Assessing Convergence in Monte Carlo k_{eff} Problems

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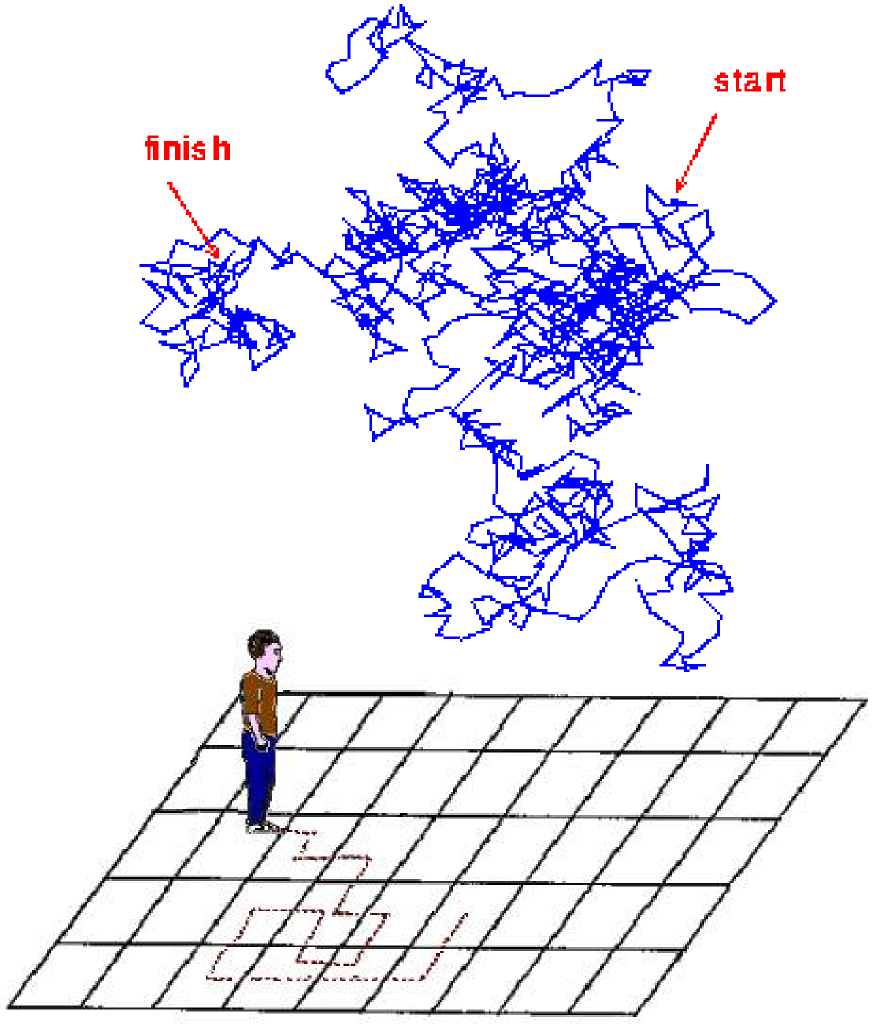
Overview

- Monte Carlo methods in nuclear simulation
- Different needs of reactor physics and criticality safety
- Methods of source convergence assessment
- Alternative means of assessment

The Monte Carlo Method

- The Monte Carlo approach is a statistical method where the expected behavior of particles (neutrons, photons, electrons) in a system is estimated by simulating the lives, or “**histories,**” of a large number of individual particles.

- Using random numbers a computer can generate a random history for the life of each particle (i.e., Random Walk).



Monte Carlo algorithms for k_{eff} calculation

- Neutron histories are grouped into cycles, batches, or generations.
- In iterated source (k_{eff}) problems, each generation of neutrons creates fissions that give birth to the next generation of neutrons.
- The fission site distribution converges during initial “skipped” generations.
- The later “active” generations are used to estimate k_{eff} and potentially other parameters, like flux and reaction rate.
  - k_{eff} will statistically fluctuate from generation to generation due to variance in the histories and fission sites.
  - The overall estimate of k_{eff} should converge as the number of histories and generations increases.

Needs for Monte Carlo calculations for different communities

- Criticality Safety
  - k_{eff} is primary metric of importance
  - Good estimates may be possible without well known global flux estimate
  - Practitioners often work with limited computational resources
- Reactor Physics
  - k_{eff}, reactivity coefficients, control rod worths, power peaking measures, activation calculations
  - Flux distribution must be known with greater accuracy in order to have confidence in spatially dependent parameters
  - If they work with MC, computer power is often good

Methods of assessing source convergence

- Shannon Entropy tests on source distribution
- KENO uses a default uniform source distribution in the fissile material
- "Best estimate k_{eff}" from Keno will report k_{eff} lowest variance number of generations skipped rather than requested value
- Plot of k_{eff} vs. number of generations and the number of generations skipped.
- Normality test on the active generations

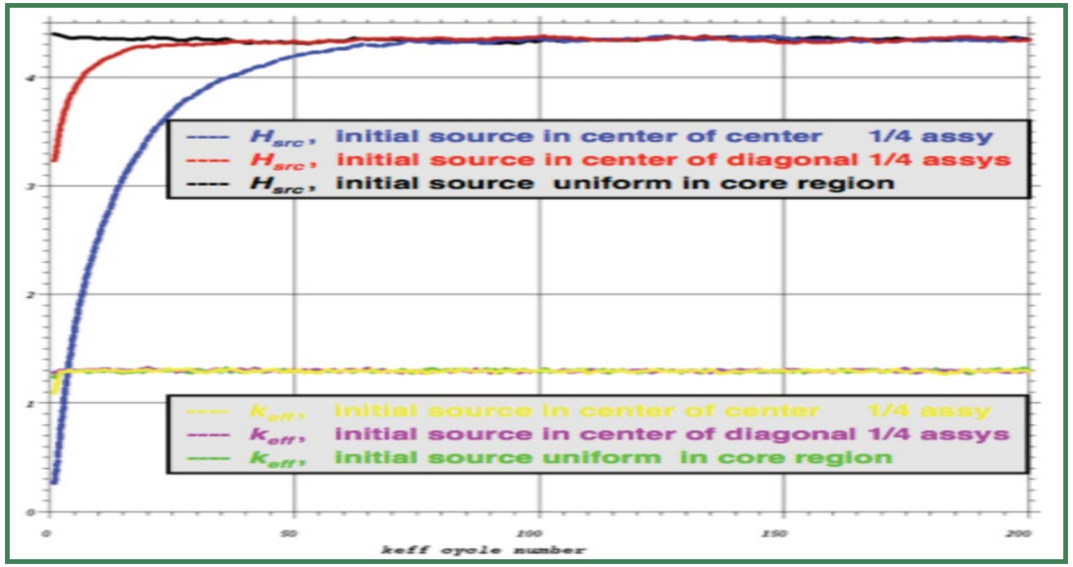
Shannon Entropy Convergence Diagnostics

- Shannon Entropy is a concept from Information Theory that measures the amount of information contained in messages in a data stream.

- Brown and Ueki have employed Shannon Entropy to diagnose convergence of the fission source in eigenvalue calculations.

$$H = -\sum_{n}^{N} p_n \ln(p_n)$$

p_n= Fraction of information in message n.

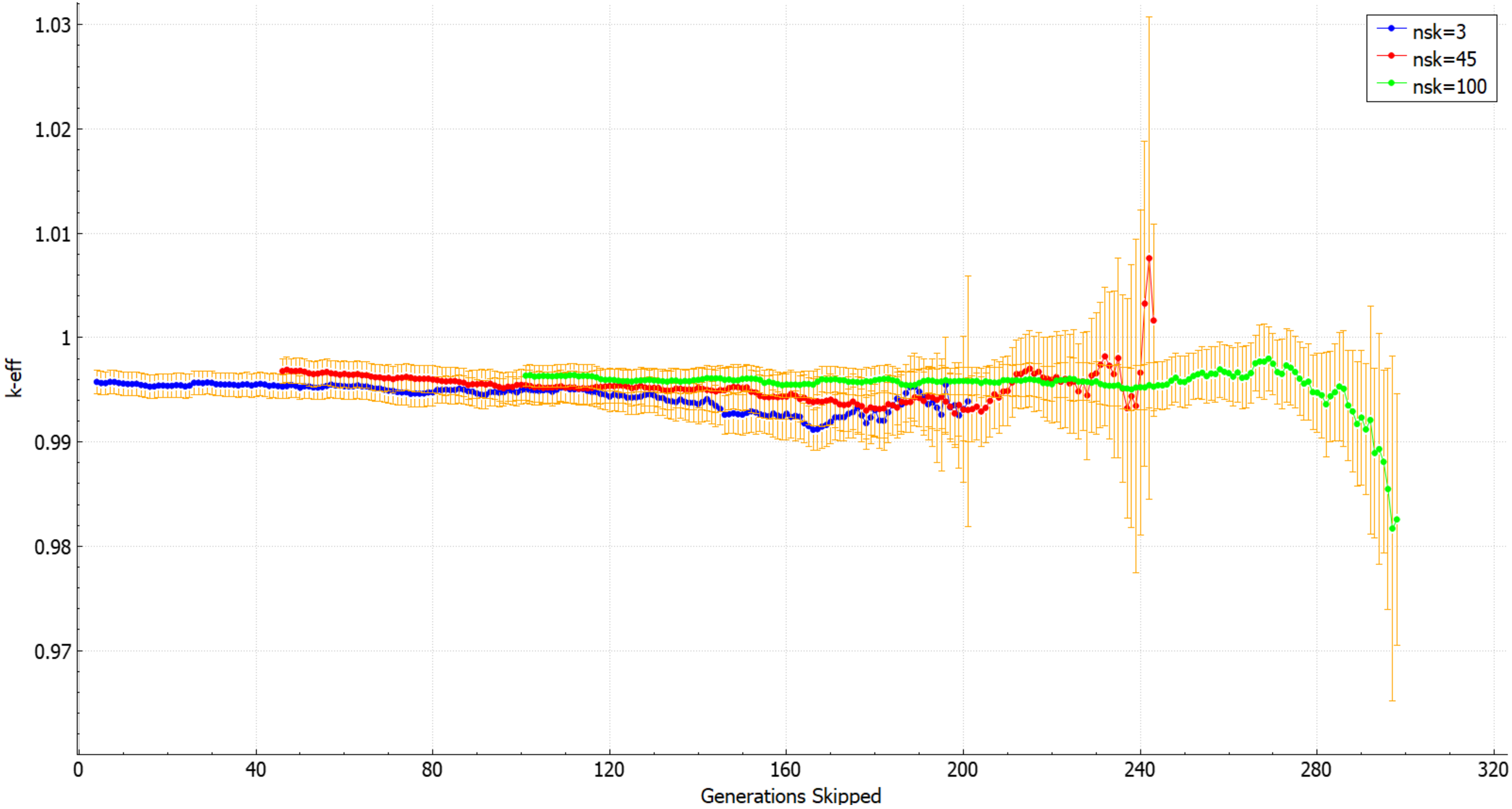


Convergence of Shannon Entropy in a 2D Full Core PWR Calculation
[Brown, 2011]

Entropy Convergence Tests

- KENO contains three statistical tests to check whether the Shannon Entropy is converged.
  - **Test 1:** Is the uncertainty in the Entropy larger than the Entropy?
  - **Test 2:** Does the Entropy score from any of the active generations differ significantly from the total average Entropy?
    - Note: It is expected that many of the generations will fall more than 1-sigma from the average, so failing this test is not necessarily worrisome.
  - **Test 3:** Does the Entropy from the second half of the active generations differ significantly from the Entropy from all generations?

K_{eff} by generation skipped



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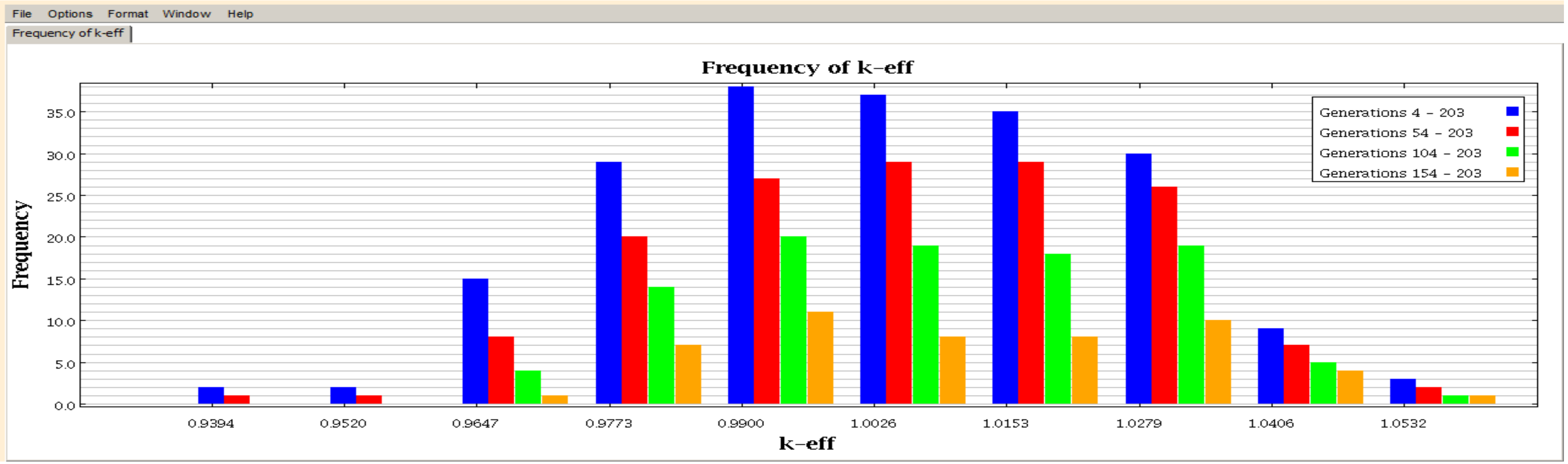
Distribution of Generations

- k_{eff} estimates from the active generations are expected to be normally distributed
- KENO performs a χ^2 test and reports result in final results block as one of:
  - Satisfy at 95% level
  - Fail at 95% but pass at 99% level
  - Fail
- Histograms of generations in output for all active generations as well as the last 75%, 50% and 25% of active generations
  - Examine plots for normality and to ensure the distribution doesn't change as problem progresses

k_{eff} Plots

Javapeno applet embedded in HTML output



Plot in text output

```
0.9394 to 0.9520     **
0.9520 to 0.9647     **
0.9647 to 0.9773     ***************
0.9773 to 0.9900     *****************************
0.9900 to 1.0026     **************************************
1.0026 to 1.0153     *************************************
1.0153 to 1.0279     ***********************************
1.0279 to 1.0406     ******************************
1.0406 to 1.0532     *********
1.0532 to 1.0659     ***
```

Shannon Entropy for Criticality Safety

- Users often have requirement to pass these tests in order to consider calculation converged.
- Focus should be placed on convergence of k_{eff} for criticality safety problems
- If you pass them great, if not fall back on more traditional techniques
- If those still look weird then skip more generations and potentially increase the number of particles per generation
- It would be good to separate the conversations on source and k_{eff} convergence
- Beware potentially “hot spot” or decoupled problems