overall K_{path}, $K_{collision}$, & $K_{absorption}$ for the problem & the standard deviations.

- The Keff estimators from each cycle (K_{path}, $K_{collision}$, $K_{absorption}$) can also be combined to produce a minimum-variance combined result, $K_{combination}$. This combination must account for correlations between the path, collision, & absorption estimators

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

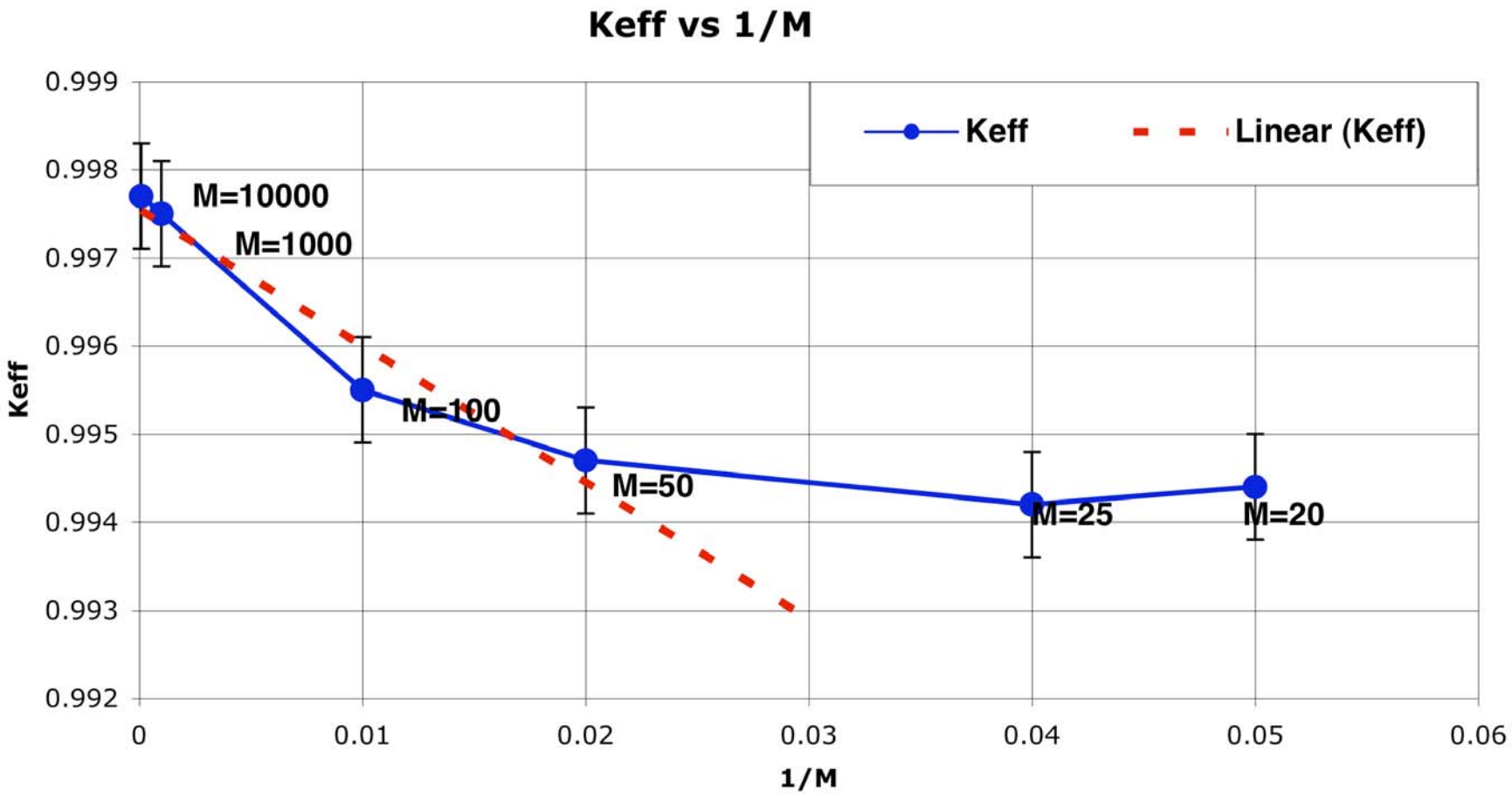
$$\text{bias in } K_{eff} = -\frac{\sigma_k^2}{K_{eff}} \cdot \begin{pmatrix} \text{sum of correlation coeff's} \\ \text{between batch K's} \end{pmatrix}$$

  - 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)]

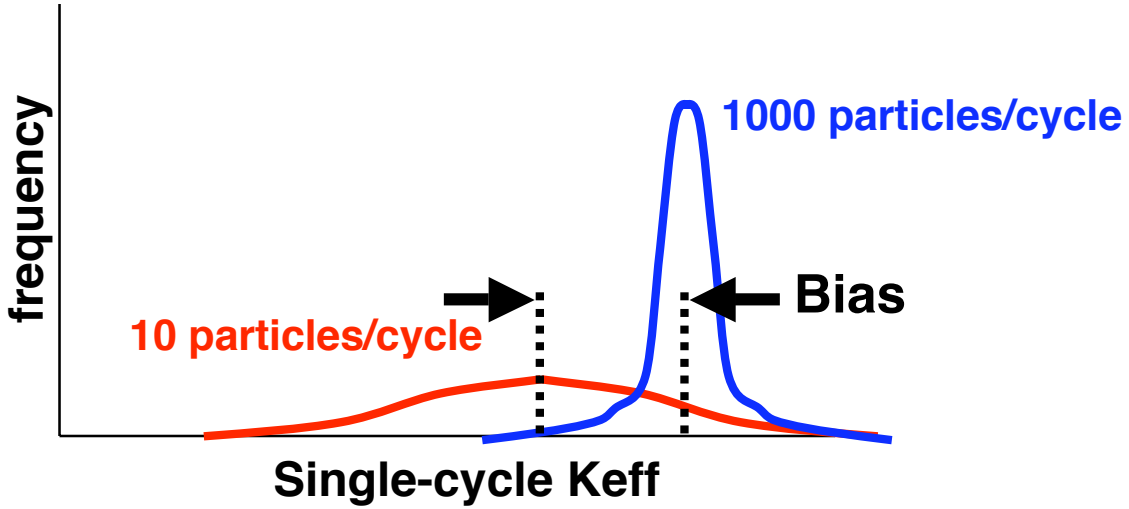
K-Calculations — Bias

- 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 1000 or more particles/cycle, preferably 5000, 10000, or more**

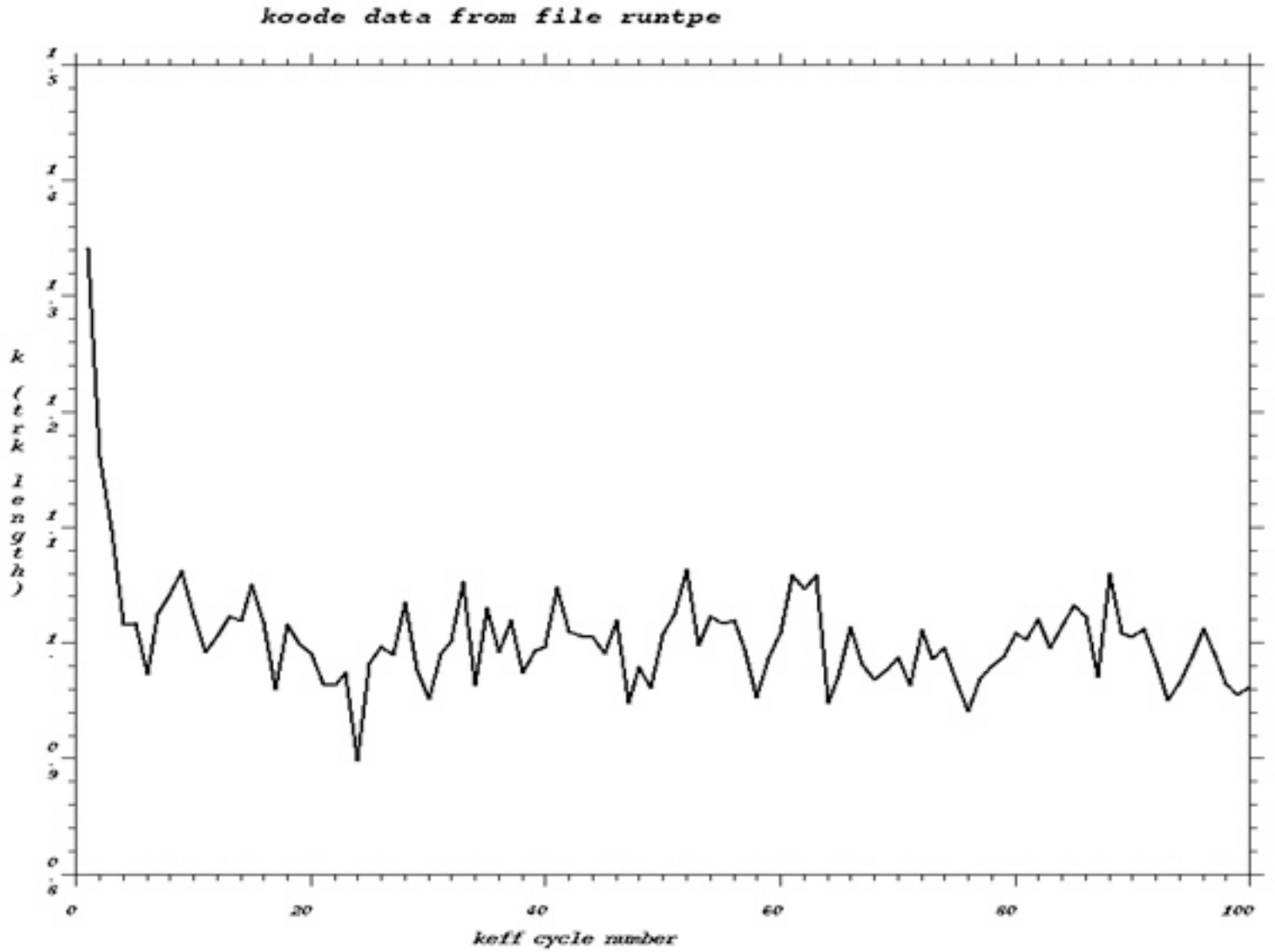
K-Calculations — Convergence

- **Some number of initial cycles must be discarded**
  - The source distribution & Keff are not known initially
  - Guess at the source & Keff
  - Iterate, discarding tallies
  - When converged, iterate to accumulate tallies

- **Number of iterations to discard depends on the dominance ratio**
  - Dominance Ratio = K_1 / K_{eff}
    - K_{eff} = eigenvalue of fundamental eigenmode
    - K_1 = eigenvalue of first higher eigenmode, $K_1 < K_{eff}$
  - If DR close to 1 (e.g., .999…), 100s or 1000s of initial iterations may be required for initial source distribution errors to die away
  - Most statistical tests for convergence are *ex post facto* tests to look for trends
  - Most common practice is to examine plots of Keff vs. cycles

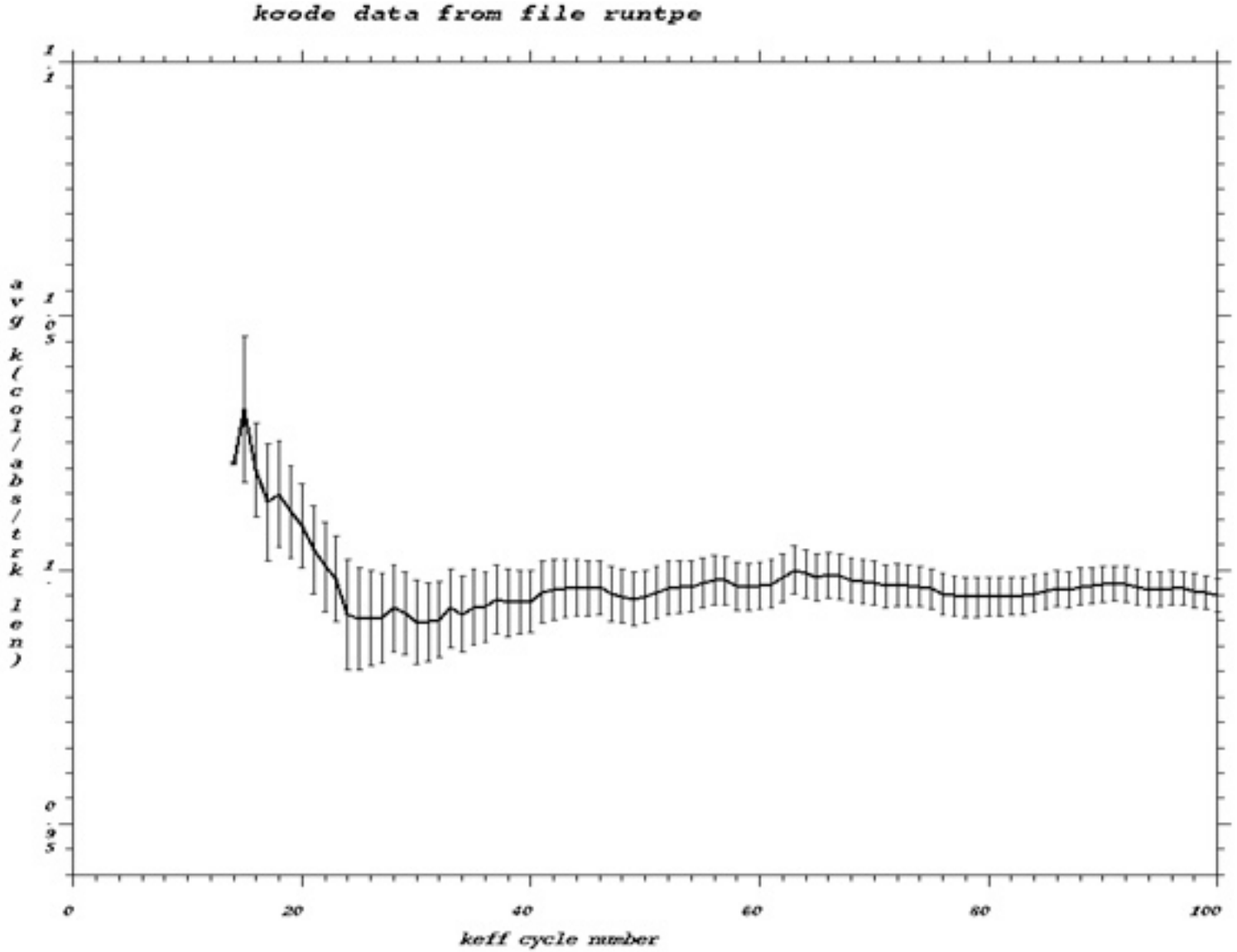
K-Calculations — Convergence

- Plots of single-cycle Keff vs. cycle number



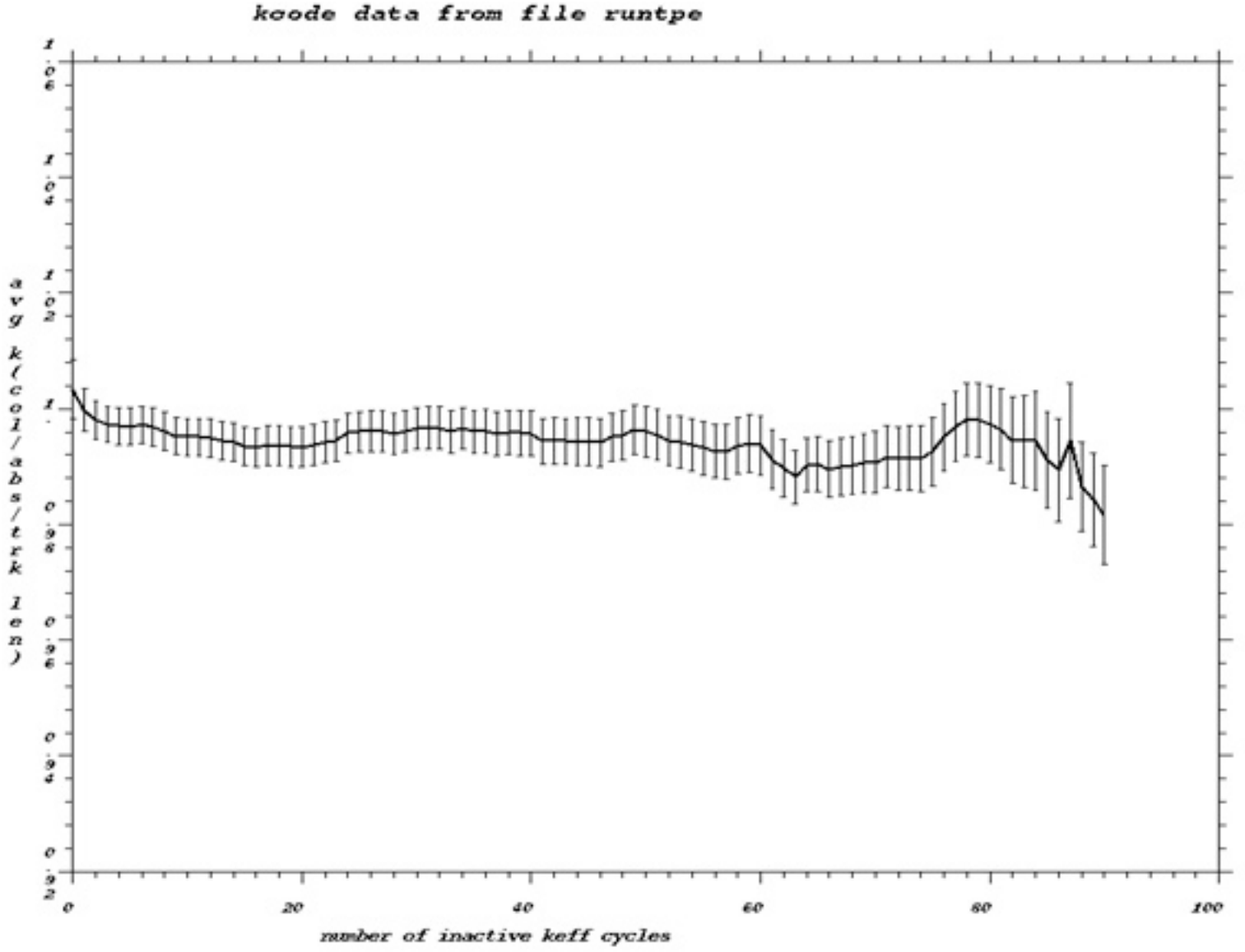
K-Calculations — Convergence

- Plots of cumulative Keff vs. cycle number



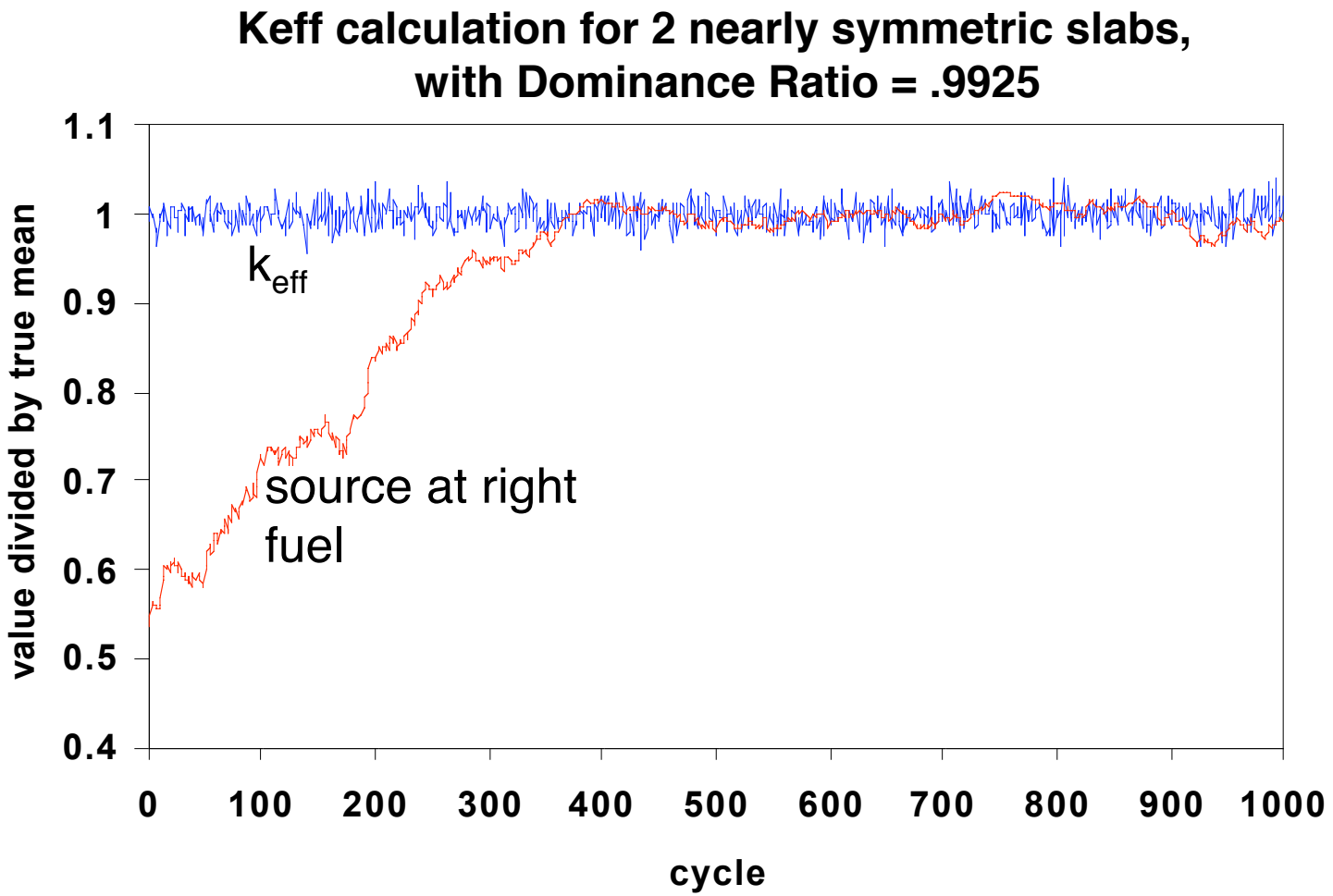
K-Calculations — Convergence

- Plots of cumulative Keff vs. number of initial cycles discarded



K-Calculations — Convergence

- Keff is an integral quantity – converges faster than source shape



K-Calculations — Convergence

- Choose the number of cycles to discard by examining convergence plots
- Then, choose the total number of cycles to be large enough so that relative errors are "small enough"
  - Always run >25 cycles for tallies, to get good estimates of σ^2
  - Always try to run a few 100 or 1000 cycles for tallies
    - Statistical tests on convergence more reliable if more cycles
    - Better plots for assessing convergence
- **Summary**
  - **Particles per cycle - > 1000**
  - **Discarded cycles - varies, check plots**
  - **Tally cycles - > 100**

α-Eigenvalue Calculations

- Eigenvalue equation with **both** K_{eff} & α
  - α **is a fixed number**, not a variable

$$\left[\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E) + \max(\frac{\alpha}{v},0) \right] \Psi_\alpha(\vec{r},E,\vec{\Omega})$$

$$= \max(\frac{-\alpha}{v},0)\Psi_\alpha(\vec{r},E,\vec{\Omega}) + \iint \Psi_\alpha(\vec{r},E',\vec{\Omega}')\Sigma_S(\vec{r},E'\rightarrow E,\vec{\Omega}\cdot\vec{\Omega}')d\vec{\Omega}'dE'$$

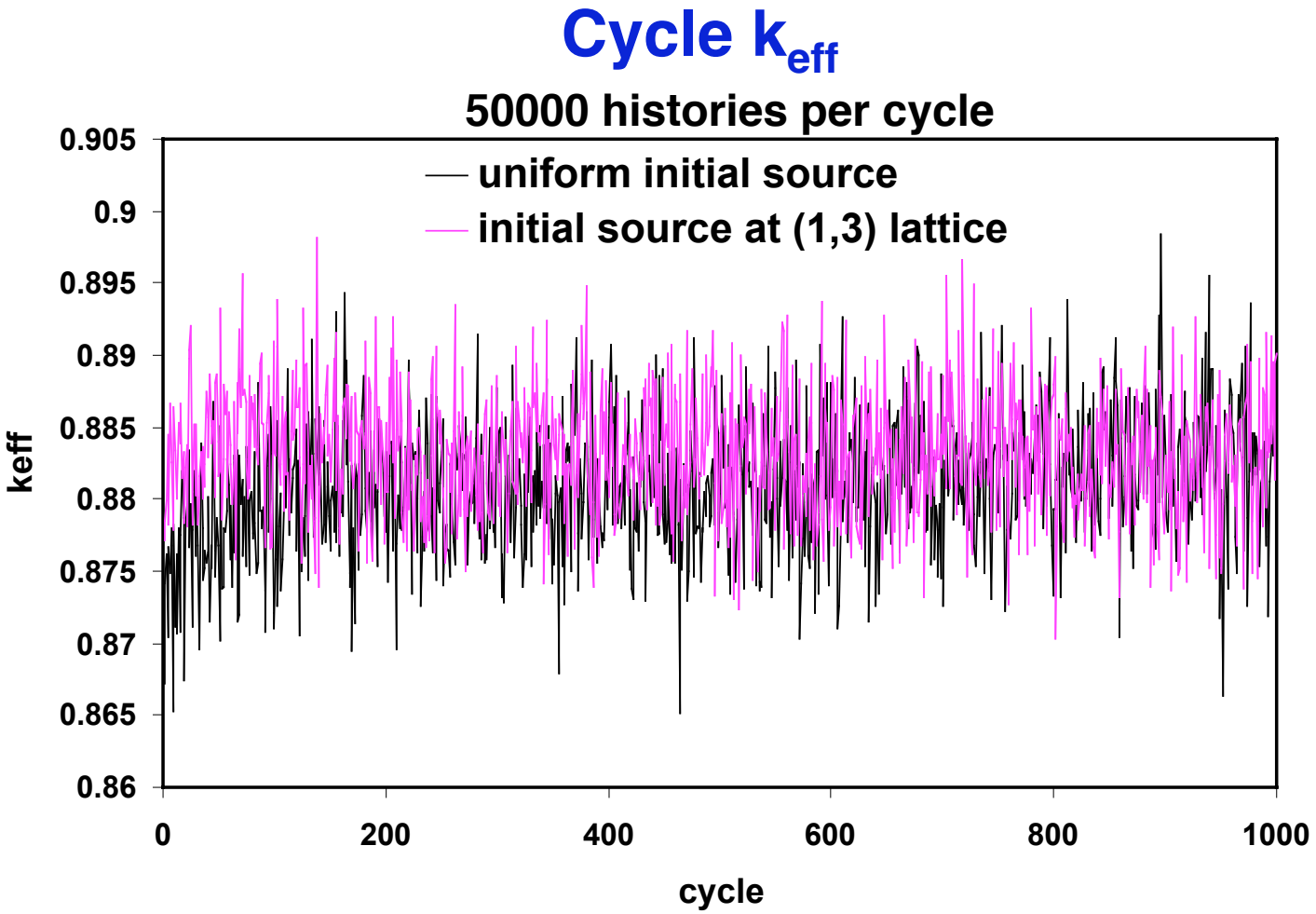
$$+ \frac{1}{K_{eff}}\cdot\frac{\chi(E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\Psi_\alpha(\vec{r},E',\vec{\Omega}')d\vec{\Omega}'dE'$$

- Note on the max(α/v, 0) and max(-α/v, 0) terms
  - If α < 0, real absorption plus time absorption could be negative
  - If α < 0, move α/v to right side to prevent negative absorption,
  - If α < 0, -α/v term on right side is treated as a delta-function source

- 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

Special Topic – Stationarity Tests

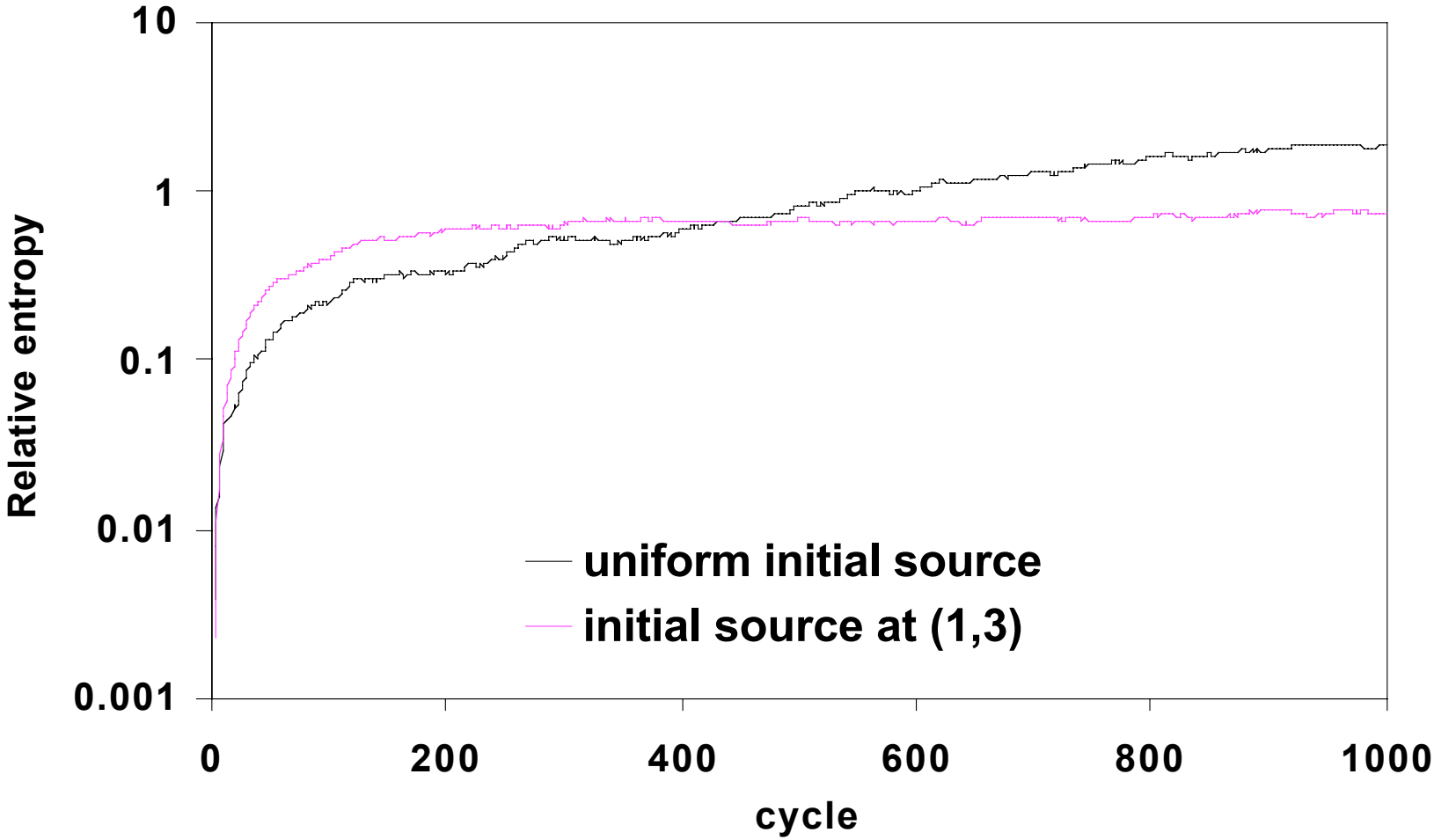
- Plots of single-cycle Keff or cumulative Keff are difficult to interpret when assessing convergence



Special Topic – Stationarity Tests

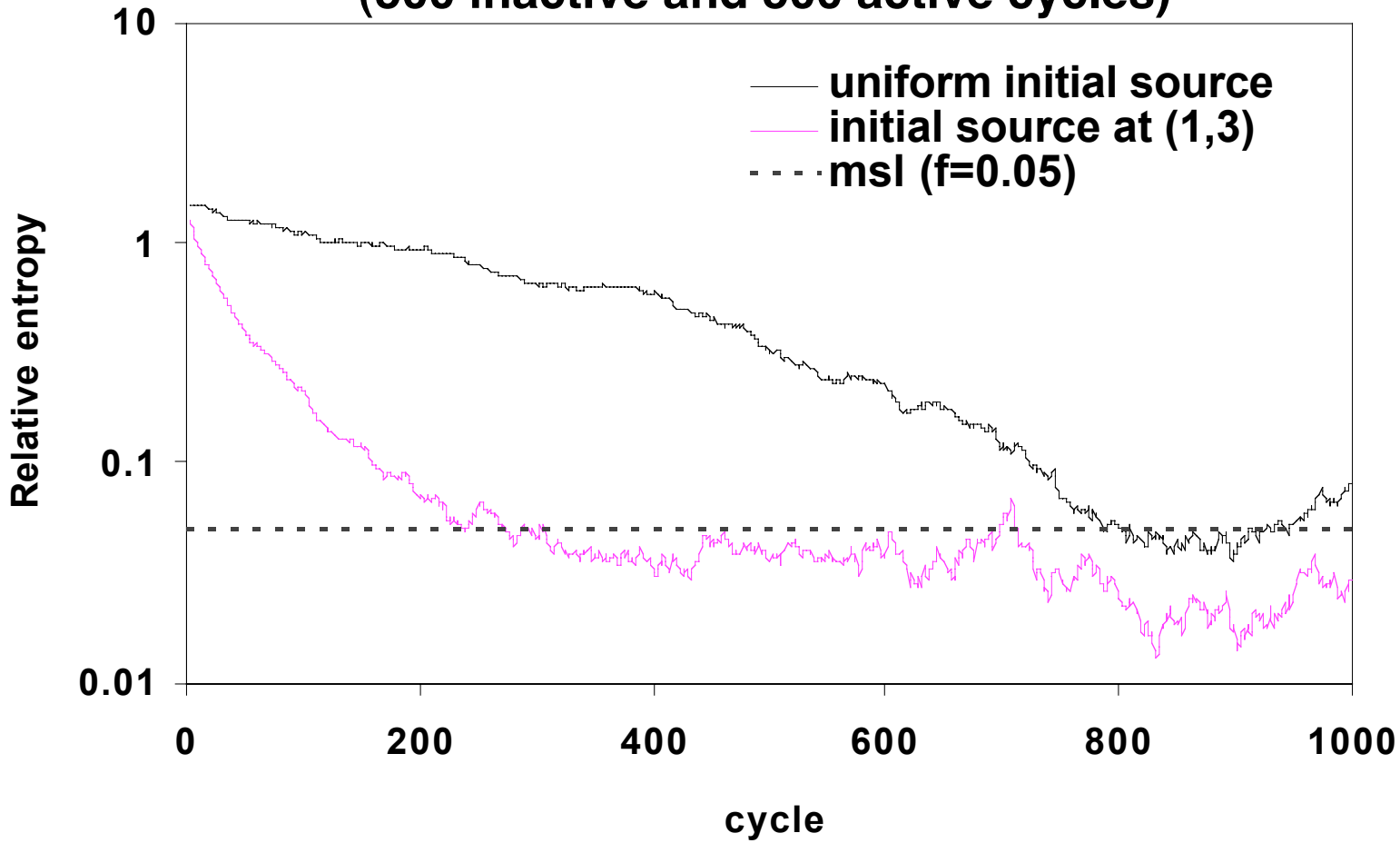
- The MCNP team has been investigating new stationarity tests

Progressive relative entropy

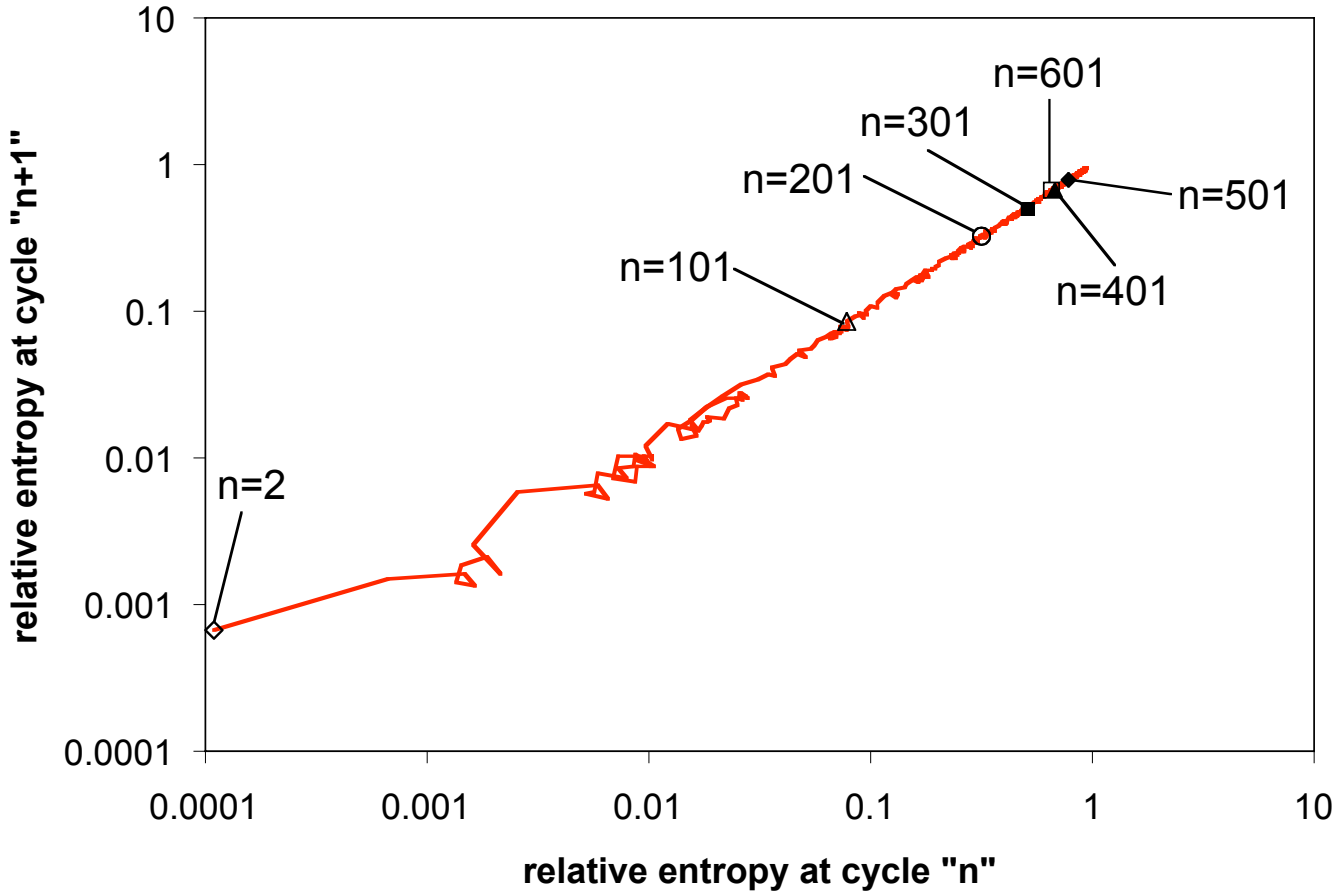


Posterior relative entropy

(500 inactive and 500 active cycles)



Special Topic – Stationarity Tests



Special Topic – Stationarity Tests

- In a series of related papers, we have significantly extended the theory of Monte Carlo eigenvalue calculations, explicitly accounting for correlation effects.

LA-UR-02–0190:	T Ueki, "**Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations**", Nucl. Sci. Eng. (2002)
LA-UR-01–6770:	T Ueki & FB Brown, "**Autoregressive Fitting for Monte Carlo K-effective Confidence Intervals**", ANS Summer Meeting, (June 2002)
LA-UR-02–3783:	T Ueki & FB Brown, "**Stationarity Diagnostics Using Shannon Entropy in Monte Carlo Criticality Calculations I: F Test**", ANS Winter Meeting (Nov 2002)
LA-UR-02–6228:	T Ueki & FB Brown, "**Stationarity and Source Convergence in Monte Carlo Criticality Calculations**", ANS Topical Meeting on Mathematics & Computation, Gatlinburg, TN (April, 2003)
LA-UR-03–0106:	T Ueki, FB Brown, DK Parsons, "**Dominance Ratio Computation via Time Series Analysis of Monte Carlo Fission Sources**" , ANS Annual Meeting (June 2003)
LA-UR-02–5700:	T Ueki, FB Brown, DK Parsons, & DE Kornreich, "**Autocorrelation and Dominance Ratio in Monte Carlo Criticality Calculations**", Nucl. Sci. Eng. (Nov 2003)
LA-UR-03–3949:	T Ueki & FB Brown, "**Informatics Approach to Stationarity Diagnostics of the Monte Carlo Fission Source Distribution**", ANS Winter meeting (Nov 2003)
LA-UR-03–5823:	T Ueki, FB Brown, DK Parsons, JS Warsa, "**Time Series Analysis of Monte Carlo Fission Source: I. Dominance Ratio Calculation**", Nucl. Sci. Eng. (Nov 2004)
LA-UR-03-????:	T Ueki & FB Brown, "**Stationarity Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations**," submitted to Nucl. Sci. Eng.