Correlated Sampling

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SNU/NUKE/EHK

Perturbation Calculation

- To determine the effect of small changes in the problem parameters on the solution to the problem.
- To examine the sensitivity of a solution to uncertainties in such factors as cross sections, material composition, geometry, source characteristics, etc.
- To identify the portions of a problem that must be specified to a high degree of accuracy and the portions that may be approximated without detriment to the solution.
- <u>To have any validity</u>, two independent Monte Carlo calculations, that are used to analyze a perturbation in a system should have statistical uncertainties in the individual answers that are significantly smaller than the difference between those two results.

Perturbation Calculation (cont.)

- To estimate two quantities I_1 and I_2

$$I_1 = \int g(x) f_1(x) dx \quad (1) \quad and \quad I_2 = \int g(y) f_2(y) dy \quad (2)$$

where $f_1(x)$ and $f_2(y)$ are probability density functions that reflect the baseline and perturbed cases, respectively.

- With the corresponding estimates θ_1 and θ_2,

$$\Delta\theta = \theta_1 - \theta_2 = \frac{1}{N}\sum_{i=1}^{N} g(x_i) + \frac{1}{N}\sum_{i=1}^{N} g(y_i) = \frac{1}{N}\sum_{i=1}^{N} \Delta_i \quad (3)$$

where $\Delta_i = g(x_i) - g(y_i)$ (4)

Perturbation Calculation (cont.)

- The variances are

$$\sigma_1{}^2 = E[(\theta_1 - I_1)^2] \quad (5) \quad \text{and } \sigma_2{}^2 = E[(\theta_2 - I_2)^2] \qquad (6)$$

- Then the variance <u>in difference</u> b/w two <u>estimates</u> is

$$var(\theta_1 - \theta_2) = var(\theta_1) + var(\theta_2) - 2cov(\theta_1, \theta_2), \text{ or}$$

$$\sigma^2 = \sigma_1{}^2 + \sigma_2{}^2 - 2cov(\theta_1, \theta_2) \qquad (7)$$

$$\text{where } cov(\theta_1, \theta_2) = E[(\theta_1 - I_1) \cdot (\theta_2 - I_2)]. \qquad (8)$$

Perturbation Calculation (cont.)

- *If* the estimates θ_1 and θ_2 are statistically independent, by estimating $I_1 - I_2$ using statistically independent Monte Carlo calculations for the baseline and perturbed results, then $cov(\theta_1, \theta_2) = 0$ and thus

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 , \qquad (9)$$

– This variance places a stringent limit on the reliability (or certainty) to which the change induced by the perturbation can be determined.

Perturbation Calculation (cont.)

- The result in (7) can be improved by using correlated calculations, instead of attempting to calculate two highly precise but statistically independent results, to reduce the uncertainty in the estimated difference.

- When the estimates θ_1, θ_2 are positively correlated, $cov(\theta_1, \theta_2) > 0$, the variance in estimate for $\Delta\theta$ can be much less than that in (9).

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 - 2cov(\theta_1, \theta_2) \qquad (7)$$

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 \qquad (9)$$

$$\sigma^2\left[ag(x) + bh(x)\right] = a^2\sigma^2\left[g(x)\right] + b^2\sigma^2\left[h(x)\right] + 2ab\left[\overline{g(x)h(x)} - \bar{g}(x)\bar{h}(x)\right] \qquad (15)$$

Correlation Sampling

- *Positive correlation b/w the results can be obtained by correlated sampling i.e., by ensuring that every particle random walk, that does not involve an interaction in the perturbed portion of the problem, is the same in both of the calculations.*
- *The only difference between those two calculations is the changes produced by particle interactions or other events involving the perturbed region of the problem. This can be achieved by using the same sequence of random numbers for sampling both sets of random configurations x_i and y_i.*
- *It is not essential that the individual uncertainties in the two answers be small, but only that the uncertainty in the difference between the two results be small.*

$$\sigma^2(\theta_1 - \theta_2) = \sigma^2(\theta_1) + \sigma^2(\theta_2) - 2cov(\theta_1, \theta_2) \qquad (7)$$

Correlation Sampling (cont.)

$$\sigma^2(\theta_1-\theta_2) = \sigma^2(\theta_1) + \sigma^2(\theta_2) - 2cov(\theta_1, \theta_2) \qquad (7)$$

- As the effect of the perturbation goes to zero, those two calculations converge to the same result, independent of the statistical uncertainty in the individual answers, provided the same number of particles are tracked in both calculations.

- Although the absolute uncertainty in the result remains as determined in the individual calculations, the uncertainty in the difference between those two calculations goes to zero as the calculation becomes identical..

$$\sigma^2(\theta_1) = \sigma^2(\theta_2), \text{ and}$$

$$cov(\theta_1, \theta_2) = E[(\theta_1 - I_1)\cdot(\theta_2 - I_2)] = E[(\theta_1 - I_1)^2].$$

Hence, $\sigma^2(\theta_1-\theta_2) = 2\sigma^2(\theta_1) - 2\sigma^2(\theta_1) = 0$

Correlation Sampling (cont.)

- The key to correlated sampling in MC transport is to make sure that corresponding particle tracks in the baseline and the perturbed calculations use the same random number string.
  - Any particle that does not encounter the perturbed region of the problem scores the same in both calculations.
  - by using a <u>second,</u> <u>separate,</u> <u>and</u> <u>independent</u> random number generator.
  - There is always a risk that a portion of random number used in random walk of a particle be repeated.

Perturbation Calculation: example

- Sensitivity of the number of particles passing through a slab to the thickness of the slab?

  → To examine the effect of an uncertainty in the thickness z [unit in the number of mean-free-path] of the slab on the number of particles passing through the slab.

- The probability of a normally incident particle passing through the baseline slab is

$$P_b = e^{-z},$$

while the probability of a particle passing through the perturbed slab is

$$P_{pt} = e^{-z'}.$$

Perturbation Calculation: example (cont.)

- Assume a start particle weight of one, then the average of the weights of particles passing through the slab is

$$\langle x \rangle = \lim_{n\to\infty} \frac{1}{n} \sum_n x_i = e^{-z}$$

where $x_i = 1$ for particles that pass through the slab, and zero otherwise.

– Since $\langle x^2 \rangle = \langle x \rangle$ ($x_i = 1$ or 0), the standard deviation of $\langle x \rangle$ is

$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x \rangle - \langle x \rangle^2} = \sqrt{e^{-z} - e^{-2z}}$$

which gives σ ($z = 1$) and σ' ($z'=1.01$).

Perturbation Calculation: example (cont.)

- For normally incident particles on a purely absorbing material, the change in the number of particles passing through the slab, with respect to the thickness of the slab, is

$$\frac{dP}{dz} = \frac{d}{dz}e^{-z} = -e^{-z},$$

where P is the probability in fraction of an incident particle passing through the slab.

– A linear approximation calculated analytically with the value z = 1 and z' = 1.01 gives

$$\left.\frac{dP}{dz}\right|_{z=1} \cong \frac{P_{pt} - P_b}{z' - z} = \frac{e^{-z'} - e^{-z}}{z' - z} = \frac{e^{-1.01} - e^{-1.00}}{0.01} = -0.3660/\text{unit length}$$

Monte Carlo Estimators

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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.)

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

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

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

  – For monoenergetic, isotropic scattering in L system,

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

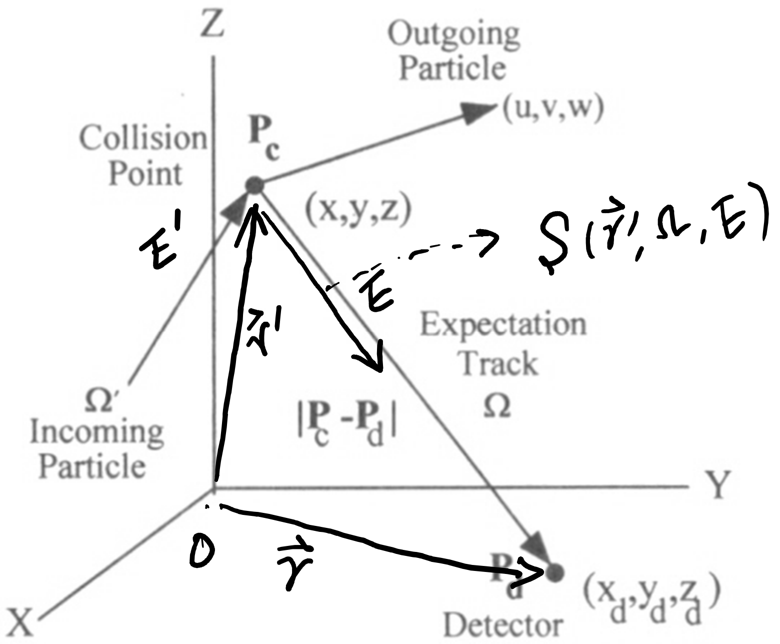
Next–Event Estimator (cont.)

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

- *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 ,*

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

Next-Event Estimator (cont.)



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

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 scattering 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 <u>per unit volume</u>, 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

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

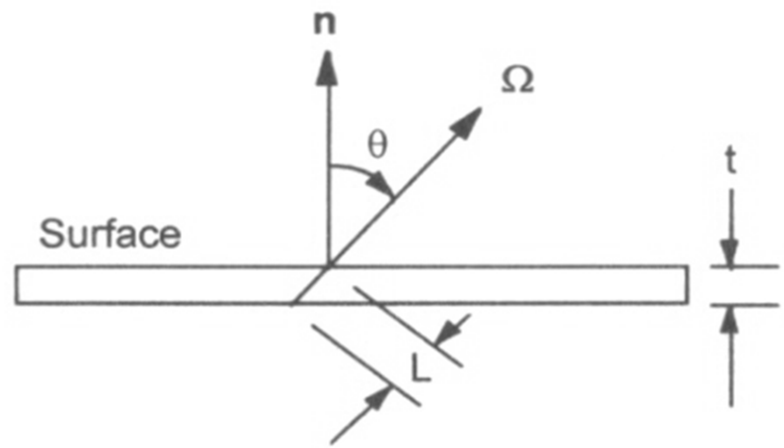
$$\cong W \cdot \frac{L}{V} \leftarrow$$

– 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.

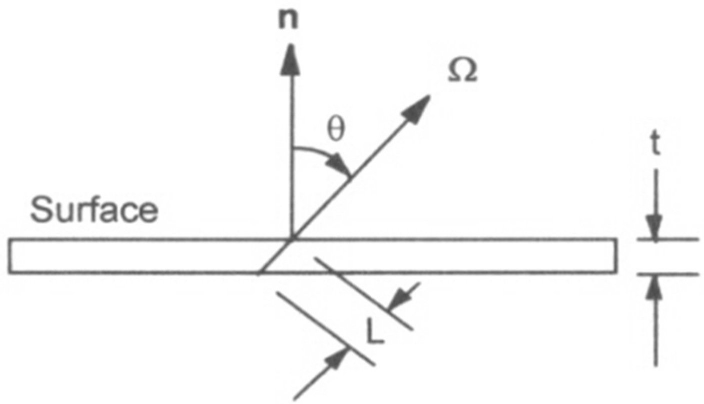
Surface-Crossing Flux Estimator



- 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

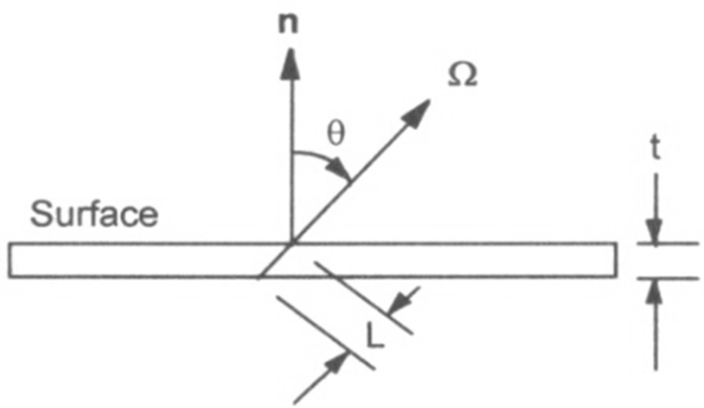
$$P(L) = 1 - e^{-\Sigma_t L} \; . \qquad (17)$$

- 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

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

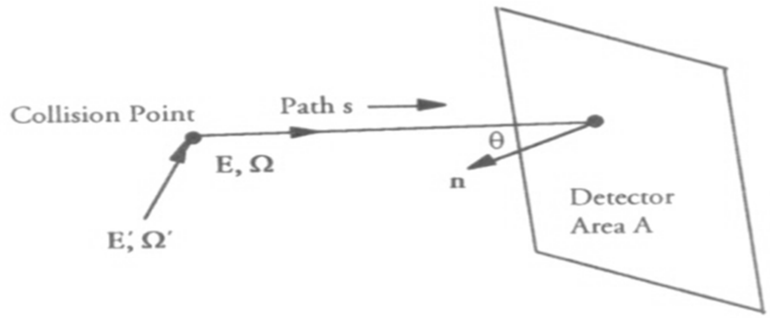
- Applying (16), and taking the limit as $t \rightarrow 0$ and applying L'Hospital's rule,

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

Expectation 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.

<u>Expectation</u> Surface-Crossing Flux Estimator (cont.)



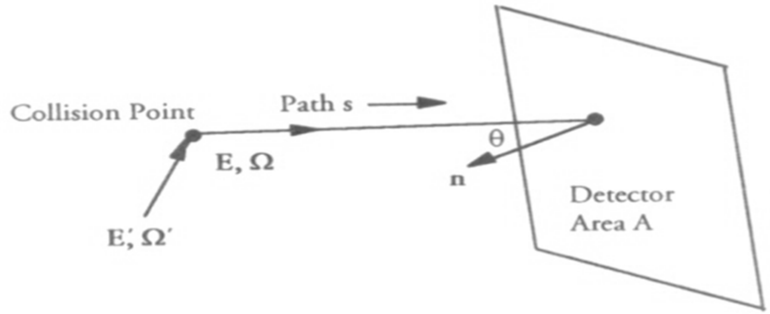
- The probability of a particle traveling a distance r without suffering an intervening collision is

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

- If a detector is placed at a distance r <u>along the path of the particle</u> 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 $E_{non-rel} = m_0v^2/2$ in non-relativistic expression

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

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

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

- 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.