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Title: (U) Introduction to Monte Carlo Methods

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(U) Introduction to Monte Carlo Methods

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April 4, 2017

Abstract

Monte Carlo methods are very valuable for representing solutions to particle transport problems. Here we describe a "cook book" approach to handling the terms in a transport equation using Monte Carlo methods. Focus is on the mechanics of a numerical Monte Carlo code, rather than the mathematical foundations of the method.

(U) Introduction to Monte Carlo Methods

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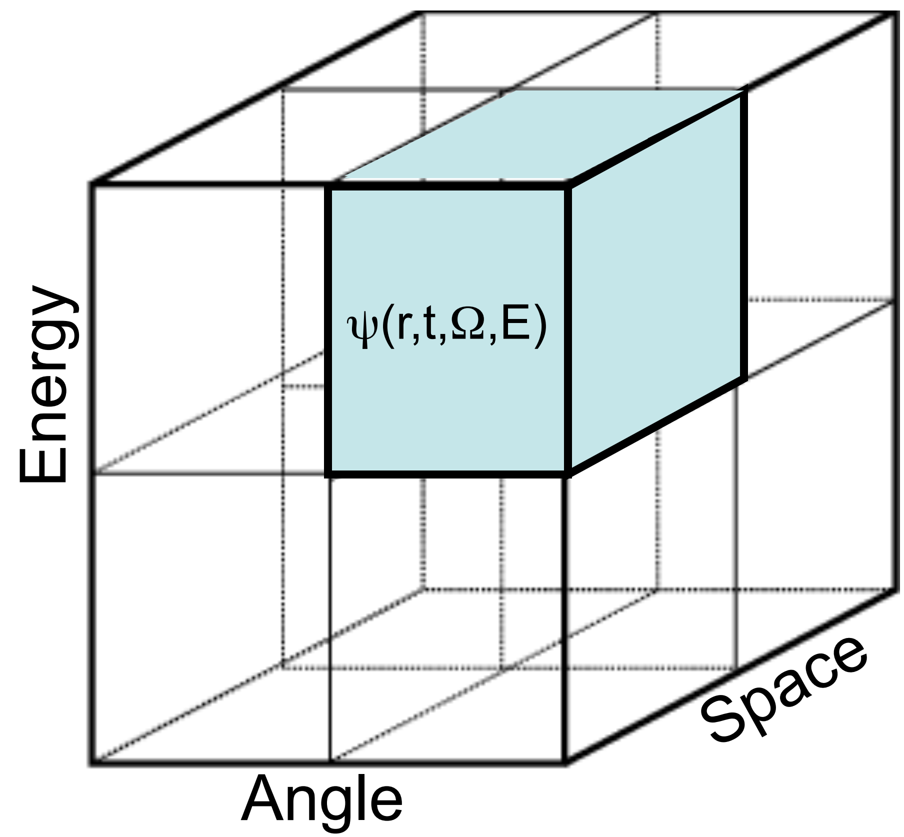
Outline

Particle vs. Continuum Methods
Function Sampling Techniques
Transport Equation: Term by Term
Monte Carlo Estimators

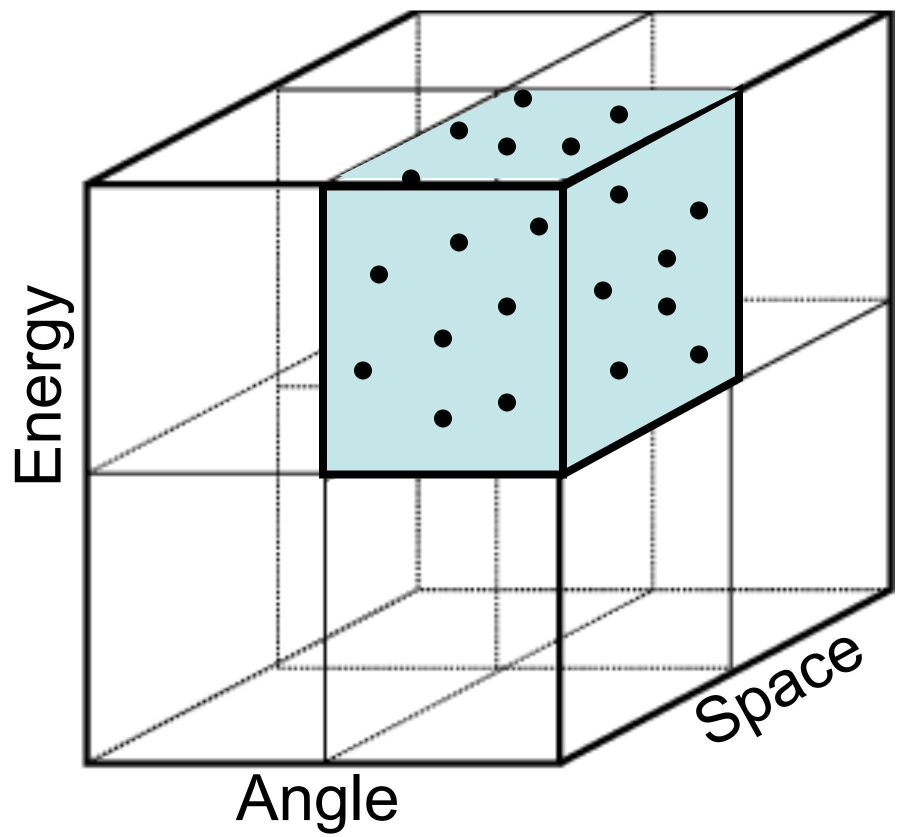
Deterministic Methods

- Take a differential volume in phase space (energy, angle, space,time)
- ψ represents sort of an average solution in the phase space volume.
- Evolve ψ in every phase space volume according to the transport equation.



Particle Methods

- Pick out points on the function
  - not phase space volumes
  - individual instances of the sol'n
- Evolve them according to the microphysics that the terms in the transport equation represent
- In the limit as $N_{packet} \rightarrow N_{particles}$ in the system, then we are modeling the true microphysical processes of nature
- Generally, each packet represents some large number of neutrons or photons.



Comparison: Particle vs Deterministic

Particle

- Inherently local
  - Conservation enforced on an event by event basis
- No ψ
  - Only when we back out and look at all of our instances in an ensemble do we have a sense of ψ as a function
- If we want to know mean values of a function, we must keep a separate tally for it

Deterministic

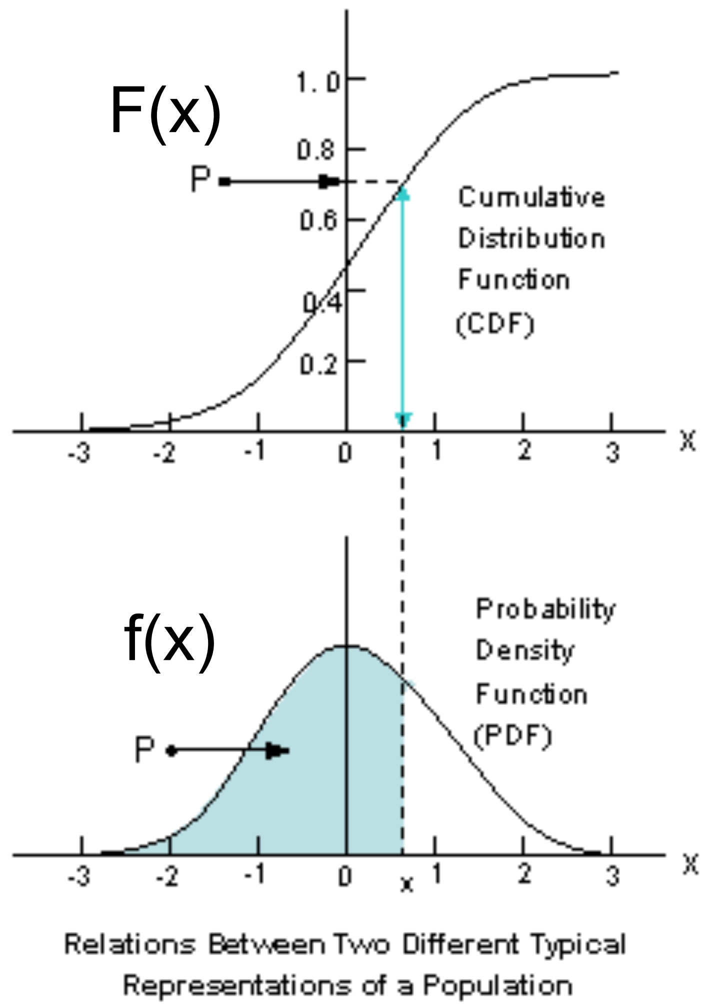
- Global Solutions
  - We do the same solution for every phase space volume
- ψ is what we are tracking, so any value computed from ψ is readily available everywhere
- We must pay for the whole solution, even if we only care about a small piece of it

Sampling - Inversion

- 2 Classes
  - Inversion
  - Rejection

- Cumulative Distribution Function

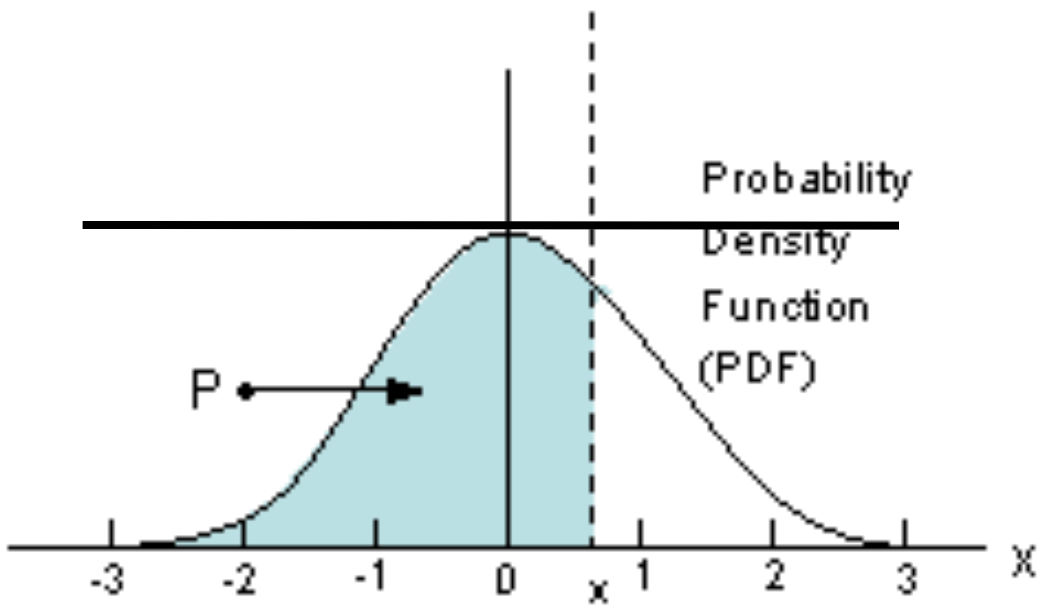
$$F(x) = \frac{\int_{-\infty}^{x} f(x')dx'}{\int_{-\infty}^{\infty} f(x')dx'}$$



http://home.ubalt.edu/ntsbarsh/Business-stat/CdfAndPdf.gif

Sampling - Rejection

- Choose x from a uniform distribution.
- Choose a random number ξ on [0,1]
- If f(x) > ξ then keep x as a sample.
- Else reject x as a sample and start over.



Sampling - Rejection

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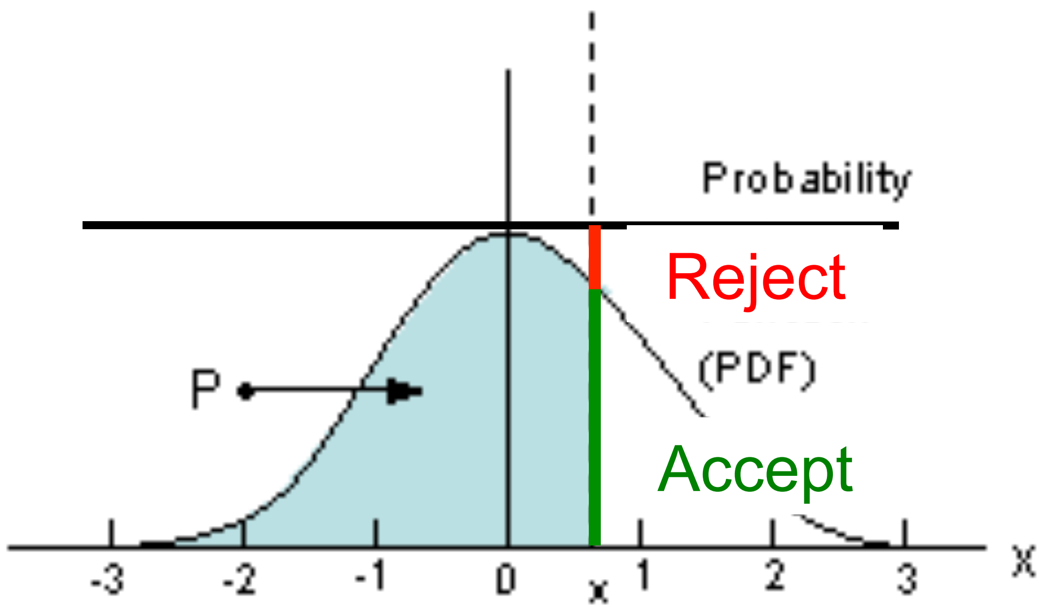
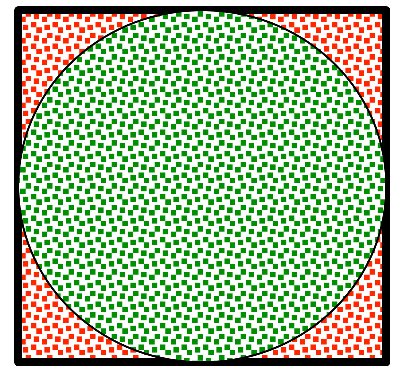
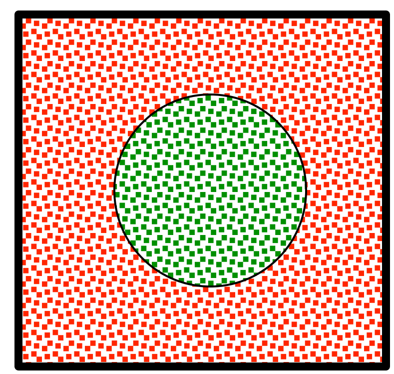


Calculate the area of a shape by throwing random darts at a square board.

$$\frac{A_{shape}}{A_{square}} = \frac{\#_{green\_darts}}{\#_{total\_darts}}$$

Red = Reject
Green = Accept





Transport Equation

Streaming and Removal Term

Scattering Term

$$\frac{1}{v_n}\frac{\partial\Psi}{\partial t}+\Omega\bullet\nabla\Psi+(\sigma_f+\sigma_s)\Psi=\int\int\Psi(r,t,\Omega',E')\sigma(E'\rightarrow E,\Omega'\rightarrow\Omega)d\Omega'dE'+$$

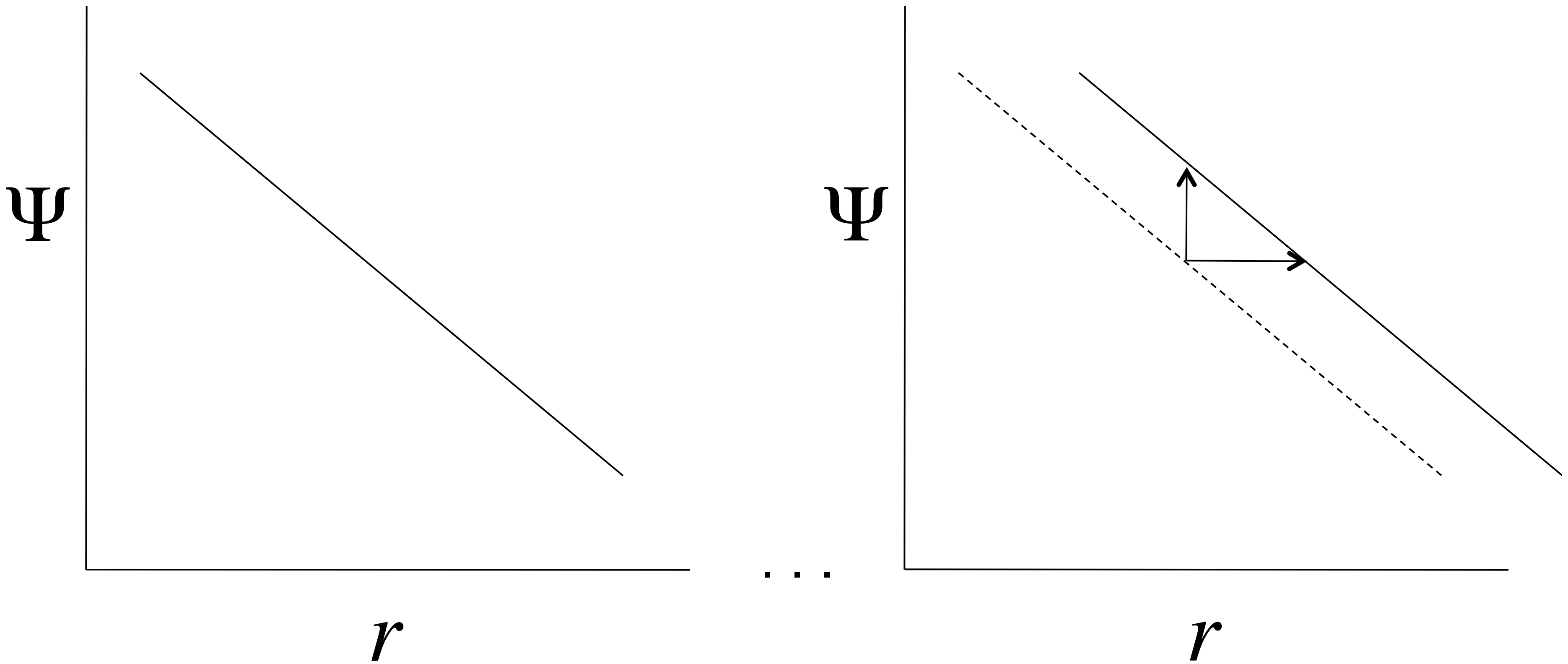
Fission Term

Source Term

$$\int\int\Psi(r,t,\Omega',E')\sigma_f(E',\Omega')\nu'(E',\Omega')S_f(E,\Omega)d\Omega'dE'+Q(r,t,\Omega,E)$$

Streaming Term

$$\frac{1}{v_n}\frac{\partial \Psi}{\partial t} + \Omega \bullet \nabla \Psi$$



Streaming Term

$$\frac{1}{v_n}\frac{\partial\Psi}{\partial t}+\Omega\bullet\nabla\Psi$$

- Basically a translation of the former solution in space
- Direction Ω and Energy E of packet are unchanged
- New values for position and time are updated:
  - $r_{new} = r_{old} + v_n \partial t$
  - $t_{new} = t_{old} + \partial t$

Removal Term

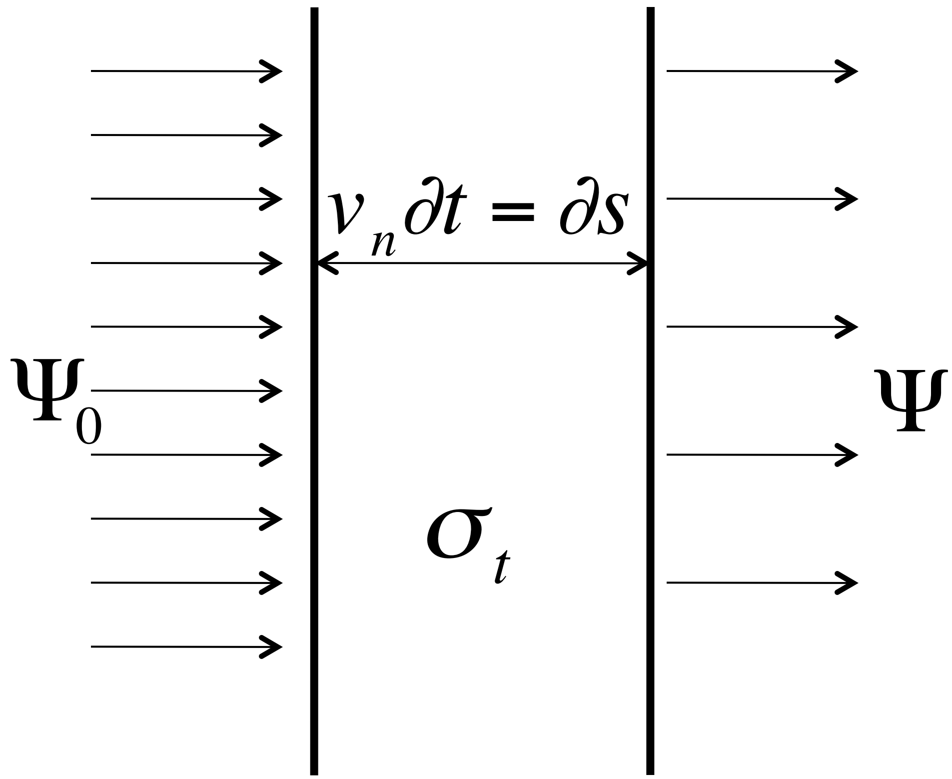
$$\frac{1}{v_n}\frac{\partial \Psi}{\partial t} + (\sigma_f + \sigma_s)\Psi$$

$$\frac{\partial \Psi}{\partial s} + \sigma_t \Psi = 0$$

$$\frac{1}{\Psi}\partial \Psi = -\sigma_t \partial s$$

$$\ln \Psi = -\sigma_t s + C$$

$$\Psi = \Psi_0 e^{-\sigma_t s}$$



Fraction of original angular flux remaining is given by an exponential distribution in *s*.

Sample a Distance to Collision (by inversion technique)

- PDF ➔ $$f(x) = e^{-\sigma x}$$

- CDF ➔ $$F(x) = \frac{\int_0^x e^{-\sigma x} dx}{\int_0^\infty e^{-\sigma x} dx} = 1 - e^{-\sigma x} = \xi$$

Random Number

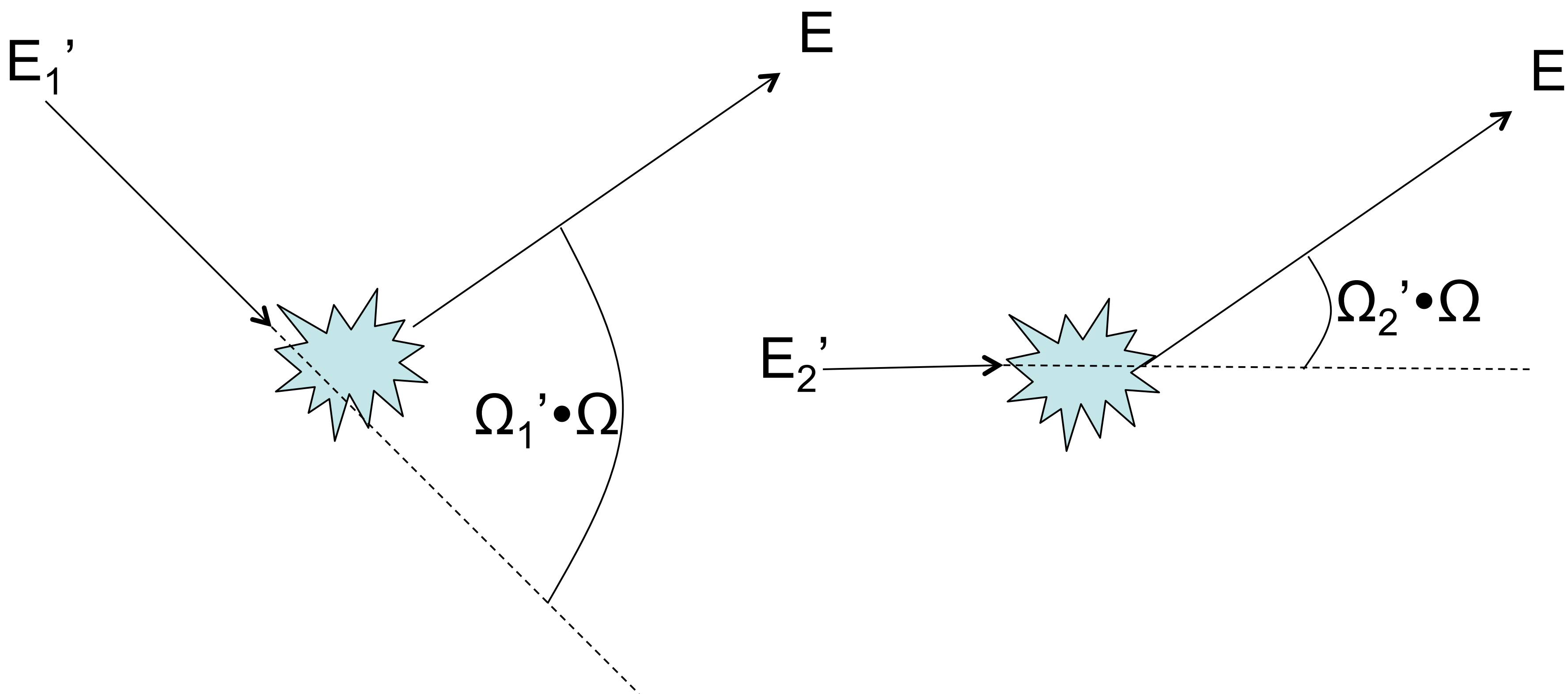
» $$x = \frac{-\ln(1-\xi)}{\sigma}$$

Distance to Collision (Homework Problem)

- Write a code to sample an exponential function
- Use the two sampling techniques discussed:
  - Inversion
  - Rejection
- What is the efficiency of the rejection scheme
  - i.e. what fraction of samples are accepted?
- Could use ran2 program (random number generator from Numerical Recipes.)

Scattering Term

$$\int\int \Psi(r,t,\Omega',E')\sigma(E'\rightarrow E,\Omega'\rightarrow\Omega)d\Omega' dE'$$



$$\sigma(E_1'\rightarrow E,\Omega_1'\rightarrow\Omega)\neq\sigma(E_2'\rightarrow E,\Omega_2'\rightarrow\Omega)$$

Scattering Example (isotropic, coherent)

- Sample angle uniformly in solid angle

$$f(\Omega) = C$$

$$d\Omega = \sin\theta d\theta d\phi$$

$$F(\Omega) = \frac{\int_0^{\phi} d\phi \int_0^{\theta} \sin\theta d\theta}{\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta}$$

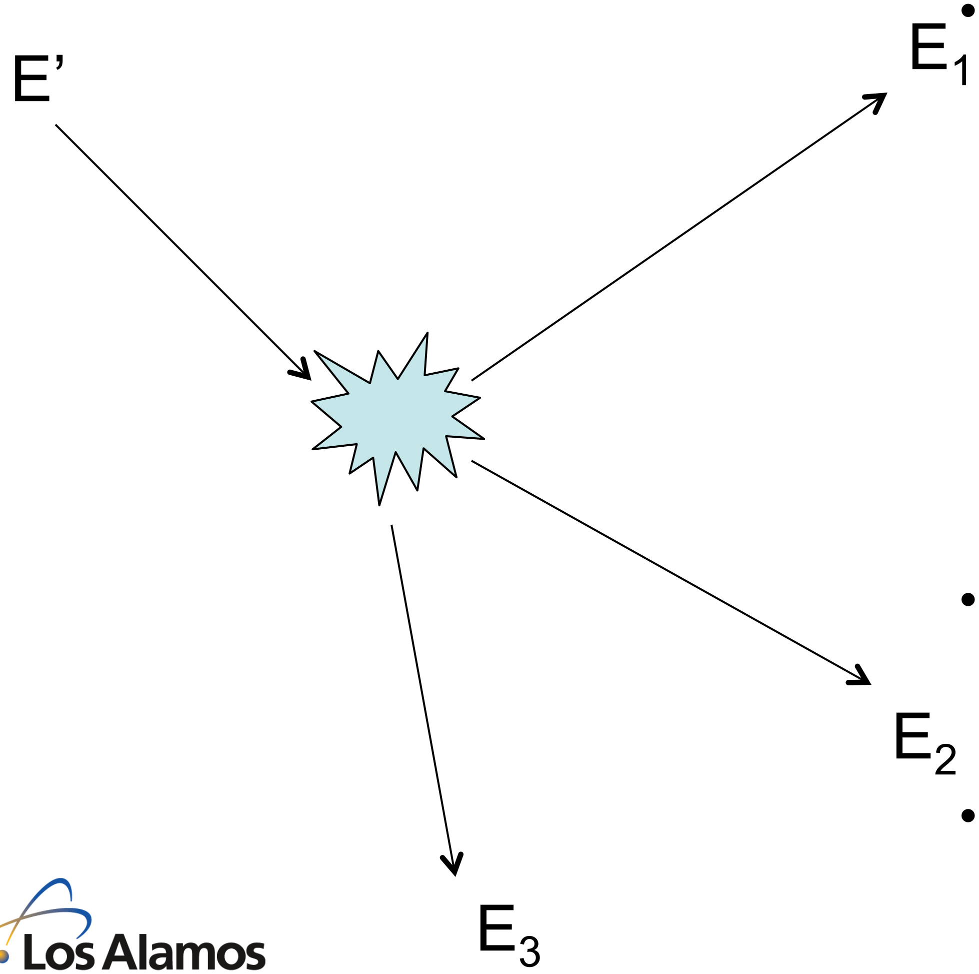
$$\Rightarrow F(\theta) = \frac{\int_0^{\theta} \sin\theta d\theta}{\int_0^{\pi} \sin\theta d\theta} = \frac{(\cos\theta - 1)}{2} = \xi$$

$$\Rightarrow F(\phi) = \frac{\int_0^{\phi} d\phi}{\int_0^{2\pi} d\phi} = \frac{\phi}{2\pi} = \xi$$

- Outgoing energy is same as incoming energy

Fission Term

$$\int\int \Psi(r,t,\Omega',E')\sigma_f(E',\Omega')\nu'(E',\Omega')S_f(E,\Omega)d\Omega' dE'$$



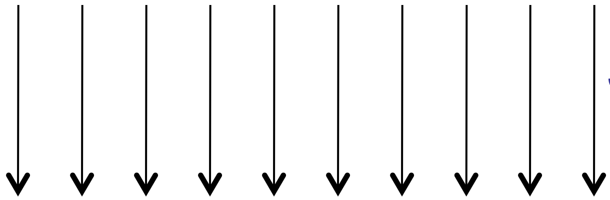
- Can rewrite

$$\sigma_f(E',\Omega')S_f(E,\Omega) = \sigma_f(E',\Omega',E,\Omega)$$

  - Looks a lot like scattering kernel, except for the v' term
  - Scattering with more than one daughter product

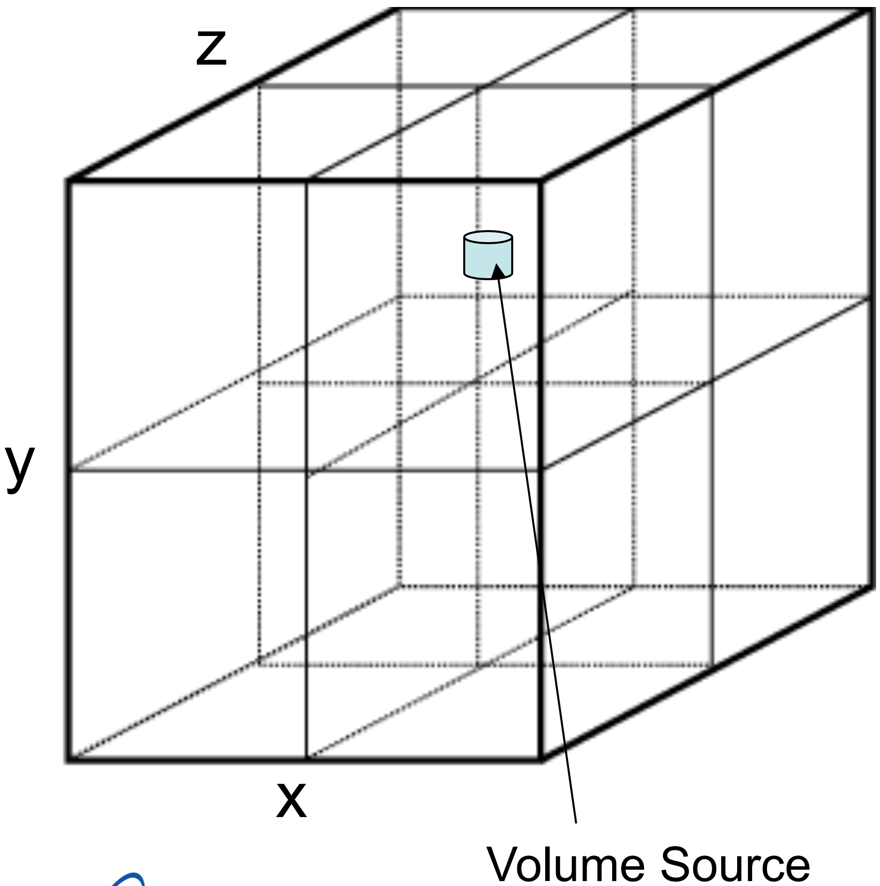
- v'(E',Ω') must be sampled for an integer

- $S_f(E,\Omega)$ provides outgoing distribution for energy and angle



Source Term

$Q(r,t,\Omega,E)$



- Surface Source
  - External Flux
  - Boundary Condition

- Volume Source
  - Radioactive Decay
  - Thermal Emission

Los Alamos NATIONAL LABORATORY EST. 1943

NNSA

Source Term
Thermal Emission Example

- Sample angle uniformly in solid angle

$$f(\Omega) = C$$
$$d\Omega = \sin\theta d\theta d\phi$$
$$F(\Omega) = \frac{\int_0^{\phi} d\phi \int_0^{\theta} \sin\theta d\theta}{\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta}$$
$$\Rightarrow F(\theta) = \frac{\int_0^{\theta} \sin\theta d\theta}{\int_0^{\pi} \sin\theta d\theta} = \frac{(\cos\theta - 1)}{2} = \xi$$
$$\Rightarrow F(\phi) = \frac{\int_0^{\phi} d\phi}{\int_0^{2\pi} d\phi} = \frac{\phi}{2\pi} = \xi$$

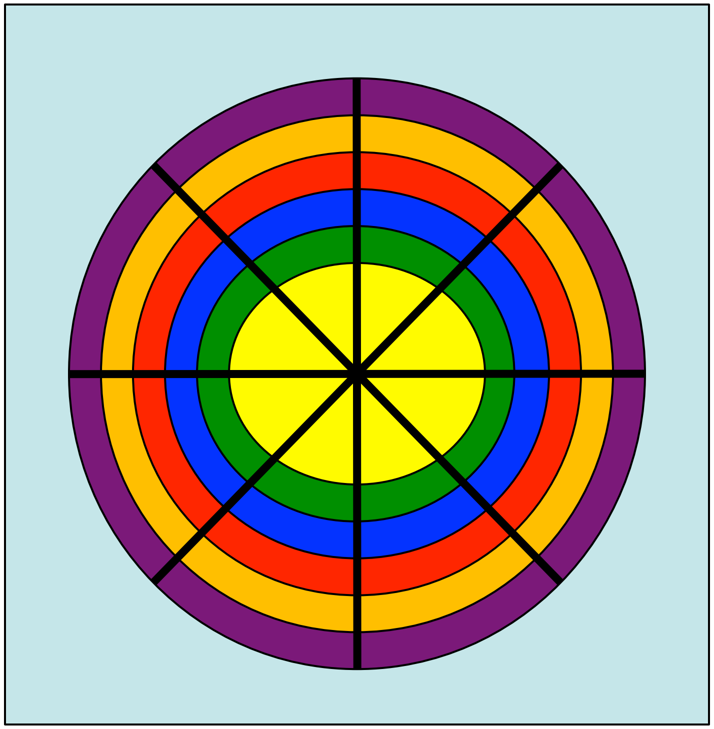
- Sample energy from opacity weighted planckian

- Kirchoff's Law gives emissivity $\eta = \kappa B$
  (usually this is sampled from a table)

Monte Carlo Estimators

- Angular flux $\psi(r,t,\Omega,E)$ doesn't show up directly in our particle treatment
  - If you want it, you'd need to tally it…
  - When have you ever actually used this directly?
- How do I multiply it by σ_f to get a reaction rate?
- How do I convolve it with my detector's response function?
- How do I take its first moment to get a current?

Tally ψ



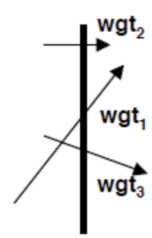
- 100 groups X 100 angles
- 10,000 quantities to store per grid cell each time step

Monte Carlo Estimators (Neutron Current Example)

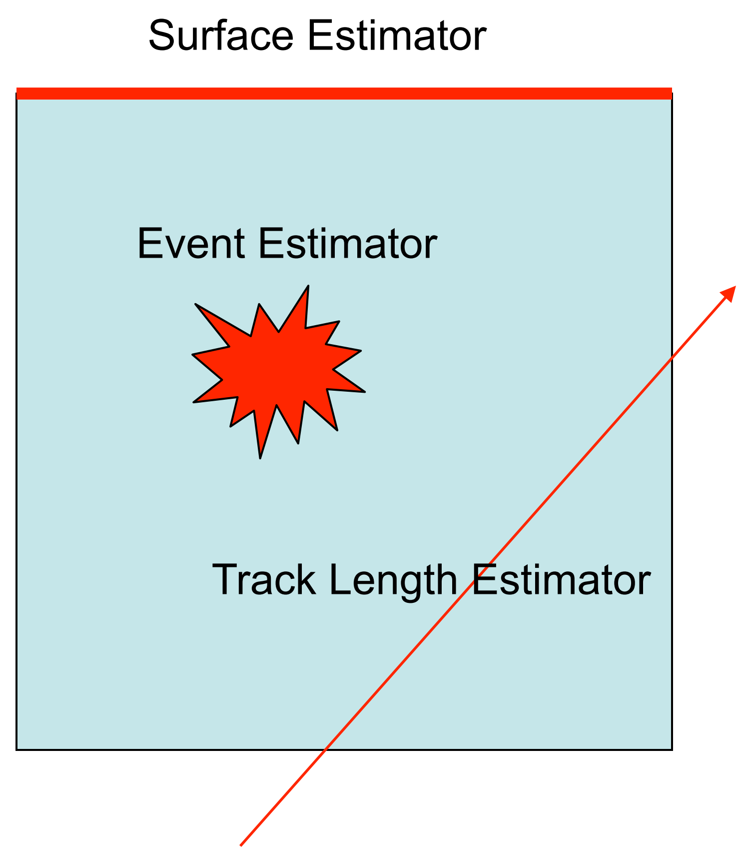
- Why not just keep a tally of the quantities we want?
  - Multiple tally types or approaches exist

- Neutron Current (via Surface Estimator)
  - For every packet that crosses a surface, tally the packet weight

$$J = \frac{1}{\Delta t\, A} \sum_{\substack{\text{all} \\ \text{particles} \\ \text{crossing} \\ \text{surface}}} wgt_j$$

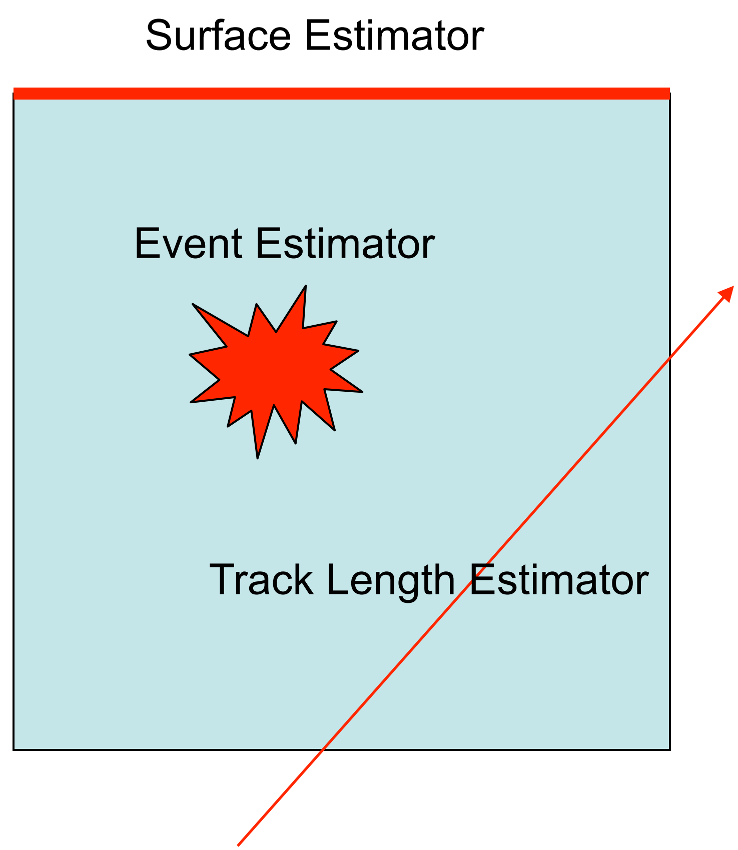


  - Divide by surface area A and timestep Δt to get **neut/cm²-sec**



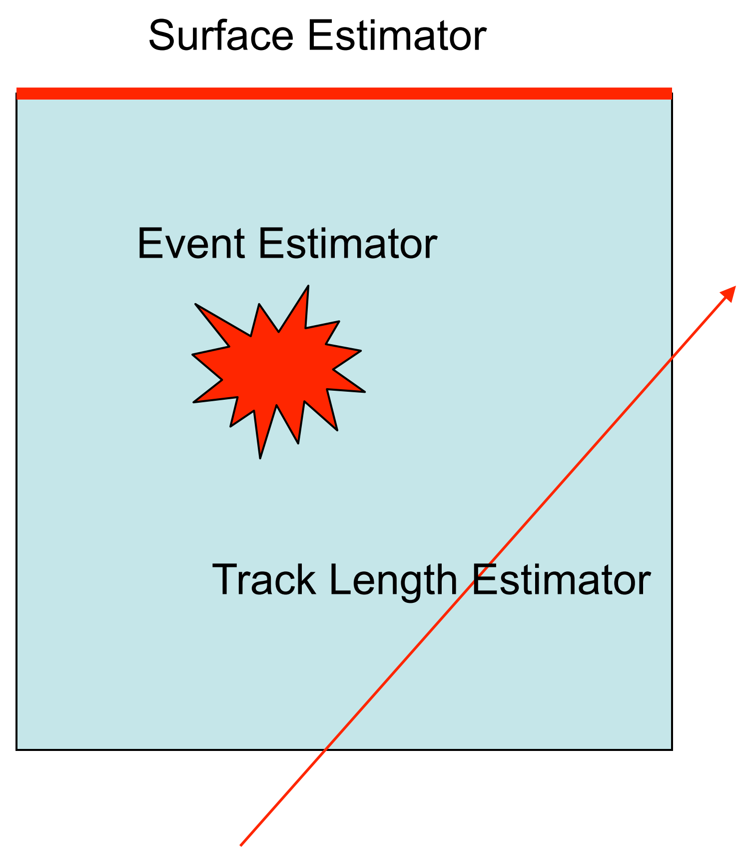
Monte Carlo Estimators (Reaction Rate Example)

- Reaction Rate (via Event Estimator)
  - Tally the packet weight for every packet that undergoes the reaction you are interested in.
    - Fission
    - Absorption (by a particular isotope)
  - Divide timestep Δt to get **reactions/sec**



Monte Carlo Estimators (Flux Examples)

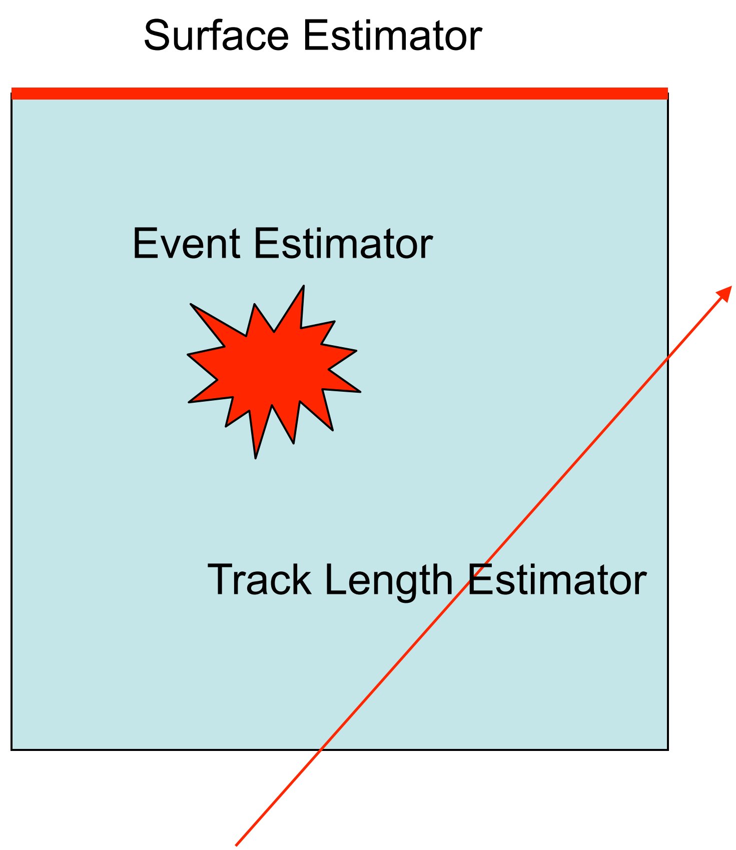
- $\varphi = \int \Psi \, d\mu$
- $J = \int \mu \, \Psi \, d\mu$
  - **Surface estimator Σ wgt**
  - **Get φ from surface estimator Σ wgt/μ**
- $R_x = \int \sigma_f \, \Psi \, d\mu$
  - **Event estimator Σ wgt**
  - **Get φ from event estimator Σ wgt/σ_f**
- **Multiple ways to tally the same thing**



Monte Carlo Estimators (Continuous Moment Tallies)

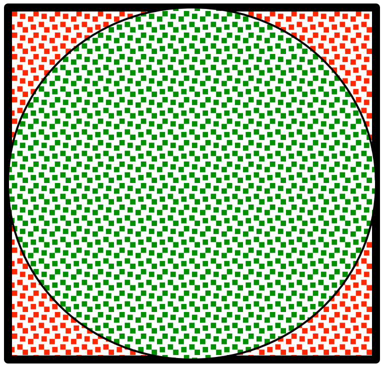
- What if you really needed the angular flux?
  - Memory intensive to tally into space, time, angle and energy bins.

- Why not tally a functional form that represents the angular flux?
  - As example, consider just the angular dependence of ψ.

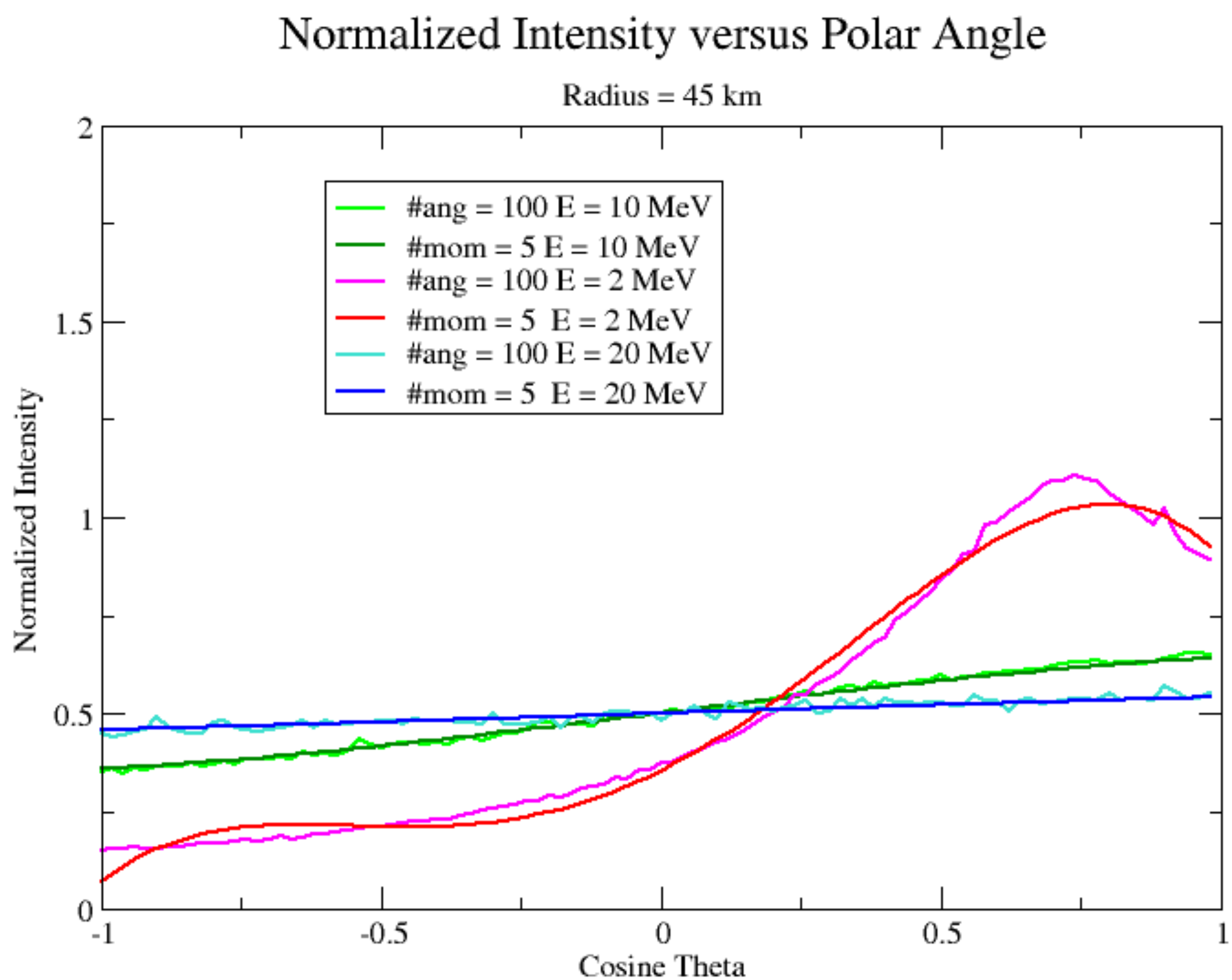


Legendre Moment Tallies

- Imagine representing the phase space distrib'n function in terms of a set of orthogonal basis functions
  - For example, Legendre Polynomials in 1D (Pn)
  - Spherical Harmonics in 3D
- Any function can be represented as a sum of Legendre Polynomials
  - $$F(\mu) = \sum_{k=1}^{\infty} \mathrm{a_k P_k}(\mu)$$
- Taking advantage of the orthogonality of the basis set
  - $$\mathrm{a_n} = \frac{2\mathrm{n}+1}{2} \int_{-1}^{1} \mathrm{F}(\mu)\mathrm{P_n}(\mu)\ \mathrm{d}\mu$$
- Monte Carlo is great for calculating integrals!



Legendre Moment Method Comparison



Step by Step

- Create a new packet according to $S(r,t,E,\Omega)$
- Choose a distance to collision
- Update position and time to arrive at collision location
- Sample what type of collision
  - Fission
  - Scatter
- Sample outgoing packet properties
- Start over again by choosing a distance to collision

Step by Step (want material motion correction?)

- Create a new packet according to S(r,t,E,Ω)
- Choose a distance to collision
- Update position and time to arrive at collision location
- Sample what type of collision
  - Fission
  - Scatter
- Sample outgoing packet properties
- Start over again by choosing a distance to collision

- Transform to lab frame
- Transform to fluid frame
- Transform back to lab frame

Step by Step (want thermal up-scatter?)

- Create a new packet according to S(r,t,E,Ω)
- Choose a distance to collision
- Update position and time to arrive at collision location
- Sample what type of collision
  - Fission
  - Scatter
- Sample outgoing packet properties
- Start over again by choosing a distance to collision

- Transform to lab frame

- Transform to fluid frame
- Sample a target from a Maxwellian, and transform to the target frame
- Double transform back to lab frame

Particle Man Meets Deterministic Man
(apologies to They Might Be Giants)

- Monte Carlo packets are not always tracked continuously in all variables
- Often we smear the particles out in energy
  - Multigroup or gray MC
  - Each packet represents an energy averaged particle
  - Sort of like a deterministic phase space dimension in energy