

**NE 155**

**Introduction to Numerical Simulations in  
Radiation Transport  
Geometry and Collisions**

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# OUTLINE

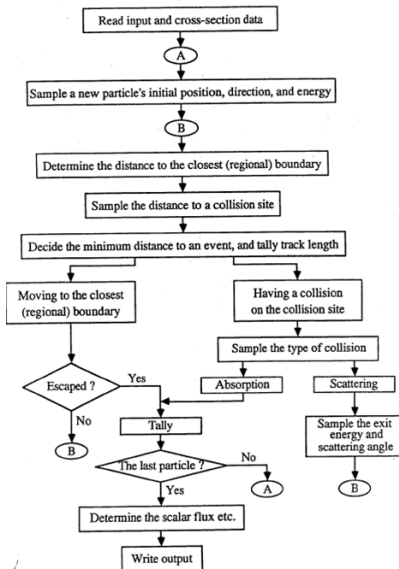
- ❶ Overview of Monte Carlo for Neutron Transport
- ❷ Determining next event location
  - Sampling flight path
  - Distance to boundary
  - Next event selection
- ❸ Collision Physics
  - Sampling target nuclide
  - Sampling reaction type
  - Sampling exit direction
  - Sampling exiting particles

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

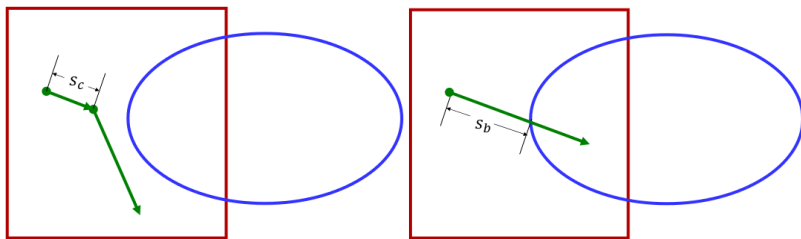


# POSSIBLE FUTURES FOR A PARTICLE

After we've gotten to **Circle B** on the chart, 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?



**Figure 1:** Collision../figs/Surface Crossing

# SAMPLING DISTANCE TO COLLISION

Collisions are probabilistic

- Note that  $\Sigma_t$ , 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*:

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

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

- This is the probability of interaction per unit distance  $\times$  probability of traveling  $s$  without interacting
- 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,  $n_c$

- $p(n_c)dn_c = e^{-n_c}dn_c$
- $P(n_c)dn_c = 1 - e^{-n_c}$
- Directly invert to get:  $n_c = -\ln(1 - \xi)$   
(note  $1 - \xi$  is equivalent to  $\xi$ )
- 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

# OPTION A: COLLISION

$n_b > n_c$ :

- Boundary is further away than collision
- Collision occurs
- Using physics models and/or cross-sections
  - Sample target nuclide
  - Sample reaction type
  - Sample new direction
  - Sample new energy
  - Sample exiting particles
- Some of these may depend on each other
- Repeat
  - Sample new  $n_c$  following collision
  - Calculate new  $n_b$  in new direction

## 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  $\Sigma_t$

# 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

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

- Sample **reaction type** for a 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

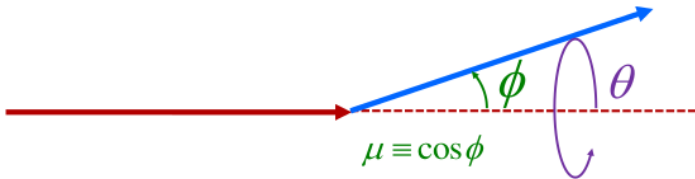
- Particle maybe absorbed
- Particle may continue its history in a *different direction* and with a *different energy*
- Energy-angle distributions are tabulated in different formats
  - Scattering laws have analytic forms with parameters in data tables (Direct inversion or rejection sampling)
  - Tabulated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

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**