Introduction to Monte Carlo simulations of neutron transport in nuclear reactors

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Outline

1. Introduction

2. Principles of analog simulation of MC neutron transport

3. Neutron transport in fissile materials
Introduction
What is the Monte Carlo method?

The Monte Carlo method is a way of solving a deterministic problem by a stochastic approach using random numbers.

A number $n$ of independent observations (e.g. neutron histories) are collected. The result is derived from the averaged observation.

The Monte Carlo method is commonly applied on deterministic problems that are **difficult** to solve by deterministic methods.

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General advantages and disadvantages of the MC method

**General advantages**

- Complex problems can be solved without simplifications.
- Precision of the results can be improved simply by running the simulation longer (making more observations).
- Governing equations do not need to be formulated for the quantities of interest.

**General disadvantages**

- Large computing cost to achieve a good precision of some results.
- Statistical uncertainty in the results.
Specific advantages and disadvantages of the MC method in reactor physics

Specific advantages

- Geometry of the nuclear reactor does not need to be discretised and homogenised, as in case of deterministic methods.
- Microscopic neutron cross sections and other data can be treated with an accurate dependence on neutron energy.
- A single MC criticality code can simulate a great variety of nuclear reactors.

Specific disadvantages

- Quantities with spatial dependence (local power or flux) are hard to compute.
- Acceleration methods common in deterministic calculations ineffective due to presence of the random noise.
Major components of the Monte Carlo method

- Probability distribution function (pdf’s) that describe the system
- Random number generator
- Sampling rules
- Scoring (tallying) the outcomes
- Error estimation
- Variance reduction techniques
Application

Application in nuclear engineering

- Benchmarking of deterministic codes
- R&D of new reactors
- Computation of quantities in complex shielding and criticality problems (mainly in research), such as:
  - multiplication factor
  - neutron flux
  - reaction rates, group cross sections, etc.

Major Monte Carlo codes for reactor physics

- MCNP - Monte Carlo N-Particle Transport Code (Los Alamos National Laboratory, USA)
- TRIPOLI (CEA, France)
- KENO (Oak Ridge National Laboratory, USA)
- SERPENT (VTT, Finland)
Basic principles of analog simulation of MC neutron transport
Principles of analog simulation of MC neutron transport

- In analog Monte Carlo simulation, neutrons are simulated from “birth” (originating from the source) to “death” (absorption or leakage from the system).
- The birth-to-death simulation is called a neutron “history”.
- The average behaviour of neutrons is estimated via simulating of a large number of neutron histories.
Quantities in analog simulation of MC neutron transport

Transition kernel

\[ T(\vec{r}', \vec{r}, E, \vec{\Omega})dV = \text{probability for a neutron starting at } \vec{r}' \text{ with energy } E \text{ and direction } \vec{\Omega} \text{ to have its next collision in } dV \text{ at } \vec{r}. \]
Quantities in analog simulation of MC neutron transport

Collision kernel

\[ C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})dE d\Omega = \text{probability for a neutron entering a collision at } \vec{r} \text{ with energy } E' \text{ and direction } \vec{\Omega}' \text{ to exit the collision with energy } E \text{ in } dE \text{ and direction } \vec{\Omega} \text{ in } d\Omega. \]
Sampling neutron histories

If we can sample

- the source $S$, (i.e. $r, \vec{\Omega}$ and $E$)
- the transition kernel $T$, (i.e. $\vec{r}$, given $\vec{r'}$, $\vec{\Omega}$ and $E$)
- the collision kernel $C$, (i.e. $\vec{\Omega}$ and $E$, given $\vec{r}$, $\vec{\Omega'}$ and $E'$)

then

we are solving a neutron transport problem without even deriving the transport equation!
Schematic representation

- Neutron starting a flight path
- Neutron entering a collision
- Neutron exiting a collision
## Sampling the source $S(\vec{r}, E, \vec{\Omega})$

### Sampling $S(\vec{r}, E, \vec{\Omega})$

- sample position $\vec{r}$ (known for fixed source problems)
- sample direction $\vec{\Omega}$ (often isotropic)
- sample energy $E$

(e.g. Watt fission spectrum $f_S(E) = Ce^{-aE} \sinh(\sqrt{bE})$)
Sampling the transition kernel

**Transition kernel**

\[
T(\vec{r}', \vec{r}, E, \hat{\Omega})dV = \Sigma_t(\vec{r}, E)e^{-\Sigma_t s}ds
\]

where:

- \( s = |\vec{r} - \vec{r}'| \), i.e. \( \vec{r} = \vec{r}' + s\hat{\Omega} \)
- \( \Sigma_t(\vec{r}, E) = \sum_i N_i \sigma_{t,i}(\vec{r}, E) \) is the total macroscopic cross section of a material, where
  - \( N_i \) is atomic density of \( i \)-th isotope in the material
  - \( \sigma_{t,i} \) is the total microscopic cross section of \( i \)-th isotope
Sampling the transition kernel

- The transition kernel $T$ is the pdf $f_s$ for the distance $s$.
- We can sample $s$ by the inverse method if we know the cdf function $F_s$.
- $F_s = \int_0^s \Sigma_t(\vec{r}, E) e^{-\Sigma_ts'} ds' = 1 - e^{-\Sigma ts}$

Sampling the distance $s$

- Generate random number $u$ from (0,1)
- Solve $u = 1 - e^{-\Sigma ts}$ for $s$.
- $\Rightarrow s = -\frac{1}{\Sigma t} \ln(1 - u)$
- You can also use $s = -\frac{1}{\Sigma t} \ln(u)$
Sampling the transition kernel

How to sample $s$ in inhomogeneous media?
Sampling the transition kernel

How to sample $s$ in inhomogeneous media?

Neutron has no memory, so once a neutron has reached an interface, start a new flight path.

Algorithm

Select $s$ as $s = -\frac{1}{\Sigma t_1} \ln(u_1)$

- if $s < s_1$ then the collision point was found
- if $s \geq s_1$ then position neutron at interface boundary and select a new flight path as $s = -\frac{1}{\Sigma t_2} \ln(u_2)$

Note

Tracking the distances to the boundaries may be difficult in complex geometries...
Sampling the collision kernel

**Collision kernel**

\[
C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) = \sum_i \sum_j \frac{\Sigma_{ji}(\vec{r}, E')}{\Sigma_t(\vec{r}, E')} p_{i,j}(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})
\]

where:

- \(i\) sums over the isotopes
- \(j\) sums over the reaction types (elastic, inelastic, (n,2n), ...)
- \(p_{i,j}\) conditional probability for changing \(\vec{\Omega}\) and \(E\) knowing \(j\)-th reaction occurred on \(i\)-th isotope
Sampling the collision kernel

Sampling procedure

- select $i$-th nuclide with probability $p(i) = \frac{\sum_{t} t_i (\vec{r}, E')}{\sum_{t} t (\vec{r}, E')}$
- select reaction type $j$ with probability $p(j|i) = \frac{\sum_{i,j} j,i (\vec{r}, E')}{\sum_{t,i} t,i (\vec{r}, E')}$
- select energy $E$ and direction from $p_{i,j}(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$
- then we have selected from the pdf given by the collision kernel.
Sampling the collision kernel

Sampling the new angle and energy

- Scattering (often) isotropic in CM-system $\Rightarrow$ select $\mu_C$ 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.
Sampling the collision kernel

Transformation of angle from CM- to L-system

\[ \tilde{\Omega} = \frac{1}{\sqrt{A^2 + 2A\mu_C + 1}} (A\tilde{\Omega}_C + \tilde{\Omega}') \]
Neutron Transport in Fissile Materials
Neutron Transport in Fissile Materials

Problem
The distribution of the fission source is not known in fissile systems.

Solution
The fission source (together with the fundamental neutron flux and eigenvalue $k_{\text{eff}}$) need to be established over a simulation of a number of successive neutron generations (iterations).
Active/inactive cycles

- The iterations are called “cycles” in MC terminology.
- Unlike in deterministic calculations, the cycles have to continue after the convergence is reached in order to sample well the required result.
- The cycles where the source converges are called inactive, and no results are collected during these cycles.
- When the source is converged, active cycles can start, and results can start to be collected.
- Active cycles can be stopped when the results are computed to the required precision.