22.211 Lecture 4

Monte Carlo methods - Eigenvalue

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Outline

1. Objectives
2. Fixed Source
3. Eigenvalue
4. Conclusions

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Objectives

- Fixed source MC
- Eigenvalue MC and estimators
- Source stationarity

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Basic Particle Simulation Algorithm

```
for i = 1 → nps do
    Sample position, direction, velocity
    loop
        Sample travel distance
        Move particle to new location or material boundary
        if Leak then
            Exit loop
        else if Material Boundary then
            Cycle loop from new position
        elseCollision in region
            Sample collision isotope
            Sample collision type
            if Absorption then
                Exit loop
            else
                Sample direction, velocity
                Cycle loop
            end if
        end if
    end loop
end for
```

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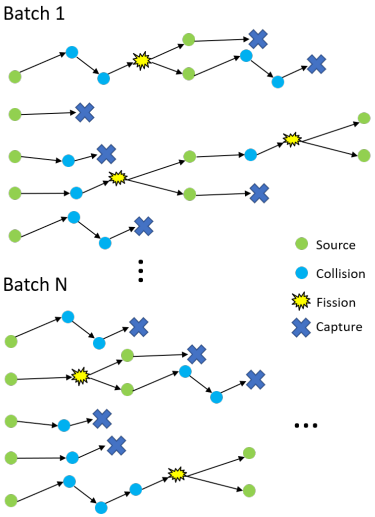
Fixed Source MC



- Neutrons are followed throughout their entire history which includes all of its offspring
- Batches of source neutrons are simulated independently (varying starting seeds) from which mean and variance can be computed
- Only possible when the multiplication factor is less then 1 (subcritical medium), otherwise chains never end!

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Batching

- Typically, fixed source calculations will use batches of particles.
- Each batch will provide one random sample of a given tally and Central Limit theorem states that the random sample will come from a normal distribution.
- Multiple batches provide multiple random samples from a normal distribution which meets the requirements for the Student t-distribution from which we can estimate confidence interval.
- It is possible to use only a single batch and still calculate mean and standard deviation from the individual samples, but it is not guaranteed that each sample comes from a normal distribution.

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Secondary Particles/Fission Neutrons

- Many ways of doing this
- One possibility
  - Add fission neutrons only when fission reaction is selected
  - Sample directly from $\nu(E)$

$$n = int(\nu + \xi)$$

- Another possibility
  - Add fission neutrons after each collision
  - Sample from expected number of neutrons per collision

$$r = \nu\sigma_f/\sigma_t \quad n = int(r + \xi)$$

- Particles are banked and must be simulated before starting a new particle

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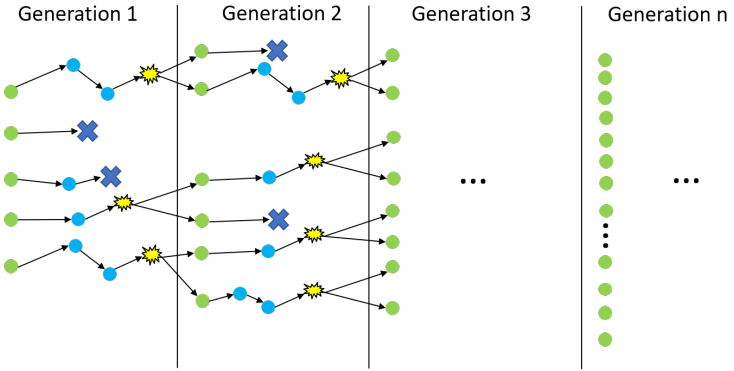
MC by generation



- k is estimated as the ratio of fission neutrons between each generation and averaged over many generations
- Population grows uncontrollably for supercritical cases
- Population goes to 0 for subcritical cases

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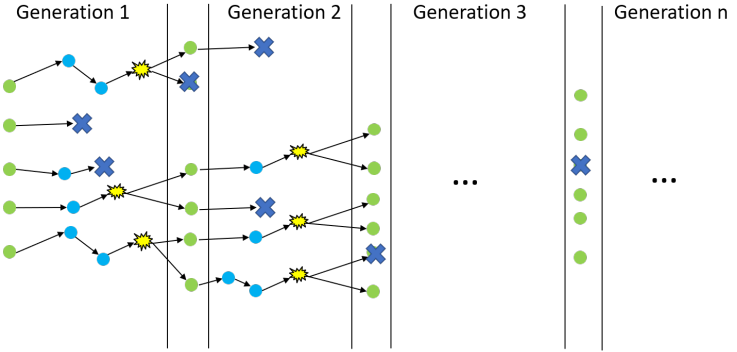
MC by generation - with Normalization



- Population control is applied after each batch so that population remains constant
  - If too many neutrons are generated, we randomly select the ones that survive
  - If too few are generated, we random select a neutron to duplicate

Source
Collision
Fission
Capture

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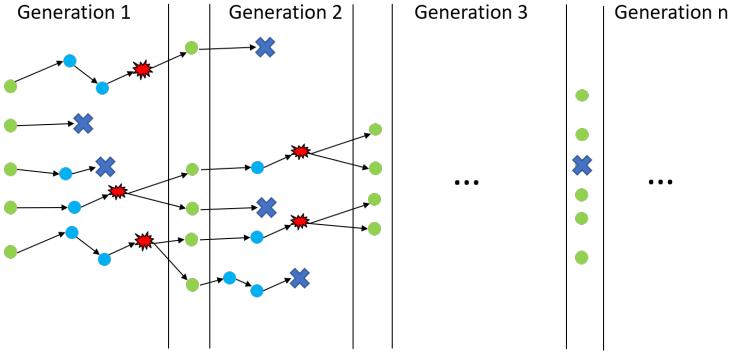
MC by generation - with Normalization and Population Control



- The fission cross-section is divided by the estimated k.
- k is now the previous multiplied by the ratio of successive generation
  - When k "converges", the expected neutron population at each generation is constant
  - Population control is used to tamper statistical fluctuations

Source
Collision
Fission / k
Capture

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k_{eff} Collision Estimator

This eigenvalue estimator is tallied at every collision site.

$$k_{eff}^{C} = \frac{1}{N} \sum_{i} w_i \frac{\sum_k f_k \bar{\nu}_k \sigma_{f,k}}{\sum_k f_k \sigma_{t,k}}$$

where i is a sum of particle histories with weight w_i, k is a sum over nuclides, f_k is the nuclide fraction, $\bar{\nu}$ is the average number of neutrons produced by fission, σ_f is the microscopic fission cross-section and σ_t is the microscopic total cross-section.

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k_{eff} Analog Absorption Estimator

This eigenvalue estimator is tallied at every absorption event with nuclide k.

$$k_{eff}^{AA} = \frac{1}{N} \sum_i w_i \frac{\bar{\nu}_k \sigma_{f,k}}{\sigma_{a,k}}$$

where i is a sum of particle histories with weight w_i, k is the nuclide with which an absorption event has happened, $\bar{\nu}$ is the average number of neutrons produced by fission, σ_f is the microscopic fission cross-section and σ_a is the microscopic absorption cross-section (which includes the fission cross-section).

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k_{eff} Implicit Absorption Estimator

This eigenvalue estimator is tallied at every collision event with nuclide k (where absorption is no longer an option).

$$k_{eff}^{IA} = \frac{1}{N} \sum_i w_i \frac{\sigma_{a,k}}{\sigma_{t,k}} \frac{\bar{\nu_k} \sigma_{f,k}}{\sigma_{a,k}}$$

where i is a sum of particle histories with weight w_i, k is the nuclide with which an absorption event has happened, $\bar{\nu}$ is the average number of neutrons produced by fission, σ_f is the microscopic fission cross-section, σ_a is the microscopic absorption cross-section (which includes the fission cross-section) and σ_t is the microscopic total cross-section.

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k_{eff} Track Length Estimator

This eigenvalue estimator is tallied for every path sampled.

$$k_{eff}^{TL} = \frac{1}{N} \sum_i w_i \rho d \sum_k f_k \bar{\nu}_k \sigma_{f,k}$$

where i is a sum of particle histories with weight w_i, k is a sum over nuclides, ρ is the nuclide density of the material, f_k is the nuclide fraction, d is the distance traveled by the neutron in the cell, $\bar{\nu}$ is the average number of neutrons produced by fission and σ_f.

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Combined k_{eff}

The estimators are obviously correlated, so simply averaging them does not necessarily reduce variance. For example, the implicit absorption and collision estimators are identical for the case of a single fissile nuclide and are thus 100% correlated. Monte Carlo calculations typically provide 3 estimators and combine them into a single one. The correlation is evaluated and propagated in the final estimate.

$$\bar{k} = \frac{k_1 + k_2 + k_3}{3}$$

$$\sigma_{\bar{k}}^2 = \frac{1}{9N} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{i,j}^2 = \frac{1}{9N} (\sigma_{1,1}^2 + \sigma_{2,2}^2 + \sigma_{3,3}^2 + 2\sigma_{1,2}^2 + 2\sigma_{1,3}^2 + 2\sigma_{2,3}^2)$$

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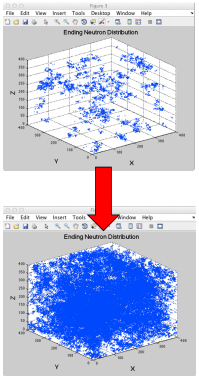
Clustering

Neutrons have a tendency to cluster over multiple generations!



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Uncorrelated samples

If samples are uncorrelated, the variance of a sum can be expressed as

$$Var\Big(\sum_{i=1}^{N} X_i\Big) = \sum_{i=1}^{N} Var(X_i)$$

This expression also allows us to calculate the variance of a mean

$$Var(\bar{X}) = Var\Big(\frac{1}{N}\sum_{i=1}^{N} X_i\Big) = \frac{1}{N^2}\sum_{i=1}^{N} Var(X_i) = \frac{1}{N^2} N \times Var(X_i) = \frac{\sigma^2}{N}$$

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Correlated samples

If samples are correlated, the variance of a sum can be expressed as

$$Var\Big(\sum_{i=1}^{N} X_i\Big) = \sum_{i=1}^{N}\sum_{j=1}^{N} Cov(X_i, X_j)$$

This expression also allows us to calculate the variance of a mean for a known average correlation (ρ)

$$Var(\bar{X}) = Var\Big(\frac{1}{N}\sum_{i=1}^{N} X_i\Big) = \frac{\sigma^2}{N} + \frac{N-1}{N}\rho\sigma^2$$

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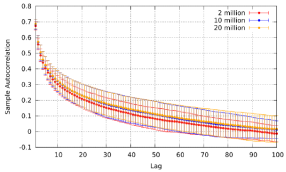
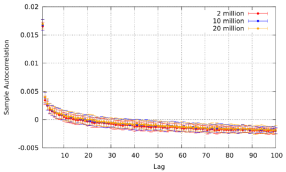
Correlation of fission source sites

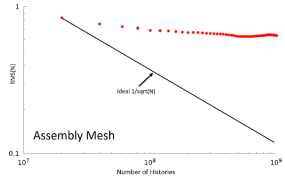
- In our case, the correlation is not constant and tends to 0 after many batches.
- Fission neutrons are produced at the fission site, and how far they travel depends on the optical thickness of the medium.
- The correlation depends largely on the size of the tally-size of interest, the larger the tally region size, the more correlated the samples are.



(a) Autocorrelation coefficients assembly-size tally



(b) Autocorrelation coefficients pin-size tally



(c) RMS Convergence assembly-size tally

Correlated samples

If we include the effect of the lag, k, seen in the correlation, we can compute the variance of the mean as

$$Var(\bar{X}) = \frac{\sigma^2}{N}\left(1 + 2\sum_{k=1}^{N-1}\left(1 - \frac{k}{N}\right)\rho(k)\right)$$

where

$$\rho(k) = \frac{Cov\big(X(n), X(n+k)\big)}{\sqrt{Var\big(X(n)\big)\,Var\big(X(n+k)\big)}}$$

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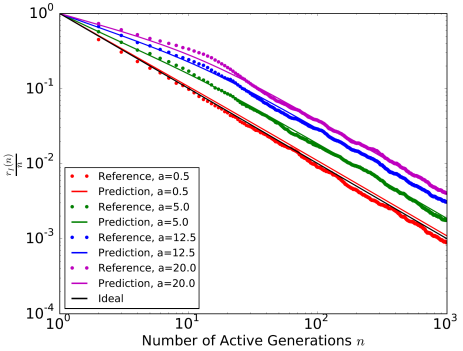
How to account for correlation effects?

- All Monte Carlo codes will ignore correlation effects by default!
- The only sure way to capture the correlation effects is to perform multiple independent simulations (with different seeds) and compute mean and variance from these.
- Other approaches rely on de-correlating batches by creating batches-of-batches, which in OpenMC we call generations-per-batch.
- Correlations are important in very large systems and large tally regions.



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How many particles/batches/... to use?

- MC eigenvalue simulations require setting the number of particles, the number of total batches and the number of total batches to skip.
- Too few particles per batch will lead to tally bias (>10,000 is usually good for k only)
- Too few particles will also lead to visible clustering (>300,000 is usually needed in PWR to reduce strong clustering effects)
- Number of batches to skip will depend on the size of the problem, suitability of the initial guess, and number of particles per batch.

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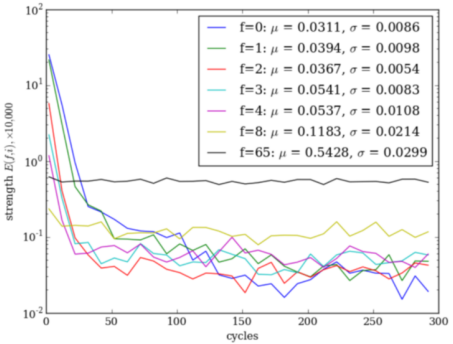
Convergence?

Monte Carlo simulations never truly converge like in the same sense as a deterministic calculation. We instead reach a level of stationarity where fluctuations are constant magnitude. The following plot shows a frequency transform of the source. The black line is the inherent noise of the simulation from the stochastic process. The source convergence process reduces the low order frequencies and stationarity is achieved when their fluctuations is comparable to the noise.



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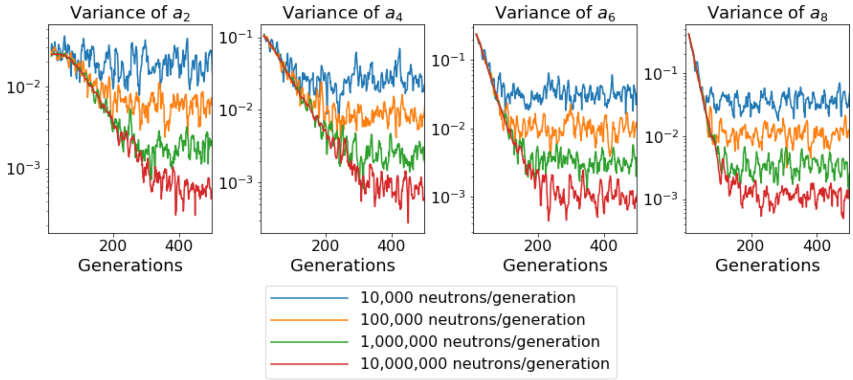
Dependence on particle count

As you increase the number of particles per batch you reduce the inherent noise of the simulation which increases the number of batches needed to reach stationarity.



Shannon Entropy

While not perfect, the most broadly used metric is called Shannon entropy. It relies on the use of a spatial mesh on which we determine the fraction of fission source sites in eash mesh, $p_m(n)$, where m is the mesh index and n the batch number.

$$S(n) = -\sum_m p_m(n) \ln \left(p_m(n) \right)$$

Shannon entropy, $S(n)$ returns a single scalar that captures fluctuations of the fission source. Once the value of S stops changing significantly, we can assume that stationarity has been reached. It is sensititive to the mesh size selection and runs into difficulty in high dominance ratio problems.

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Why not use MC for all core analysis?

- Monte Carlo methods are slow!
- A single steady-state calculation of a full core PWR can take roughly 100,000 CPU-hours to properly quantify heat deposited in 35,000,000 pellets.
- Reactor design, operation and safety analysis requires 1,000-10,000's of simulations.
- Transients would add a few more order of magnitude of runtime!

So what can we do? and what is Monte Carlo useful for?

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Recap

- Always verify that you truly have a pdf before sampling
- Always favor direct sampling if possible
- Think like a neutron!

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References

- F. Brown Lecture Notes: Google: LANL MCNP
- I. Lux, L. Koblinger: Monte Carlo Particle Transport Methods: Neutron and Photon Calculations
- OpenMC online documentation (https://docs.openmc.org/en/latest/)

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