

NE 255

Numerical Simulations in Radiation Transport

Geometry, Collisions, and Scoring

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MAJOR COMPONENTS OF MC ALGORITHM

- **PDFs:** the physical/mathematical system must be described by a set of pdfs.
- **Random number generator:** a source of random #s uniformly distributed on the unit interval.
- **Sampling rule:** prescription for sampling the pdf (given having random #s)
- **Scoring:** *the outcomes must be accumulated/tallied for quantities of interest*
- **Error estimation:** an estimate of the statistical error (variance) of the solution
- **Variance Reduction:** methods for reducing the variance and computation time simultaneously
- **Parallelization:** efficient use of computers

OUTLINE

① Determining next event location

- Sampling flight path
- Distance to boundary
- Next event selection

② Collision Physics

- Sampling target nuclide
- Sampling reaction type
- Sampling exit direction
- Sampling exiting particles

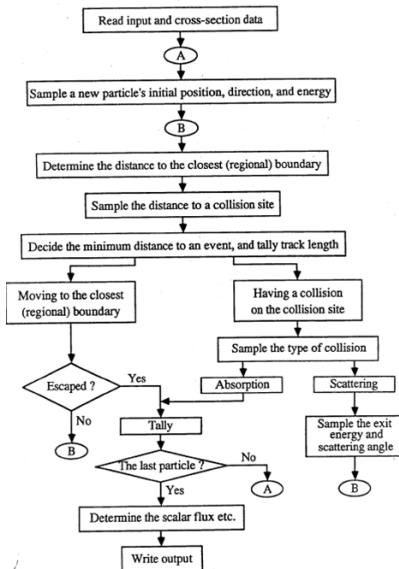
③ Scoring

Notes derived from Jasmina Vujic and Paul Wilson

LEARNING OBJECTIVES

- ① 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
- ② Understand what sampling needs to happen after a collision
- ③ Understand how to translate interactions into a score

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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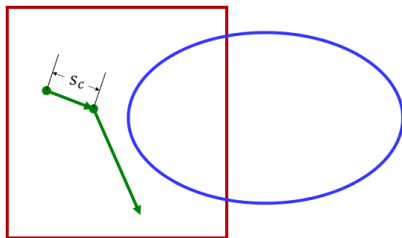


Figure 1 : Collision

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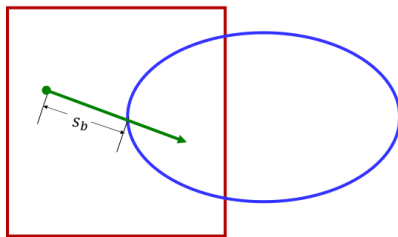


Figure 1: fig/Surface Crossing

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*:

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

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

- 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

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

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

- 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: $n_c = -\ln(1 - \xi)$
[note $(1 - \xi)$ is equivalent to ξ]
- In the absence of material boundaries ($\Sigma_t \neq f(s)$), 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 s_b , just know that we can find it using the internal geometry representation

OPTION A: COLLISION

$n_b > n_c$:

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- Using physics models and/or cross-sections
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 - Sample reaction type
 - Sample new direction
 - Sample new energy
 - Sample exiting particles
- Some of these may depend on one another

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- Some of these may depend on one another
- Repeat
 - Sample new n_c following collision
 - Calculate new n_b in new direction

OPTION B: CELL BOUNDARY

$$\underline{n_b < n_c:}$$

- Boundary is closer than collision
- Boundary crossing occurs

OPTION B: CELL BOUNDARY

$n_b < n_c$:

- Boundary is closer than collision
- **Boundary crossing occurs**
- Move particle along ray
 - Update $n_c = n_c - n_b$
- **DO NOT SAMPLE** for new n_c

OPTION B: CELL BOUNDARY

$n_b < n_c$:

- Boundary is closer than collision
- **Boundary crossing occurs**
- Move particle along ray
 - 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

$$p_i = \frac{\Sigma_{t,j}}{\Sigma_t}$$

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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

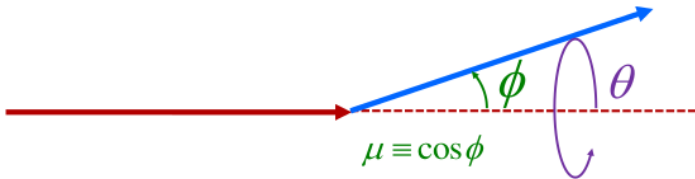
- Particle maybe absorbed
- Particle may continue its history in a *different direction* and/or with a *different energy*
- Energy-angle distributions are tabulated in different formats
 - Scattering laws have analytic forms with parameters in data tables (Direct inversion or rejection sampling)
 - Tabulated 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 $(\sin(\phi) \cos(\theta), \sin(\phi) \sin(\theta), \cos(\theta))$

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



SUMMARY OF PART I

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

- Basic Algorithm

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

- Basic Algorithm
- We can determine if particles have collisions or cross boundaries
- *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**