# OpenMC Module: Monte Carlo Theory

#### Computational Reactor Physics Group

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# Solving the Neutron Transport Equation

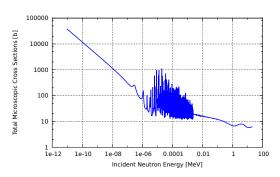
• Assume  $\partial \psi / \partial t = 0$  and scale fission term

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

- ullet Eigenvalue problem for k and  $\psi_k$ 
  - where  $\phi_k = \int d\Omega \psi_k(\mathbf{\Omega})$
- Monte Carlo method invovles simulating individual neutrons
- Random numbers are sampled from probability distributions that represent physics

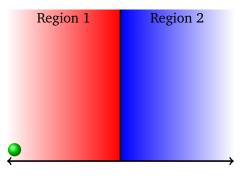
### Cross Section Data Needed

- 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 or directly from NEA (JEFF)



## Basic Monte Carlo Algorithm - Eigenvalue

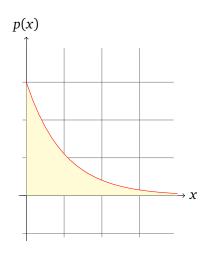
```
Guess initial source distribution and k
for i = 1 \rightarrow n_{batches} do
   for j = 1 \rightarrow n_{particles} do
       Sample neutron from source distribution
       while Neutron is alive do
           Sample distance to collision
           Determine isotope in collision
           Sample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



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

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

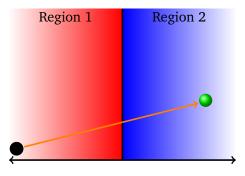
- If a surface is crossed, neutron is resampled from this surface
- If a surface is not crossed, a neutron has collided



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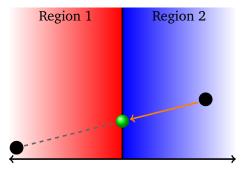
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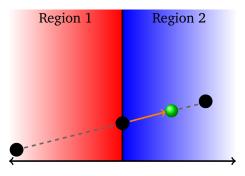
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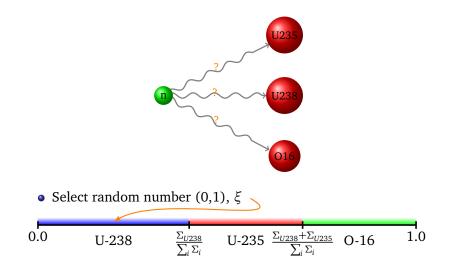


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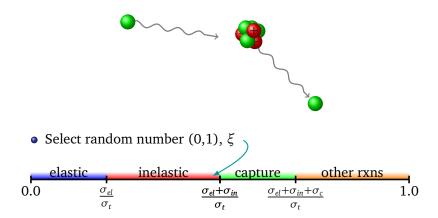
$$p(x)dx = \Sigma_t e^{-\Sigma_t x} dx$$

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## Choosing the isotope involved in collision



## Sampling the Interaction Physics



• Physics is performed by sampling from ACE data

## Implicit Fission Model – Eigenvalue Calculations

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

$$n = \left\lfloor w \frac{v \Sigma_f}{\Sigma_t} + \xi \right\rfloor \quad \text{fission sites}$$

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) ! diretional cosines
  real(8) :: E ! energy
end type Bank
```

• Note: w is the statistical neutron weight

# **Estimating Effective Multiplication Factor**

Analog

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

Collision

$$k_{col} = \sum_{i} \frac{w_i v \Sigma_f}{W \Sigma_t}$$

Absorption

$$k_{abs} = \sum_{i} \frac{w_i v \Sigma_f}{W \Sigma_a}$$

Track-length

$$k_{track} = \sum_{i} \frac{w_i v \Sigma_f d}{W}$$

# **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:

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

- $w_i$ : neutron statistical weight, where W is total starting weight
- $R_i$ : response function (flux=1, reaction rates= $\Sigma$ )
- $\phi$ : estimator (analog=1, collision= $\Sigma_t^{-1}$ , 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!