Monte Carlo Methods and Simulations in Nuclear Technology

Principles of analog Monte Carlo criticality simulations

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Principles of analog simulation of MC neutron transport

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What is the analog MC simulation of neutron transport?

In analog Monte Carlo simulation, neutron transport is simulated according to reality, from neutron "birth" (originating from the source) to "death" (absorption or leakage from the system).

What is the "neutron history"?

The simulation of all collisions of a single neutron is called a neutron "history".

How are the final results derived?

The average behaviour of neutrons is estimated via simulating a large number of neutron histories.

Principles of analog simulation of MC neutron transport

What procedures are involved in the simulation of a single neutron history?

Simulation of a single neutron history (assuming we know its initial position, direction and energy):

1. Sample the distance to next collision.
2. If the neutron moves outside the system (with black BC) then end this history.
3. Select the nuclide for the collision.
4. Select the reaction type.
5. If the selected reaction is:

- capture then end this neutron history.
- fission then end this neutron history and simulate the histories of the new fission neutrons (stable solution is obtained only for sub-critical systems).
- scattering then transform the neutron direction and energy and go to step 1.

Sampling the distance to next collision

Sampling the distance to next collision

What is the transition kernel?

The transition kernel T is the pdf of the distance s to next collision

$$T = \Sigma_t(\vec{r}, E)e^{-\Sigma_t s}$$

How can we sample the distance s to the next collision?

Sampling the distance s to the next collision by the inverse method:

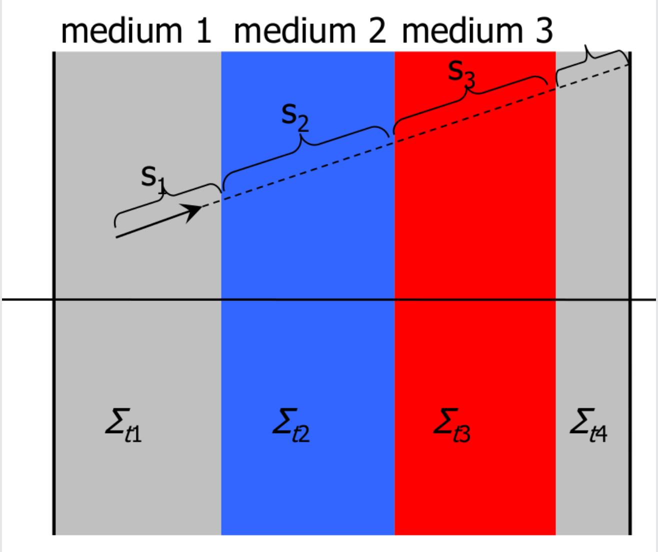
- The cdf function $F_s = \int_0^s \Sigma_t(\vec{r}, E)e^{-\Sigma_t s'} ds' = 1 - e^{-\Sigma_t s}$ (homogeneous material)
- Generate random number u from (0,1)
- Solve $u = 1 - e^{-\Sigma_t s}$ for s:

$$s = -\frac{1}{\Sigma_t} \ln(1 - u)$$

- Since $1 - u$ is also a random number from (0,1) $\Rightarrow s = -\frac{1}{\Sigma_t} \ln(u)$

Sampling the distance to next collision

How can we sample the distance to next collision in inhomogeneous media?



Selecting the nuclide for the collision

Selecting the nuclide for the collision

How can we select the nuclide on which the neutron collides?

A collision occurs in a material. Hence we assume we have a list of nuclides with their respective nuclide concentrations (and macroscopic cross section).

- We can assign a neutron collision probability to each nuclide i as

$$p(i) = \frac{\Sigma_{\mathrm{t},i}(\vec{r}, E)}{\Sigma_{\mathrm{t}}(\vec{r}, E)}$$

- Knowing the collision probabilities on various nuclides, we can sample the nuclide type by the inverse transform method.

Selection of the interaction type

Selection of the interaction type

How can we select the type of the collision reaction

- For the selected nuclide type i, we can assign probabilities to various neutron interactions j as

$$p(j|i) = \frac{\Sigma_{j,i}(\vec{r}, E)}{\Sigma_{t,i}(\vec{r}, E)}$$

- Knowing the probabilities for various neutron interactions, we can again sample the interaction type by the inverse transform method.

Scattering reaction

Scattering reaction

How can we sample the new angle and energy of the neutron after the scattering collision?

- Scattering (often) isotropic in CM-system $\Rightarrow$ select μ_C as $\mu_C = \cos\theta_C = 1 - 2u$.
- Energy and scattering angle are related, so calculate E from

$$\frac{E}{E'} = \frac{A^2 + 2A\mu_C + 1}{(A+1)^2},$$

  where A is the mass number of the nucleus that the neutron collided with.
- Transformation of angle from CM- to L-system

$$\vec{\Omega} = \frac{1}{\sqrt{A^2 + 2A\mu_C + 1}}(A\vec{\Omega}_C + \vec{\Omega}')$$

Criticality simulations

Criticality simulations

What do we mean by the term "criticality simulation"?

Criticality simulations output the steady-state neutron flux in a fissile system (e.g. nuclear reactors).

Is there some principle problem in criticality simulations?

- In criticality simulations the fission source is not known, which is **a problem**. The fission source is given by the steady-state neutron flux itself (which is the solution of the problem).
- Moreover, the steady-state solution in fissile systems without an external source of neutrons is possible only in exactly critical systems.

Criticality simulations

How can we solve the problem with the unknown fission source?

- We can divide neutron histories into generations (called cycles in Monte Carlo terminology).
- We guess the distribution of the source in the first cycle.
- During each cycle, we collect the new fission neutrons, and we use them as the source for the next cycle.
- The source will converge over the cycles to the steady-state distribution.
- Once the source is converged, we can start to collect unbiased results.
- Cycles are therefore divided into "inactive" cycles (having only the function of converging the source) and "active" cycles (that are used for computing the result)

Criticality simulations

How can we ensure the number of neutrons doesn't change over successive cycles?

- We can never design the system to be exactly critical, so we need to force the simulation to obtain the steady-state solution even if the system is not critical.
- Steady-state solution can be obtained if we divide all fission cross sections by effective multiplication factor k_{eff}, so that the system becomes critical.
- Additional normalization is applied to the collected fission neutrons to ensure the required number of neutron histories is sampled at each cycle.

Criticality simulations

How is the multiplication factor calculated?

- The multiplication factor represents the average number of fission neutrons produced during a single neutron history.
- We can estimate the multiplication factor at each cycle based on the neutron histories simulated at the actual cycle. Remember, however, that we have artificially changed the fission cross sections, so we need to correct the multiplication factor being computed (by multiplying it with the multiplication factor used for changing the fission cross sections).
- The fission cross sections in the very first cycle need to be divided by a multiplication factor set by the user in the input file.

Criticality simulations

What are all the parameters that need to be set by the user in criticality simulations?

- The initial source distribution (for the first cycle).
- The multiplication factor for the first cycle.
- The number of inactive cycles.
- The number of active cycles.
- The number of neutron histories that we simulate at each cycle.