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Revisiting the "K_{eff} of the World" Problem

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The "K-effective of the World" problem was introduced nearly 30 years ago by G. E. Whitesides. The general theme was to caution Monte Carlo code users that, despite the sophistication of the codes for representing realistic geometry and physics interactions, correct results can be obtained 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. In this work, recommended best practices for criticality safety calculations are applied to the "K-effective of the World" problem. Numerical results are discussed, and causes of previously observed discrepancies identified. The general conclusion is that the model problem used is not a difficult calculation today, and correct results will be obtained if currently recommended Monte Carlo criticality practices are followed.

- K_{eff} of the World Problem
- Best Practices
- Numerical Results
- Discussion & Conclusions

A Difficulty in Computing the k-effective of the World

G. E. Whitesides (ORNL), Trans ANS 14, No. 2, 680 (1971)

In the course of applying Monte Carlo programs in the solution of criticality safety problems, a difficulty in correctly computing certain types of systems has arisen. In view of the increasing use of Monte Carlo-type programs, it is important that some statement be made about the type of systems in which the difficulty is likely to be encountered, since when one attempts to compute the multiplication factor for such a system, the result will almost always yield a low, and hence for criticality safety purposes, nonconservative result. This can occur with no hint that the computed result is in error.

The extreme example, which defines a situation in which this difficulty can exist, is the "k-effective of the world" problem. That is, **if one attempts to calculate the k_{eff} of the world using a Monte Carlo calculation, what k_{eff} would be computed assuming that there are several critical assemblies located around the world? The answer would likely be the keff of the world with no critical assemblies present.** The cause of the erroneous result is the fact that the volume of fissile material in the world would be so large relative to the volume of fissile material in the critical assemblies that most commonly used forms of sampling would almost never "see" the critical assemblies. Hence, this would not reflect their existence in the computed keff.

A more commonly encountered example in which a user of Monte Carlo programs might observe this difficulty is illustrated by a 9 x 9 x 9 array of plutonium metal spheres with a radius of ~4 cm, spaced on 60-cm centers. The array is reflected on all sides by a thick water reflector. The k_{eff} of this system is computed to be 0.93. If the sphere in the center unit of the array is replaced by a sphere of plutonium that is exactly critical as a bare unit and the calculation repeated in the standard fashion using the Monte Carlo method, the calculation will yield a k_{eff} of 0.93, reflecting the same difficulty encountered in the "world k_{eff}" problem.

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. The difficulty can range from a problem which converges so slowly that the normal number of generations examined are insufficient to assure convergence to problems that perhaps will never converge.

The answer to the problem lies in being sure that source convergence is achieved. Most Monte Carlo programs start all neutrons initially with either a flat or a cosine distribution over the fissile material in the system. For the majority of problems this is adequate and maybe even exact. Unfortunately, the choice of a standard start procedure that is adequate for a system with a region of localized multiplication that is somewhat higher than the multiplication of the major portion of the volume of the system is difficult, if not impossible, to define. One difficulty, which should not be underestimated, is trying to determine if, and where, this situation exists. Because of this, it is not the intention of this paper to offer a solution to the general problem; but only to bring to the attention of the users of Monte Carlo programs the fact that the computed multiplication may be in error for such systems.

If the region of highest multiplication can be established, it appears to be adequate to ensure eventual source convergence to the fundamental mode by starting all neutrons in this region. If there are more than one such regions, it may be necessary to run several cases varying the initial source in order to determine the initial conditions that will lead to a fundamental mode source distribution.

The Monte Carlo method has opened up the path to very precise evaluations of the criticality safety of almost any situation likely to be encountered. Its use, however, should be tempered by the realization that unless the correct fission distribution is achieved, the results will most likely be nonconservative.

- **Elliot Whitesides, 1971:**

  … if one attempts to ***calculate the*** $\boldsymbol{k_{eff}}$ ***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*** $\boldsymbol{k_{eff}}$ ***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.*** *…*

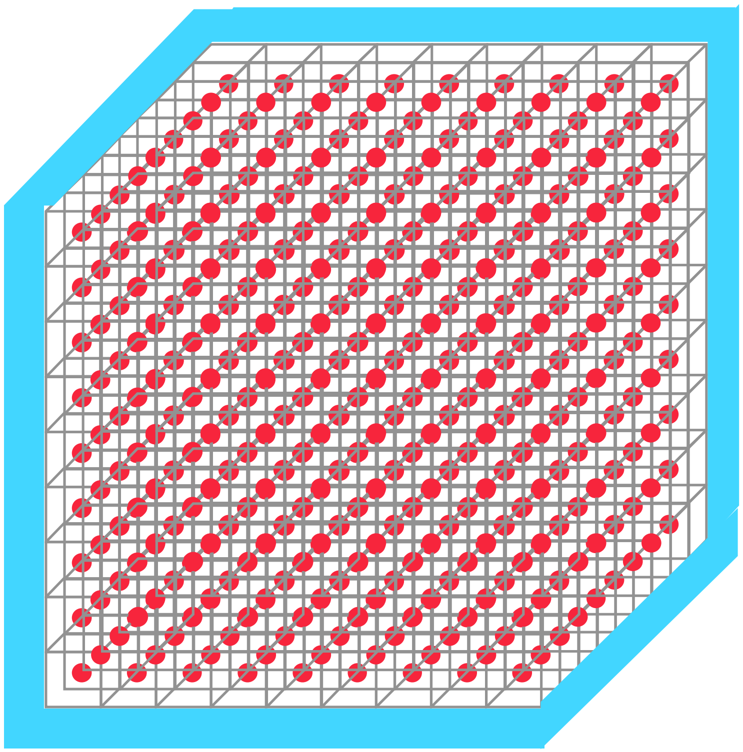
  … The Monte Carlo method has opened up the path to very precise evaluations of the criticality safety of almost any situation likely to be encountered. Its use, however, should be tempered by the realization that ***unless the correct fission distribution is achieved, the results will most likely be nonconservative****.*

- **Today:**
  - Powerful, fast computers
  - OECD/NEA/WPNCS Expert Group on Monte Carlo Source Convergence
  - Recommended "Best Practices" for Monte Carlo criticality calculations

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:

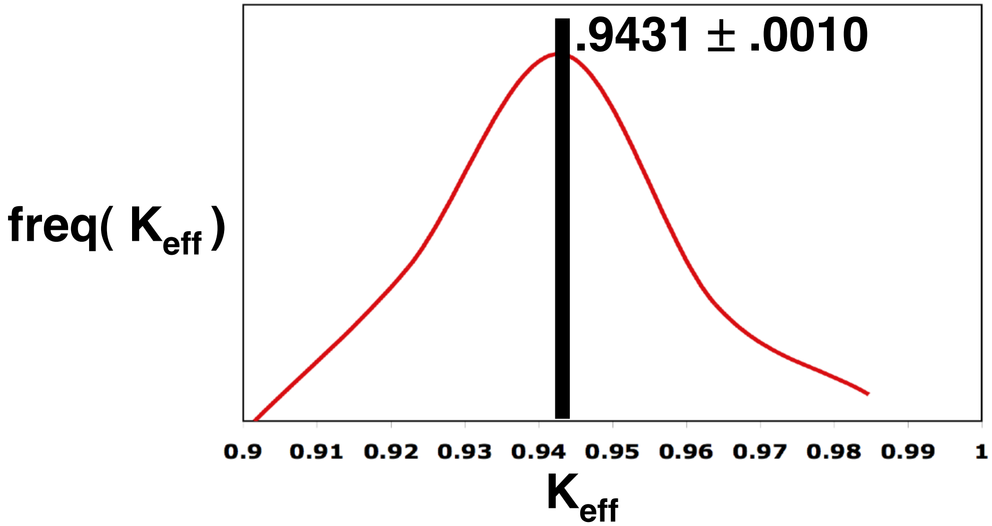
Replace center sphere of array by larger (critical) sphere

Should be supercritical - is it ?

Whitesides' Problem, circa 1971

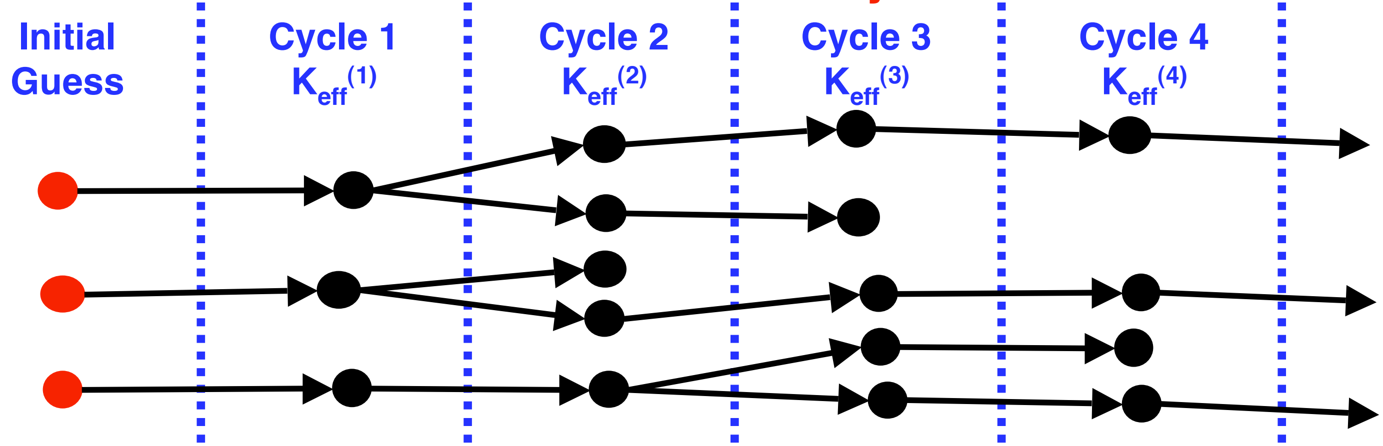
- **Due to severe computer limitations ~1971, KENO defaults were:**
  - 300 neutrons/cycle
  - Discard first 3 cycles
  - Run 100 more cycles

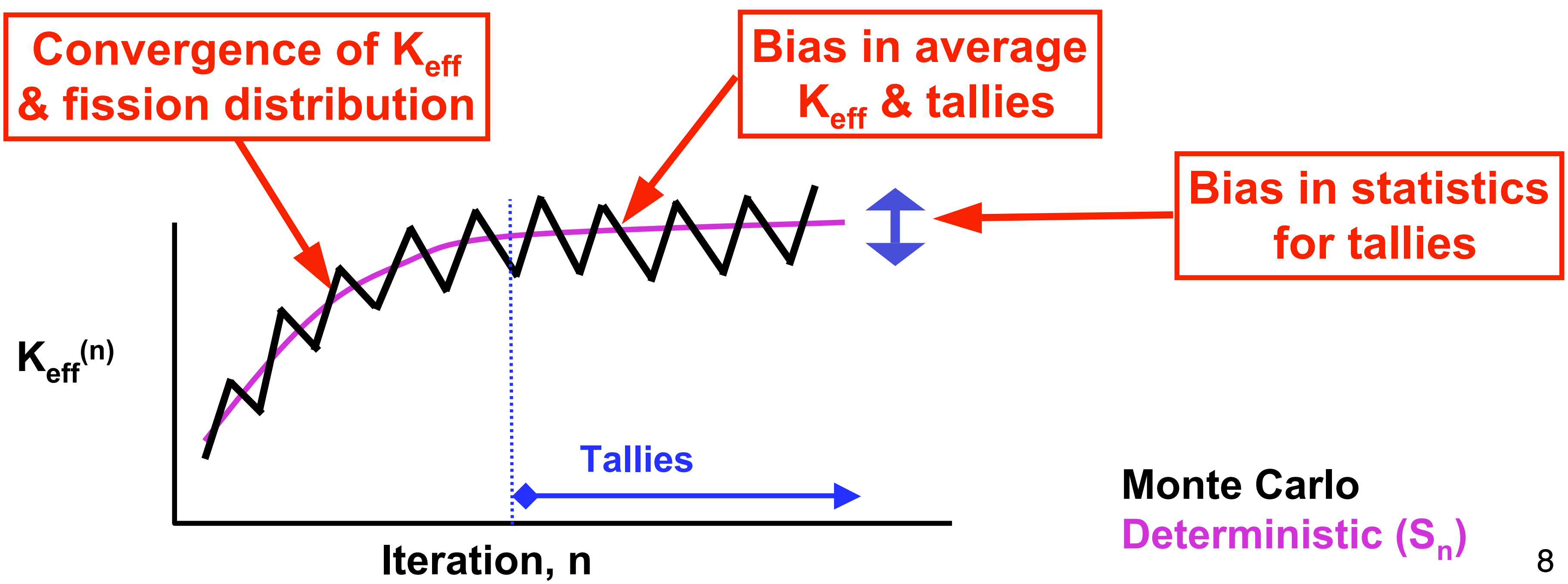
- **If MCNP5 is run using the 1971 KENO defaults, 200 independent replica calculations give:**
  - Average of 200 replicas: **K_{eff} = .9431 ± .0010**
  - None of the 200 calculations produced $K_{eff} > 1$
  - Distribution of replica results:



Concerns for MC Criticality Calculations

Power Iteration for MC Criticality Calculations





Best Practices

- Make trial run to examine convergence of both K_{eff} & the fission distribution (eg, plot K_{eff} & Shannon entropy vs cycle)

- 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

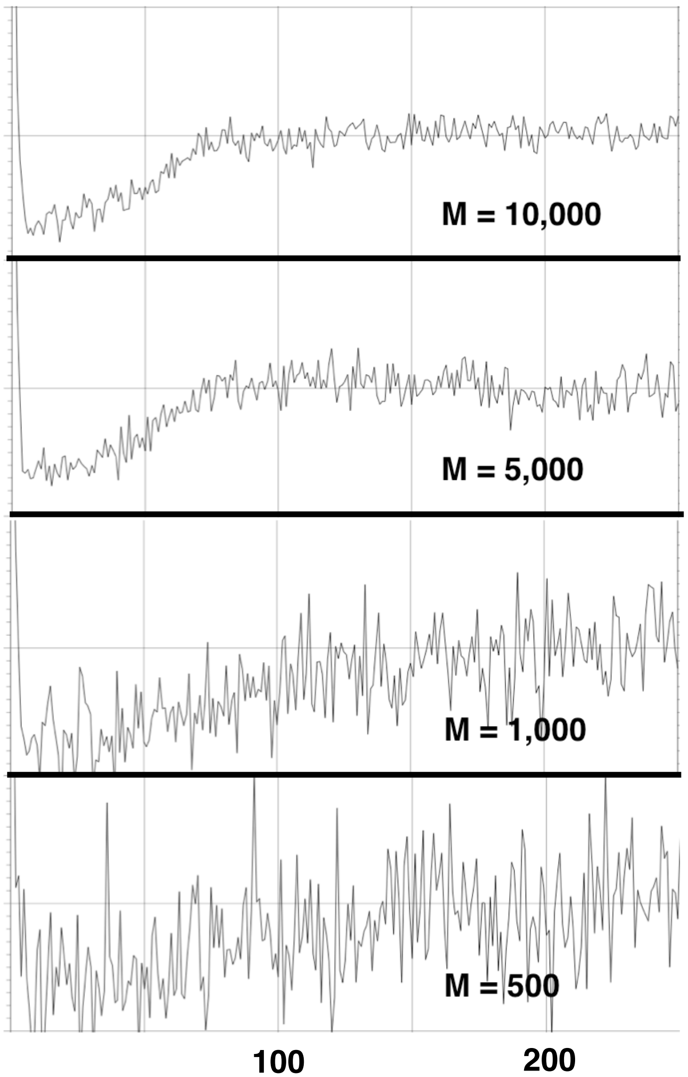
- To help with convergence:
  - Take advantage of problem symmetry, if possible
  - Use good initial source guess, cover fissionable regions

- Run at least a few 100 active cycles to allow codes to compute reliable statistics

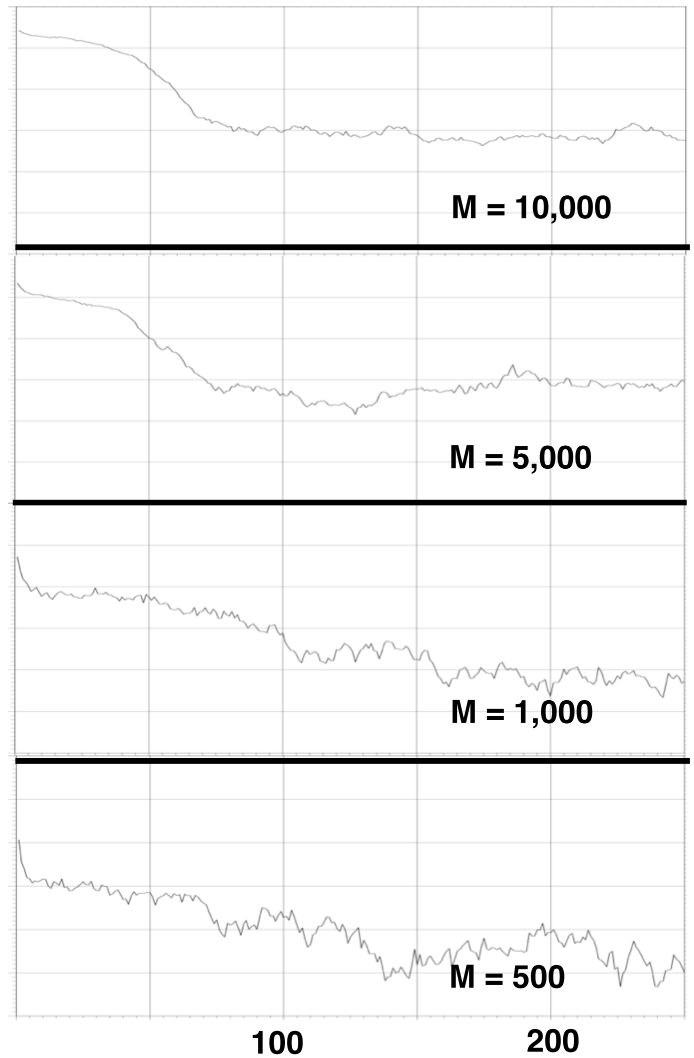
- Statistics on tallies from codes are underestimated, often by 2-5x; possibly make multiple independent runs

Whitesides Problem - Convergence

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



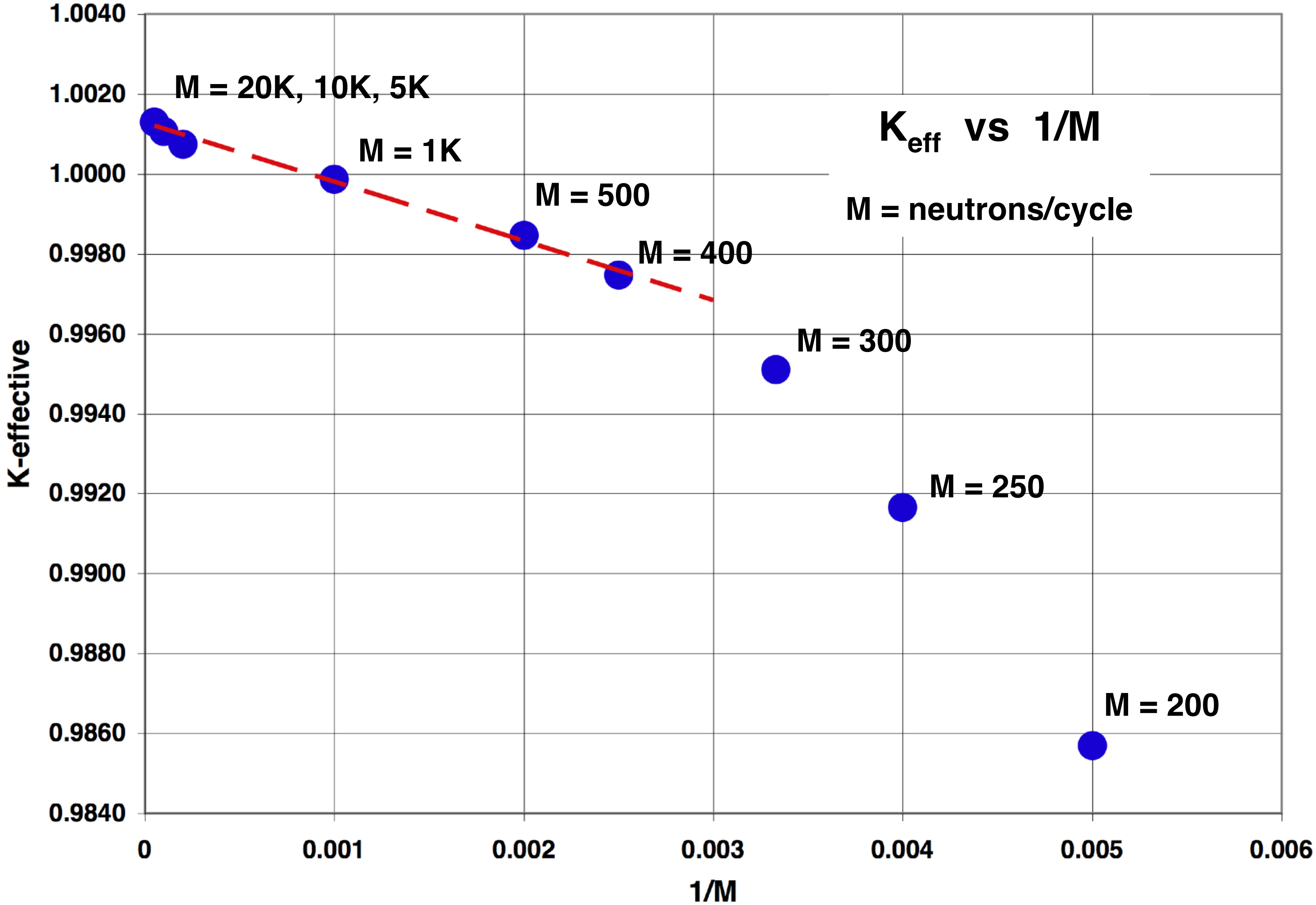
H_{src} vs cycle, various M
M = neutrons/cycle



- 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

Whitesides Problem - 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

Whitesides Problem - K_{eff} Bias

- 10M active neutrons for all cases
- First 150 cycles discarded for all cases
- MCNP5-1.60 + ENDF/B-VII.0

neutrons/cycle	K_{eff}	bias
200	0.9857 (3)	-0.0156
250	0.9917 (3)	-0.0096
400	0.9975 (3)	-0.0038
500	0.9985 (3)	-0.0028
1000	0.9999 (2)	-0.0014
5000	1.0007 (3)	-0.0006
10000	1.0011 (2)	-0.0002
20000	1.0013 (3)	-0.0000

Discussion & Conclusions

- **The original 1971 version suffered from:**
  - Computers - small memory & slow
  - Discarding only 3 initial cycles would result in K_{eff} computed from an **unconverged** problem (K_{eff} much too low, if started with uniform source)
  - Using only 300 neutrons/cycle results in **K_{eff} bias** - too low, nonconservative (best that could be done, if converged properly, would be ~ .994)
  - Using only 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),

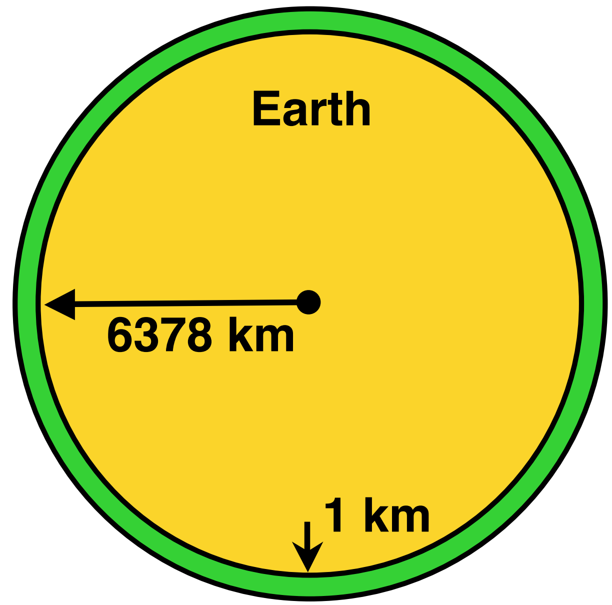
then the "K-effective of the World" problem is actually <u>not</u> a difficult problem to solve

The Real "K_{eff} of the World" Problem

- **Volumes**
  - 1 km shell at earth surface = 5.11×10^{23} cm^3
  - Whitesides' model problem = 2.16×10^{8} cm^3

- **The real "K_{eff} of the World" problem has volume ~ 2.4×10^{15} times that of Whitesides' model problem**

- **Need a really, really big computer …..**



References

- G.E. WHITESIDES, "Difficulty in Computing the k-effective of the World," *Trans. Am. Nucl. Soc.,* 14, No. 2, 680 (1971).
- R.N. Blomquist, et al., "Source Convergence in Criticality Safety Analysis, Phase I: Results of Four Test Problems," OECD Nuclear Energy Agency, OECD NEA No. 5431 (2006).
- R.N. Blomquist, et al., "NEA Expert Group on Source Convergence Phase II: Guidance for Criticality Calculations", 8th International International Conference on Criticality Safety, St. Petersburg, Russia, May 28 – June 1, 2007 (May 2007).
- F.B. BROWN, "Review of Best Practices for Monte Carlo Criticality Calculations", ANS NCSD-2009, Richland, WA, Sept 13-17 (2009).
- X-5 MONTE CARLO TEAM, "MCNP – A General N-Particle Transport Code, Version 5 – Volume I: Overview and Theory", LA-UR-03-1987, Los Alamos National Laboratory (April, 2003).
- 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**
  - **PHYSOR-2008 Monte Carlo workshop**
  - **Math & Comp 2009 Monte Carlo workshop**
  - **Paper at Nuclear Criticality Safety Division topical meeting**
  - **PHYSOR-2010 Monte Carlo Workshop**

Presentations available at
http://mcnp.lanl.gov/publication/mcnp_publications.html