

OpenMC Module: Monte Carlo Theory

Computational Reactor Physics Group

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Solving the Neutron Transport Equation

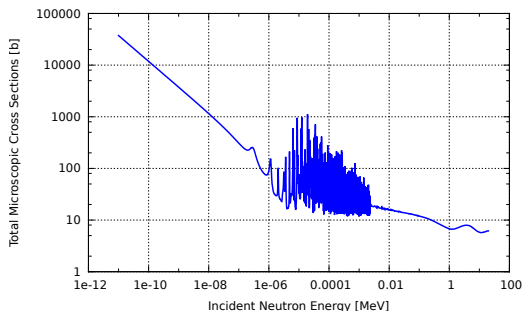
- Assume $\partial\psi/\partial t = 0$ and scale fission term

$$\begin{aligned}\hat{\Omega} \cdot \nabla \psi_k + \Sigma_t(\mathbf{r}, E) \psi_k(\mathbf{r}, \hat{\Omega}, E) = \\ \iint dE' d\Omega' \Sigma_s(\mathbf{r}, \hat{\Omega} \cdot \hat{\Omega}', E' \rightarrow E) \psi_k(\mathbf{r}, \hat{\Omega}', E') \\ + \frac{1}{k} \frac{\chi(E)}{4\pi} \int dE' \nu \Sigma_f(\mathbf{r}, E') \phi_k(\mathbf{r}, E')\end{aligned}$$

- Eigenvalue problem for k and ψ_k
- Monte Carlo method involves simulating individual neutrons
- Random numbers are sampled from probability distributions that represent physics

Cross Section Data Needed

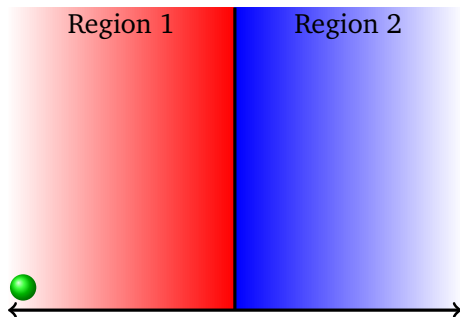
- Microscopic cross sections and other physics laws are input into Monte Carlo codes
- Data contained in ACE-formatted files
- These files are commonly generated with NJOY processing code
- Currently can be obtained via MCNP/Serpent Software



Basic Monte Carlo Algorithm – Eigenvalue

```
Guess initial source distribution and  $k$ 
for  $i = 1 \rightarrow n_{batches}$  do
  for  $j = 1 \rightarrow n_{particles}$  do
    Sample neutron from source distribution
    while Neutron is alive do
      Sample distance to collision
      Determine isotope in collision
      Sample physics
      Bank fission sites
    end while
  end for
  Sample neutrons from fission sites collected
  Calculate  $k$ 
end for
```

Distance to Neutron Collision

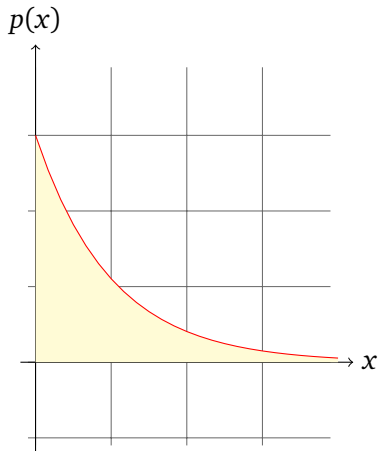


- Neutron is born or exits collision
- Neutrons are sampled from:

$$p(x)dx = \Sigma_t e^{-\Sigma_t x} dx$$

- If a surface is crossed, neutron is resampled from this surface
- If a surface is not crossed, a neutron has collided

Distance to Neutron Collision

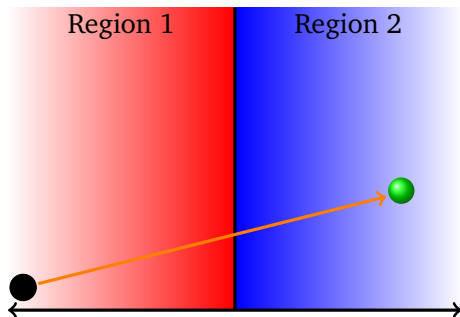


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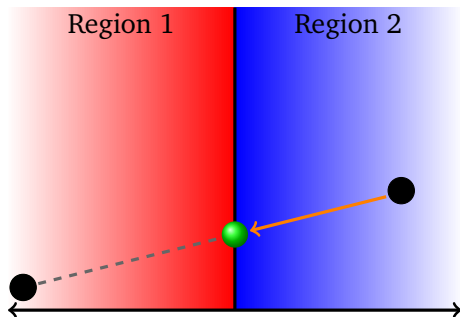


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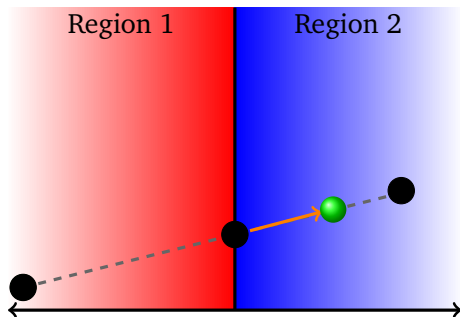


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- If a surface is crossed, **neutron is resampled from this surface**
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Distance to Neutron Collision

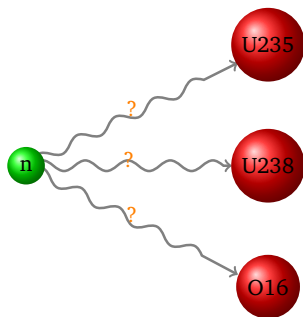


- Neutron is born or exits collision
- Neutrons are sampled from:

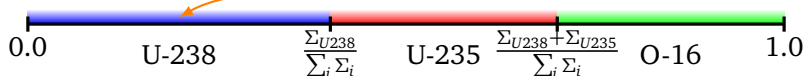
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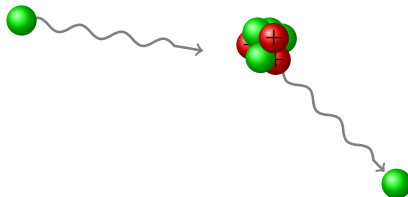
Choosing the isotope involved in collision



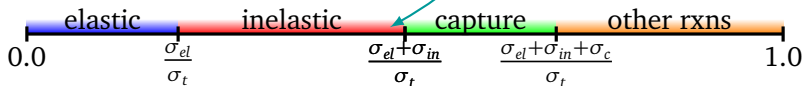
- Select random number (0,1), ξ



Sampling the Interaction Physics



- Select random number (0,1), ξ



- Physics is performed by sampling from ACE data

Implicit Fission Model – Eigenvalue Calculations

- Fission is not explicitly sampled, like other reactions
- At every collision, fission neutrons are implicitly sampled

$$n = \left[w \frac{\nu \Sigma_f}{\Sigma_t} + \xi \right] \quad \text{fission sites}$$

- Sites are banked for next batch of neutrons

```
type Bank
  real(8) :: wgt ! weight of bank site
  real(8) :: xyz(3) ! location of bank particle
  real(8) :: uvw(3) ! directional cosines
  real(8) :: E ! energy
end type Bank
```

Estimating Effective Multiplication Factor

- Analog

$$k_{ana} = \frac{\sum_{i \in \text{bank}} w_i}{W}$$

- Collision

$$k_{col} = \sum \frac{w_i \nu \Sigma_f}{W \Sigma_t}$$

- Absorption

$$k_{abs} = \sum \frac{w_i \nu \Sigma_f}{W \Sigma_a}$$

- Track-length

$$k_{track} = \sum \frac{w_i \nu \Sigma_f d}{W}$$

Tallying Physics

- Method to extract quantities out of Monte Carlo run (e.g., flux, reaction rates, current, etc.)
- Tallies are made using different estimators (e.g., analog, collision, track-length)
- When an event occurs, the following formula is used for tallies:

$$\text{tally} = \sum_{i \in \text{events}} \frac{R_i w_i \phi_i}{W}$$

- w_i : neutron statistical weight
- R_i : response function (flux=1, reaction rates= Σ)
- ϕ : estimator (analog=1, collision= Σ_t^{-1} , track= d)

Eigenvalue Calculations – Converging Fission Source

- Monte Carlo eigenvalue problem solved with Power Iteration
- Source must be guessed and iterated until converged
- May take many iterations (inactive batches) to converge depending on dominance ratio

All these batches should be discarded!