22.211 Lecture 3

Monte Carlo methods

Benoit Forget

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Outline

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Objectives

- Relation between nuclear data and distribution functions
- Introduction to pseudo-random numbers
- Understanding of basic sampling techniques
- Understanding of basic algorithm for particle simulation

Monte Carlo Neutron Transport - In a nutshell

- Simulate the stochasticity of nature by tracking neutrons randomly through our domain of interest from their birth to their death
- Use nuclear data and material properties to determine probabilities of various events
- Evaluate contribution of individual neutrons to a quantity of interest
- In addition to common modeling and data uncertainties, Monte Carlo results always present an element of statistical uncertainty
  - Average is never enough, you must always provide a measure of dispersion.

Outline

Probability Distribution Function

If X is a continuous random variable, $p(x)$ is a probability distribution function if:

- $\int_{\mathbb{R}} p(x)dx = 1$
- $p(x) \geq 0, \forall x$
- If $A \subseteq \mathbb{R}$, then $P(X \in A) = \int_A p(x)dx$

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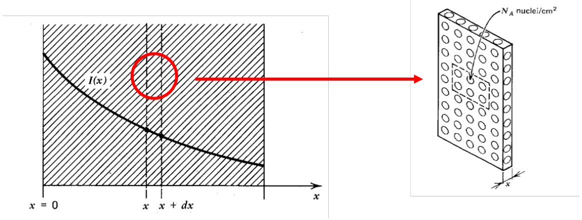
Review of Macroscopic xs



$$dR = \sigma_t I(x) dN_A = \sigma_t I(x) N dx$$

$$-dI(x) = -\left[I(x+dx) - I(x)\right] = \sigma_t I N dx$$

Dividing by dx yields a differential equation for beam intensity

$$\frac{dI(x)}{dx} = -N\sigma_t I(x)$$

Solving for $I(x)$ with an beam intensity of I_0 at boundary

$$I(x) = I_0 e^{-N\sigma_t x}$$

The macroscopic cross section is defined as the product of the nuclide density and the microscopic cross section

$$\Sigma_t = N\sigma_t$$

Interpretation

- Σ_t is the probability per unit path length traveled that the neutron will undergo a reaction with a nucleus in the sample
- $e^{-\Sigma_t x}$ is the probability that a neutron moves a distance x without any interaction
- $p(x)dx = \Sigma_t e^{-\Sigma_t x} dx$ is the probability that a neutron has its first interaction in dx after travelling a distance of x, this is at the foundation of Monte Carlo codes

$$p(x) = \begin{cases} \Sigma_t e^{-\Sigma_t x} & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

This distribution is also called the exponential distribution. $(X \sim Exp(\Sigma))$

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Example of Exponential Distribution

Suppose $X \sim Exp(1)$ (Comparable to a thermal neutron in water)

- $P(X \leq 1) = \int_0^1 e^{-x} dx = 1 - e^{-1} = 0.632$
- $P(X \leq 3) = \int_0^3 e^{-x} dx = 1 - e^{-3} = 0.950$
- $P(X \geq 5) = \int_5^\infty e^{-x} dx = e^{-5} = 0.0067$
- $P(X = 3) = \int_3^3 e^{-x} dx = 0$

This distribution defines the distance traveled by a neutron between collisions.

Uniform Distribution

If X is equally likely to be anywhere between a and b, then X has the uniform distribution on (a, b)

$$f(x) = \begin{cases} \frac{1}{(b-a)} & \text{if } a < x < b \\ 0 & \text{otherwise} \end{cases}$$

Notation $X \sim U(a, b)$
Very important distribution for sampling sources over a uniform volume.

Cumulative Distribution Function

For any random variable X, the cumulative distribution function is defined for all x by $F(x) = P(X \leq x))$

- X continuous implies

$$F(x) = \int_{-\infty}^{x} f(t)dt$$

- X discrete implies

$$F(x) = \sum_{y \leq x} f(y)$$

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Uniform Distribution cdf

Example: $X \sim U(0,1)$

$$f(x) = \begin{cases} 1 & \text{if } 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$F(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } 0 < x < 1 \\ 1 & \text{if } x > 1 \end{cases}$$

This distribution is the most commonly used in any Monte Carlo simulation.

Exponential Distribution cdf

Example: $X \sim Exp(\Sigma)$

$$f(x) = \begin{cases} \Sigma e^{-\Sigma x} & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$F(x) = \int_{-\infty}^{x} f(t)dt = \begin{cases} 0 & \text{if } x < 0 \\ 1 - e^{-\Sigma x} & \text{if } x \geq 0 \end{cases}$$

Properties of all cdf's

$F(x)$ is non-decreasing in x, i.e., $x_1 < x_2$ implies that $F(x_1) \leq F(x_2)$

$$\lim_{x \to \infty} F(x) = 1$$

$$\lim_{x \to -\infty} F(x) = 0$$

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Direct Sampling

- Direct inversion of the cdf
  - Sample random number ξ
  - Set $F(x) = \xi$
  - Invert cdf such that $x = F^{-1}(\xi)$
- Equivalent to Mathematical approach of the Monte Carlo integration
- Advantages
  - Most efficient way of sampling from a distribution
  - Straightforward approach
- Disadvantages
  - Can become quite complicated
  - Some functions cannot be inverted (i.e. Klein-Nishina photon scattering kernel)

Direct Sampling Example

Starting from the path length pdf

$$p(x)dx = \Sigma_t e^{-\Sigma_t x} dx \text{ for } 0 \leq x \leq \infty$$

We get the cdf

$$F(x) = \int_0^x p(x')dx' = 1 - e^{-\Sigma_t x}$$

Direct Sampling

$$\xi = 1 - e^{-\Sigma_t x}$$

$$e^{-\Sigma_t x} = 1 - \xi$$

$$x = -ln(1-\xi)/\Sigma_t \equiv -ln(\xi)/\Sigma_t$$

Mean Free Path

The mean or expected value of a random variable X is

$$\mu \equiv E[X] \equiv \int_{\mathbb{R}} xf(x)dx \text{ if } X \text{ is continuous}$$

- The mean gives an indication of the central tendency of X.

Average distance traveled by a neutron

$$\mu = \bar{x} = \int_0^\infty xp(x)dx = \Sigma_t \int_0^\infty xe^{-\Sigma_t x}dx = \frac{1}{\Sigma_t}$$

Variance

The variance of a random variable X is the second central moment.

$$\sigma^2 \equiv Var(X) \equiv E[(X-\mu)^2] = \int_{\mathbb{R}} (x-\mu)^2 f(x)dx$$

- The variance gives an indication of spread or dispersion.
- The standard deviation of X is $\sigma \equiv \sqrt{Var(X)}$
- Another way to evaluate $Var(X) = E[X^2] - (E[X])^2$

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Variance

$$Var(X) = E[(X-\mu)^2] = E[(X-E[X])^2]$$

$$Var(X) = E[X^2 - 2XE[X] + E[X]^2]$$

$$Var(X) = E[X^2] - 2E[X]E[X] + E[X]^2$$

$$Var(X) = E[X^2] - E[X]^2$$

Provides a form that doesn't rely on prior knowledge of the mean.

Distance Traveled

- Evaluate macroscopic total cross-section of material in which particle is located at energy E
- Use direct sampling on the exponential pdf with parameter $\Sigma_t(E)$
- Using distance traveled and direction sampled, calculate distance to nearest boundary
- If particle leaves medium, re-start sampling in new material with starting position at material boundary
  - Exponential distribution has no memory
- If distance is less than new material surface, particle makes a collision in medium

Rejection Sampling

- Random sampling of the pdf
- Equivalent to the simulation approach of the Monte Carlo integration
- Advantages
  - Very simple
- Disadvantages
  - Can become costly and/or confusing

Rejection Sampling Example

- Band pdf by a box ($g(x)$), such that $C \cdot g(x) \geq f(x)$
  - Pick $g(x)$ so that it is easy to sample
- Sample x from $g(x)$ using direct sampling
- Test to see if x is also inside $f(x)$ curve

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Discrete Sampling

- Build cdf from discrete (or continuous) pdf
- Pick a random number ξ
- Perform table search
  - Linear table search: go through each case one by one
    - Worst case performance: $O(N)$
  - Binary search: Start in the middle of the number of bins and reduce search space in half each time
    - Worst case performance: $O(log_2 N)$

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Collision Isotope

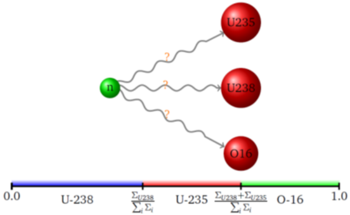
Determine which isotope of interaction by sampling the discrete pmf built from the total cross-sections of all isotopes in the material

$$p_j = N_j \sigma_{tj}(E) / \Sigma_t(E)$$

where

$$\Sigma_t(E) = \sum_j N_j \sigma_{tj}(E)$$

and j represents the isotope



Another Example

Assume a neutron of 10MeV will collide with Fe^{56}

- Evaluate all possible cross-section at that energy

$$\begin{array}{ll} (n,n) & 2.0 \text{ barns} \\ (n,n') & 0.1 \text{ barns} \\ (n,\gamma) & 0.001 \text{ barns} \\ (n,\alpha) & 0.1 \text{ barns} \end{array}$$

- Total cross-section is 2.201 barns

Another Example (2)

$$f(x) = \begin{cases} 0.9087 & \text{if } x = 1 \\ 0.0454 & \text{if } x = 2 \\ 0.0005 & \text{if } x = 3 \\ 0.0454 & \text{if } x = 4 \\ 0 & \text{otherwise} \end{cases}$$

$$F(x) = \begin{cases} 0.0 & \text{if } x \leq 0 \\ 0.9087 & \text{if } 0 < x \leq 1 \\ 0.9541 & \text{if } 1 < x \leq 2 \\ 0.9546 & \text{if } 2 < x \leq 3 \\ 1.0 & \text{if } x > 3 \end{cases}$$

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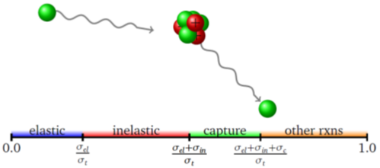
Collision Type

Once the collision isotope is selected, determine which reaction will occur by sampling a discrete pmf built from the microscopic cross-section of this isotope

$$p_k = \sigma_k(E)/\sigma_t(E)$$

where k is the reaction type and

$$\sigma_t(E) = \sigma_{n,n}(E) + \sigma_{n,n'}(E) + \sigma_{n,\gamma}(E) + \ldots$$



Collision Type

- If the collision is absorption, the particle is killed (in analog simulations)
- If the collision is scattering, sample the outgoing energy and direction from the scattering data
- If the collision is $(n, 2n)$, sample the outgoing energy and direction of each neutron. Follow each neutron individually until they are killed (or double the weight).
- ...

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Outline

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
```

Scattering

- Scattering laws are defined in either the CM or LAB system
- Simulation is performed in the LAB system
- Sample Energy and direction (sometime they are correlated)
- Example: Elastic Scattering with target at rest

$$E' = E\frac{(A^2 + 2A\mu_{CM} + 1)}{(A+1)^2}$$

$$\mu_L = \frac{1 + A\mu_{CM}}{\sqrt{A^2 + 2A\mu_{CM} + 1}}$$

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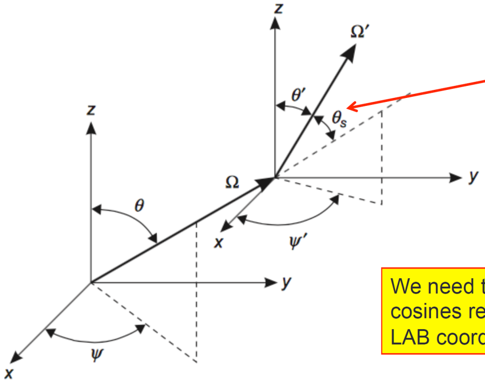
Post-collision direction



Scattering angle in LAB relative to incident angle

We need to know cosines relative to LAB coordinates

Figure 10.7 The relation between the coordinates of the particle in direction $\mathbf{\Omega}$ before a scatter and the direction $\mathbf{\Omega}'$ after the scatter. The angle between $\mathbf{\Omega}$ and $\mathbf{\Omega}'$ is the scattering angle θ_s, namely, $\cos\theta_s = \mathbf{\Omega} \cdot \mathbf{\Omega}'$.

Exit Direction

- The polar angle is given by the scattering law, μ_L
- The azimuthal angle is sample uniformly over 2π

$$u' = \mu_L u + \frac{\sqrt{1-\mu_L^2}(uw\ cos(\phi) - v\ sin(\phi))}{\sqrt{1-w^2}}$$

$$v' = \mu_L v + \frac{\sqrt{1-\mu_L^2}(vw\ cos(\phi) + u\ sin(\phi))}{\sqrt{1-w^2}}$$

$$w' = \mu_L w - \sqrt{1-\mu_L^2}\sqrt{1-w^2}\ cos(\phi)$$

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- Tally: A current score or amount.
- A Monte Carlo simulation tracks particles through a random walk. This random walk includes travel through many cells, materials and boundaries.
- During a history (i.e. 1 random walk), we will tally events of interest (e.g. reaction rates, energy deposition, flux, ...)
- After the history is complete, compute total score and its square.
- After all histories are complete, compute sample mean and sample variance

Flux Tally - Pathlength

- Flux: Total distance traveled by neutrons per cm^3 per second
- Pathlength estimator is the direct application of the definition
- For each particle travelling in a cell of interest, tally the distance traveled times the weight
- Divide by cell volume and total starting weight

$$\phi = \frac{1}{V}\frac{1}{W}\sum_{\text{all n's in cell}} d_j wgt_j$$

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

Delta Tracking - BWR Assembly

- Define a "majorant" total macroscopic cross-section that is the maximum value it can take at all energies
- Use this "majorant" cross-section when tracking

$$s = \frac{-\ln \xi_1}{\Sigma_{t,maj}(E)}$$

- Track across all geometry without stopping at material boundaries
- At collision site i, perform rejection sampling to determine if collision was real of not

$$\xi_2 < \frac{\Sigma_{t,i}(E)}{\Sigma_{t,maj}(E)}$$

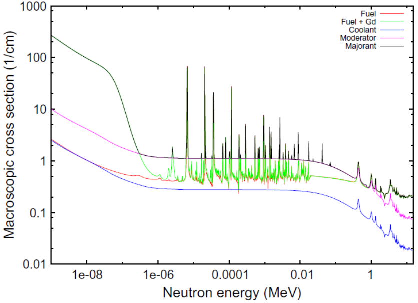

Fig. 1. Macroscopic material total cross sections and the majorant in a BWR assembly calculation with burnable absorber (cladding omitted). The majorant is dominated by the capture cross sections of gadolinium isotopes at low energy, which results in a poor efficiency in the rejection sampling loop. Above thermal region the majorant is comprised of the moderator cross section and some discrete resonance peaks from the fuel isotopes.

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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!

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/)