Monte Carlo Estimators

SNU/NUKE/EHK

Next–Event Estimator

- The flux at a point $\vec{r}$ is the sum of the probabilities of source particles and post–collision particles traveling from their original location $\vec{r}'$ to the detector point $\vec{r}$ without suffering an intervening collision.

- For the steady–state case,

$$\Psi\left(\vec{r},\vec{\Omega},E\right) = \int_0^\infty e^{-\beta}\left[S\left(\vec{r}',\vec{\Omega},E\right)+\iint\Sigma_s\left(\vec{r}';\vec{\Omega}',E' \rightarrow \vec{\Omega},E\right)\Psi\left(\vec{r}',\vec{\Omega}',E'\right)d\vec{\Omega}'dE'\right]ds \quad (1)$$

where $\vec{r}' = \vec{r} - s\vec{\Omega}$

$$\beta = \int_0^s \Sigma_t(\vec{r} - s'\vec{\Omega},E)ds' . \qquad (2)$$

Next-Event Estimator (cont.)

$$\Psi\left(\vec{r},\vec{\Omega},E\right) = \int_0^\infty e^{-\beta}\left[S\left(\vec{r}',\vec{\Omega},E\right)+\iint\Sigma_s\left(\vec{r}';\vec{\Omega}',E'\rightarrow\vec{\Omega},E\right)\Psi\left(\vec{r}',\vec{\Omega}',E'\right)d\vec{\Omega}'dE'\right]ds \qquad (1)$$

where $\vec{r}' = \vec{r} - s\vec{\Omega}$

$$\beta = \int_0^s \Sigma_t(\vec{r}-s'\vec{\Omega},E)ds' \; . \qquad (2)$$

- (1) can be written in terms of a transfer kernel.

$$\psi(\vec{P}) = \int \psi(\vec{P}')\Sigma_t(\vec{P}')K(\vec{P}'\rightarrow\vec{P})\, d\vec{P}' + S(\vec{P}) \qquad (3)$$

where ψ is the angular flux and $\vec{P}$ is a point in a phase space.

– The transfer kernel K is equal to the probability that a particle suffering a collision at $\vec{P}'$ leaves the collision and arrives at $\vec{P}$.

– $S(\vec{P})$ is the uncollided angular flux at $\vec{P}$ that arrives from externally applied sources.

Next–Event Estimator (cont.)

$$\psi(\vec{P}) = \int \psi(\vec{P}')\Sigma_t(\vec{P}')K(\vec{P}' \to \vec{P})\, d\vec{P}' + S(\vec{P}) \qquad (3)$$

- $\psi(\vec{P}')\Sigma_t(\vec{P}')$ = density of particles entering collisions in $d\vec{P}'$, where the element of phase space $d\vec{P}' = d^3\vec{r}\,dE'd\vec{\Omega}'$.
- The kernel K can be separated into two terms,

$$K(\vec{P}' \to \vec{P}) = \left\{ \begin{array}{l} \text{probability of} \\ \text{scattering from} \\ \vec{\Omega}' \text{ and } E' \text{ to } \vec{\Omega} \text{ and } E \end{array} \right\} \cdot \left\{ \begin{array}{l} \text{probability of traveling from} \\ \text{from } \vec{r}\,' \text{ to } \vec{r} \text{ without experiencing} \\ \text{an intermediate collision} \end{array} \right\}$$

where $\vec{\Omega}$ is a unit vector in the direction from $\vec{r}'$ to $\vec{r}$.

Next–Event Estimator (cont.)

$$K(\vec{P}' \rightarrow \vec{P}) = \left\{ \begin{matrix} \text{probability of} \\ \text{scattering from} \\ \vec{\Omega}' \text{ and } E' \text{ to } \vec{\Omega} \text{ and } E \end{matrix} \right\} \cdot \left\{ \begin{matrix} \text{probability of traveling from} \\ \text{from } \vec{r}' \text{ to } \vec{r} \text{ without experiencing} \\ \text{an intermediate collision} \end{matrix} \right\}$$

- Define the probability of scattering from $\vec{\Omega}'$ to $\vec{\Omega}$ per steradian and E' to E as $p(\vec{\Omega}' \bullet \vec{\Omega}, E' \rightarrow E)$. Then, if the non-absorption probability for the collision at $\vec{P}'$ is P_{na}, the first term in K can be written

$$\frac{p(\vec{\Omega}' \bullet \vec{\Omega}, E' \rightarrow E) P_{na}}{\left| \vec{r} - \vec{r}' \right|^2} \qquad (4)$$

  – For monoenergetic, isotropic scattering in L system,

$$p(\vec{\Omega}' \bullet \vec{\Omega}, E' \rightarrow E) = \frac{1}{4\pi} \qquad (5)$$

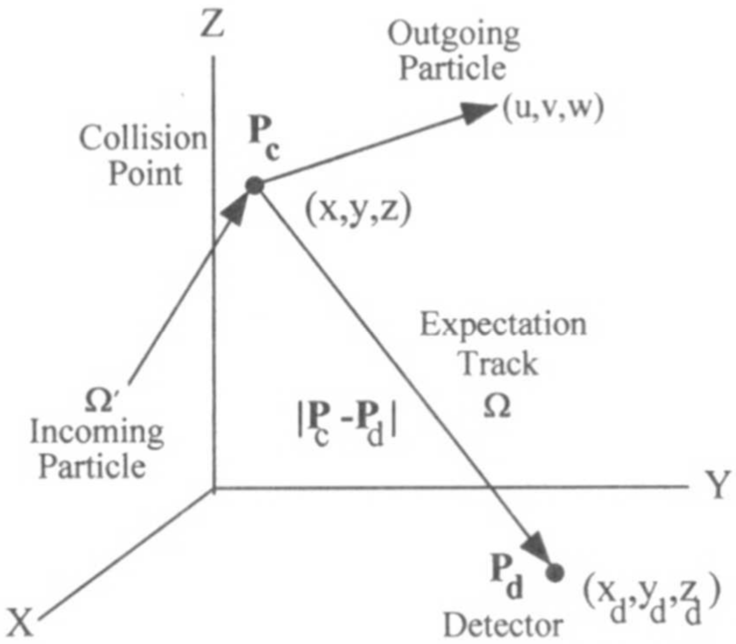
Next–Event Estimator (cont.)

$$K(\vec{P}' \rightarrow \vec{P}) = \begin{Bmatrix} \text{probability of} \\ \text{scattering from} \\ \vec{\Omega}' \text{ and } E' \text{ to } \vec{\Omega} \text{ and } E \end{Bmatrix} \cdot \begin{Bmatrix} \text{probability of traveling from} \\ \text{from } \vec{r}\,' \text{ to } \vec{r} \text{ without experiencing} \\ \text{an intermediate collision} \end{Bmatrix}$$

- The second factor in K is the attenuation factor $e^{-\beta}$, where β is given in (2).
- Applying (2) and (4) to (3) and omitting the fixed source $S(\vec{P})$ term, one obtains the flux estimate at the point ,

$$\psi\left(\vec{r},\vec{\Omega},E\right) = \iiint \psi\left(\vec{r}',\vec{\Omega}',E'\right)\Sigma_t\left(\vec{r}',E'\right)\frac{P_{na}\left(\vec{r}',E'\right)p(\vec{\Omega}'\cdot\vec{\Omega},E'\rightarrow E)}{\left|\vec{r}-\vec{r}'\right|^2}e^{-\beta}d\vec{\Omega}'dE'd^3\vec{r} \qquad (6)$$

<u>Next</u>–Event Estimator (cont.)



$$\psi\left(\vec{r},E,\vec{\Omega}\right) = \iiint \psi\left(\vec{r}',E',\vec{\Omega}'\right)\Sigma_t\left(\vec{r}',E'\right)\frac{P_{na}\left(\vec{r}',E'\right)p(\vec{\Omega}'\cdot\vec{\Omega},E'\rightarrow E)}{\left|\vec{r}-\vec{r}'\right|^2}e^{-\beta}d\vec{\Omega}'dE'd^3\vec{r} \qquad (6)$$

Next-Event Estimator (cont.)

$$\psi\left(\vec{r},E,\vec{\Omega}\right) = \iiint \psi\left(\vec{r}',E',\vec{\Omega}'\right)\Sigma_t\left(\vec{r}',E'\right)\frac{P_{na}\left(\vec{r}',E'\right)p(\vec{\Omega}'\cdot\vec{\Omega},E'\rightarrow E)}{\left|\vec{r}-\vec{r}'\right|^2}e^{-\beta}d\vec{\Omega}'dE'd^3\vec{r}' \qquad (6)$$

- The monoenergetic, post-collision particle flux with isotropic scatter in L system and for a single matter with constant cross sections, (6) becomes

$$\phi = \frac{WP_{na}e^{-\Sigma_t r}}{4\pi r^2} \qquad (7)$$

where W = the weight of the particle entering the collision per unit time;

P_{na} = the ratio of the scatter to the total cross section;

r = the distance b/w the collision point and the detector,

$$r = \sqrt{(x-x_d)^2+(y-y_d)^2+(z-z_d)^2} \qquad (8)$$

Volumetric Flux Estimator #1

- The scalar flux is related to the reaction rate per unit volume, R, by

$$R = \Sigma\phi \qquad (13)$$

where Σ is the reaction cross section.

– MC random walk provides the score of collision events per unit time, C, within a defined region of space.

– Knowing Σ within a region of volume V, one can estimate the flux by

$$\phi = \frac{C}{\Sigma \cdot V} \qquad (14)$$

Volumetric Flux Estimator #2

$$\phi = \frac{C}{\Sigma \cdot V} = \frac{W(1 - e^{-\Sigma_t L})}{\Sigma_t V} \cong \frac{W \cdot \Sigma_t L}{\Sigma_t V} \quad \text{for very small } \Sigma_t$$

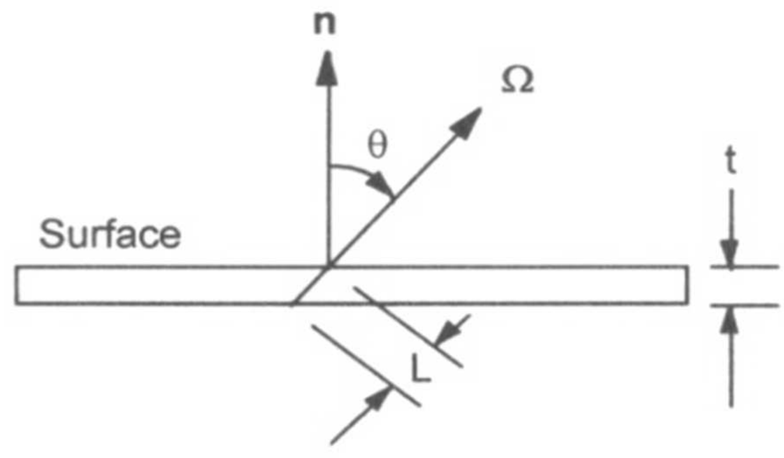
$$\cong W \cdot \frac{L}{V} \leftarrow$$

– The scalar flux is equal to the sum of the distances traveled by all neutrons of energy E that pass through a unit volume of space per unit time and energy.

---→ track length estimator

– A track length estimator scores all particle tracks within a specified volume, which requires the particle tracks to intersect the detector volume but does not require collisions to occur within the detector volume.

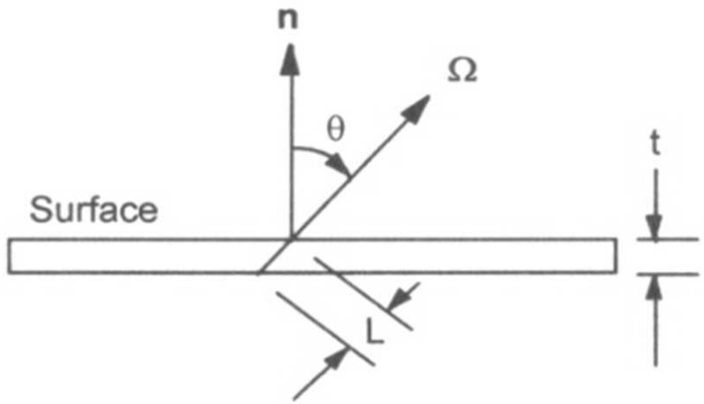
Surface-Crossing Flux Estimator



- The track length L of the particle in the layer is

$$L = \frac{t}{|\mu|} \qquad \text{where } \mu = \cos\theta = \vec{\Omega}\bullet\vec{n}. \qquad (16)$$

Surface-Crossing Flux Estimator (cont.)



- In homogeneous medium, the probability of the particle having a collision in the track length L is

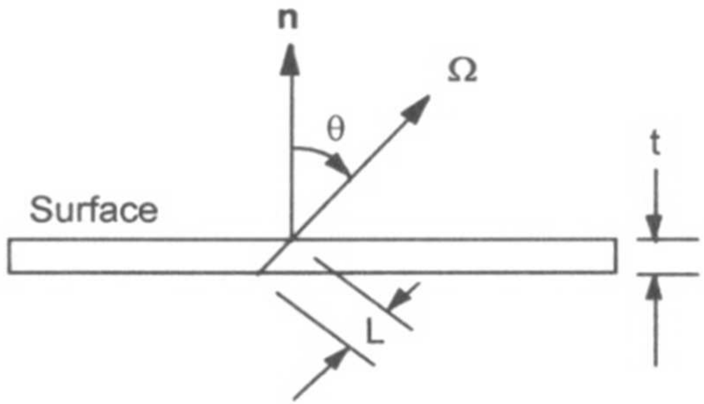
$$P(L) = 1 - e^{-\Sigma_t L} \quad . \qquad (17)$$

- One can estimate the flux on the surface of interest by the collision-density flux estimator, where the reaction rate C is

$$C = WP(L) = W(1 - e^{-\Sigma_t L}) \; , \qquad (18)$$

where W = the weight of the particle being scored per unit time.

Surface-Crossing Flux Estimator (cont.)



- Using (14), one finds the flux by

$$\phi = \frac{C}{\Sigma_t V} = \frac{W(1 - e^{-\Sigma_t L})}{\Sigma_t A t}, \quad (A = \text{the surface area}) \qquad (19)$$

- Applying (16), and taking the limit as t→0 and applying L'Hospital's rule,

$$\lim_{t\to 0}\phi = \lim_{t\to 0}\frac{W(1 - e^{-\Sigma_t t/|\mu|})}{\Sigma_t A t} = \frac{\lim_{t\to 0}\left(W\frac{\Sigma_t}{|\mu|}e^{-\Sigma_t t/|\mu|}\right)}{\lim_{t\to 0}(\Sigma_t A)} = \frac{W}{|\mu| A} \qquad (20)$$

<u>Expectation</u> Surface-Crossing Flux Estimator

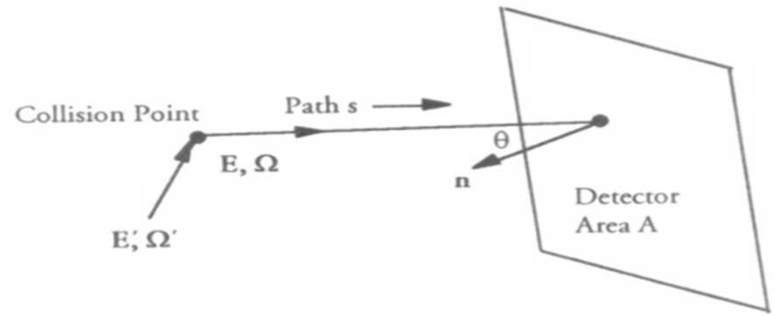
- *The standard surface-crossing flux estimator suffers from the fact that no score is made unless a particle crosses the surface being scored.*

- *The expectation surface-crossing flux estimator*

  – improves the frequency of scores in surface crossing.

  – uses an imaginary surface that is completely independent of the surface used in defining the problem geometry.

Expectation Surface-Crossing Flux Estimator (cont.)



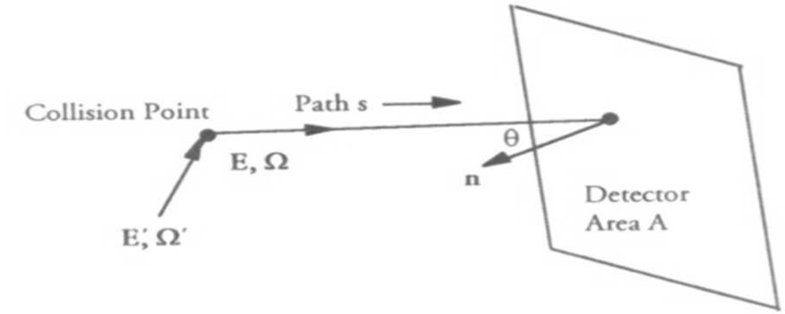
- *The probability of a particle traveling a distance r without suffering an intervening collision is*

$$p(r) = e^{-\int_0^r \Sigma_t(E,s)ds} \qquad (21)$$

- *If a detector is placed at a distance r along the path of the particle as it leaves the collision, the flux on the detector surface is, from (20) and (21),*

$$\phi(r) = \frac{W}{|\mu| A} e^{-\int_0^r \Sigma_t(E,s)ds} \qquad (22)$$

Expectation Surface-Crossing Flux Estimator (cont.)



$$\phi(r) = \frac{W}{|\mu| A} e^{-\int_0^r \Sigma_t(E,s)ds} \qquad (22)$$

– By applying (22) to every source particle and to every post collision particle whose track intersects a detector surface, one can get an estimate of the flux on the surface without requiring the particles to cross the surface.

– With the expectation estimator, one does not score particles when they actually cross the surface but score only trajectories that extrapolate to the surface.

Time-dependent Detectors

- Assign a start time to a particle track and use the speed of the particle to establish a chronology of events.

- The kinetic energy of a particle of rest mass m_0 and speed v is $E_{non-rel} = m_0 v^2/2$ in non-relativistic expression

  $E_{rel} = m_{rel}c^2 - m_0c^2$, where $m_{rel} = m_0 / \sqrt{1-(v/c)^2}$ (c = the speed of light)

  in relativistic expression.

- One can treat the <u>kinematics</u> of neutron motion non-relativistically.
  - $(E-E_r)/E_r \fallingdotseq 0.0103$ for 14 MeV neutron
  - 14.1 MeV (the neutron emission energy in a fusion reaction b/w deuteron and tritium) is a reasonable upper limit for neutron energy of interest.

Time-dependent Detectors (cont.)

- The speed of a neutron having kinetic energy E is

$$v = \sqrt{\frac{2E}{m}} \approx 1.38 \times 10^{6} \sqrt{E} \quad (v \text{ in m/sec; } m \approx 1.686 \times 10^{-24} \text{ g; } E \text{ in eV}) \ (1)$$

- If a neutron undergoes a collision at time t, leaves the collision with speed v, and then travels a distance d before its next collision, it arrives at the next collision at time t'.

$$t' = t + \frac{d}{v} \approx t + 0.723 \times 10^{-6} \frac{d}{\sqrt{E}} \quad (t \text{ in sec; } d \text{ in m; } E \text{ in eV}) \quad (2)$$

- time kill and Russian roulette to terminate tracking particles.

Homework #6