NE 155
Introduction to Numerical Simulations in Radiation Transport
Lecture 35: Geometry and Collisions

R. N. Slaybaugh
Richard Vasques

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Outline

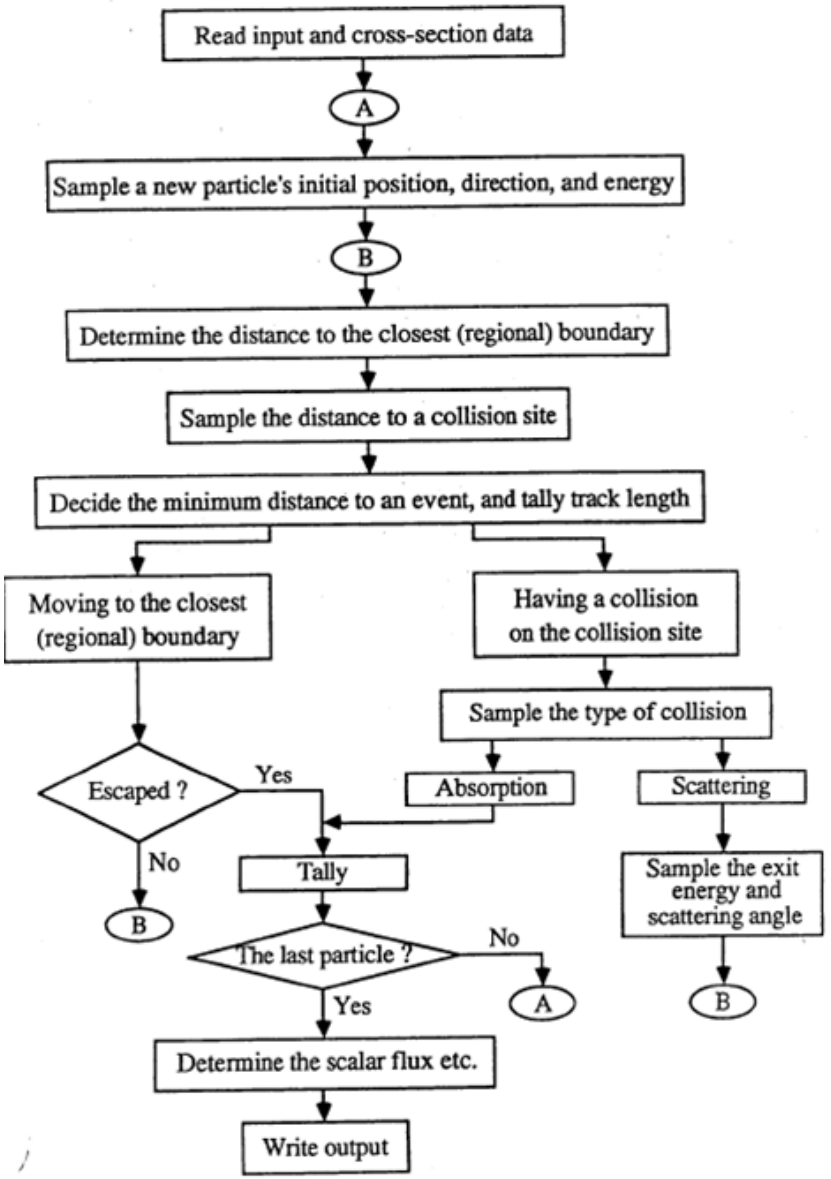
1. Overview of Monte Carlo for Neutron Transport
2. Determining next event location
   - Sampling flight path
   - Distance to boundary
   - Next event selection
3. Collision Physics
   - Sampling target nuclide
   - Sampling reaction type
   - Sampling exit direction
   - Sampling exiting particles

Notes derived from Jasmina Vujic and Paul Wilson

Learning Objectives

1. Be able to provide MC transport algorithm
2. Understand basic tracking of particles through a geometry
   - Understand the steps necessary for tracking particles
   - Understand the use of mean free path
   - Sample the distance to the next physics event
   - Determine next event
3. Understand what sampling needs to happen after a collision

Monte Carlo for Transport



Possible Futures for a Particle

After we've gotten to Circle B, we have a neutral particle:

- At point (x_p, y_p, z_p)
- Moving in direction (u, v, w)
- With energy E

What are possible next events?

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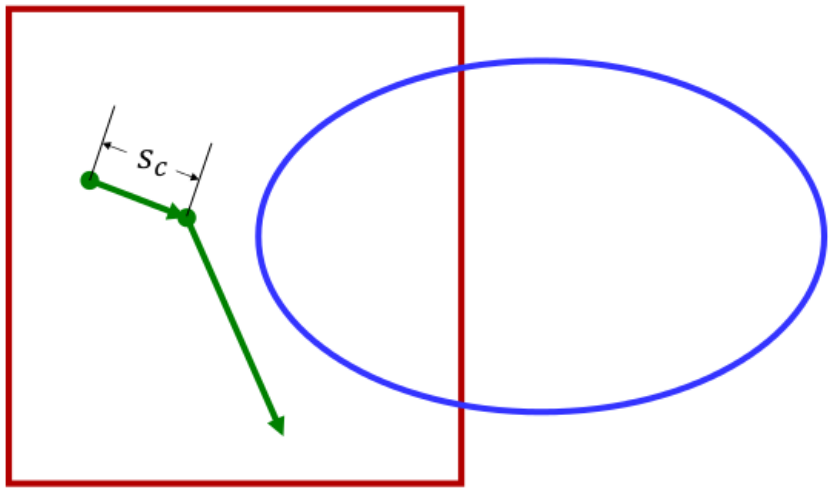

Figure 1: Collision

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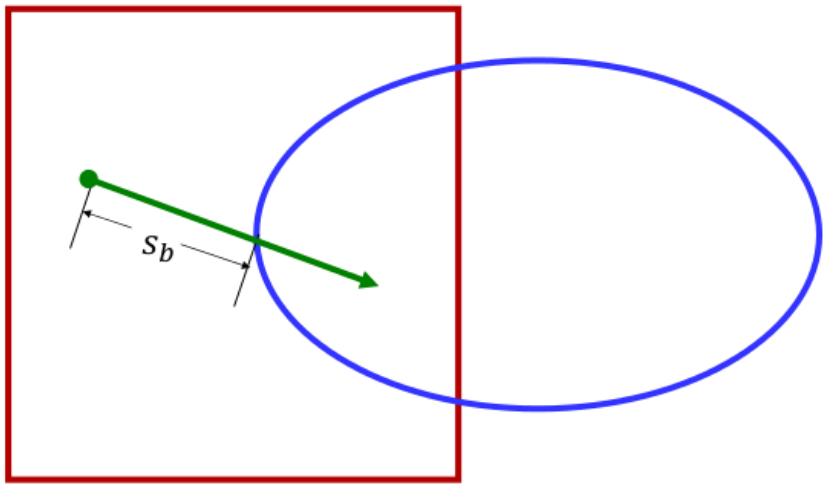

Figure 1: ../figs/Surface Crossing

Sampling Distance to Collision

Collisions are probabilistic

- Note that Σ_t, the total macroscopic cross section, will be a function of space if we have multiple materials
- Along a particular path, the *probability of a collision at distance s* from the start:

$$p_c(s) = \Sigma_t(s) e^{-\Sigma_t(s)s} ds$$

$$P_c(n) = \int_0^s \Sigma_t(s) e^{-\Sigma_t(s)s'} ds' = -e^{-\Sigma_t(s)s'}|_0^s = 1 - e^{-\Sigma_t(s)s}$$

- The cross section, $\Sigma_t(s)$, is piecewise constant, but changing

Sampling Distance to Collision

- Variable transformation: measure distance in units of *mean free path*:

$$n = \Sigma_t(s)s \ , \quad dn = \Sigma_t(s)ds$$

- We'll start with the PDF and integrate to get the CDF

$$p_c(n)dn = e^{-n}dn$$

$$P_c(n) = \int_0^n e^{-n'}dn' = -e^{-n'}|_0^n = 1 - e^{-n}$$

- Importantly, this is now independent of the material

Sampling Distance to Collision

Randomly sample to determine number of mean free paths until next collision, n_c

- $g(n_c)dn_c = e^{-n_c}dn_c$
- $G(n_c)dn_c = 1 - e^{-n_c}$
- Directly invert to get: $\boxed{n_c = -\ln(1-\xi)}$
  (note $1-\xi$ is equivalent to ξ)
- In the absence of material boundaries ($\Sigma \neq f(s)$), the distance to a collision, s_c, is

$$s_c = \frac{n_c}{\Sigma_t}$$

Calculating Distance to Boundary

- Usually have *more than one material*
- Distance to boundary is deterministic
- Algebra to determine distance between point and surface, s_b
- Convert it to units of mean free path for the current cell's material,

$$n_b = s_b \Sigma_t$$

Geometry Representations

- Combinatorial Surfaces
  - Define surfaces
  - Boolean operations combine surfaces to create cells
- Combinatorial Solids
  - Choose solid objects
  - Boolean operations combine objects to create regions
- B-Rep (Vertex-Edge)
  - Each object is a single set of vertices and edges connecting them

We're skipping how to find n_b, just know that we can find it

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  - Sample reaction type
  - Sample new direction
  - Sample new energy
  - Sample exiting particles
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- Some of these may depend on each other
- Repeat
  - Sample new n_c following collision
  - Calculate new n_b in new direction

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- Boundary is closer than collision
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  - Update $n_c = n_c - n_b$
- **DO NOT SAMPLE** for new n_c

- Calculate new n_b in new cell
  - New set of boundaries
  - New value of Σ_t

So You Had a Collision?

- Sample **target nuclide** for a mixture with J nuclides

$$\Sigma_t = \sum_{j=1}^{J} N_j \sigma_{t,j}$$

- *Discrete PDF* to determine which nuclide is hit

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- Sample **reaction type** for an nuclide with R types of reactions

$$\Sigma_{t,j} = \sum_{x=1}^{R} \Sigma_{x,j}$$

- *Discrete PDF* to determine which reaction occurs

$$p_x = \frac{\Sigma_{x,j}}{\Sigma_{t,j}}$$

Outcome of Reaction

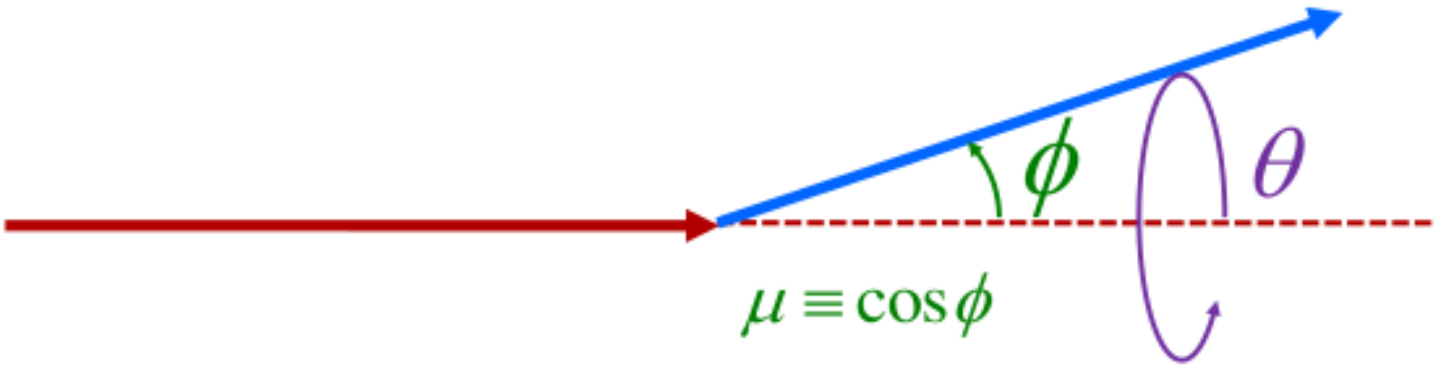
- Particle maybe absorbed
- Particle may continue its history in a *different direction* and with a *different energy*
- Energy-angle distributions are tabulated in different formats
  - Scattering laws have analytic forms with parameters in data tables (Direct inversion or rejection sampling)
  - Tabulated data that describes a piecewise analytic interpolation (Hybrid sampling; we skipped this)

Using a Scattering Angle

Scattering angles are defined relative to the original direction (considered as the z-axis)

- Polar angle, ϕ, determined by sampling from data
- Azimuthal angle, θ, determined by sampling isotropically
- The new direction is $\left(\sin(\phi)\cos(\theta), \sin(\phi)\sin(\theta), \cos(\theta)\right)$

$$= \left(\sqrt{1-\mu^2}\cos(\theta), \sqrt{1-\mu^2}\sin(\theta), \mu\right)$$



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- *After a collisions* we need to determine many things associated with the collisions (target, reaction, direction, energy)
- Repeat analysis for collisions/crossing until particle **terminates**

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We've developed a general sense of using MC for neutron transport

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- Next time: tallying results