Estimation of Physical Quantities (General)

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Reference

[1] Y. Nagaya, K. Okumura, T. Mori, M. Nakagawa, “MVP/GMVP II: General Purpose Monte Carlo Codes for Neutron and Photon Transport Calculations based on Continuous Energy and Multigroup Method,” JAERI 1381 (2005).

[2] J. F. Briesmeister (Ed.), “MCNP – A General Monte Carlo Code for Neutron and Photon Transport, Version 4A,” LA-12625-M,Los Alamos National Laboratory (1997).

Collision Estimator

- In general, the physical quantities estimated by the Monte Carlo method can be expressed with the collision density Ψ as follows:

$$Q = \int_{\mathbf{P}\in V_T} g(\mathbf{P})\Psi(\mathbf{P})d\mathbf{P}$$

  $\mathbf{P}=(\mathbf{r},E,\mathbf{\Omega},t)$ is the set of coordinates (position, energy, angle, and time) in the phase space and V_T is the region of interest in the phase space.

- $g(\mathbf{P})$ is the function to represent the contribution from the collision at $\mathbf{P}$ to the reaction of interest.
  - Macroscopic capture rate: $$g(\mathbf{P}) = \frac{\Sigma_\gamma(\mathbf{P})}{\Sigma_t(\mathbf{P})}$$
  - Flux: $$g(\mathbf{P}) = \frac{1}{\Sigma_t(\mathbf{P})}$$
  - Microscopic reaction rate: $$g(\mathbf{P}) = \frac{\sigma(\mathbf{P})}{\Sigma_t(\mathbf{P})}$$

Collision Estimator (Contd.)

- The physical quantity Q can be estimated by scoring this contribution in the collisions:

$$Q_{i,j} = g(\mathbf{P}_{i,j})W_{i,j}\delta_{V_T}(\mathbf{P}_{i,j})$$

$Q_{i,j}$ denotes the contribution of the j-th collision of history i.

$\mathbf{P}_{i,j}$ denotes the phase space point of the j-th collision of history i.

$W_{i,j}$ is the particle weight for the j-th collision of history i.

$\delta_{V_T}(\mathbf{P}_{i,j})$ is defined as

$$\delta_{V_T}(\mathbf{P}_{i,j}) = \begin{cases} 1 & \text{if } \mathbf{P}_{i,j} \in V_T \\ 0 & \text{if } \mathbf{P}_{i,j} \notin V_T \end{cases}$$

- Then the estimate of the mean, $\bar{Q}$ can be calculated by

$$\bar{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i; \quad Q_i = \sum_j Q_{i,j}$$

where N is the total number of histories.

Statistical Uncertainty

- The statistical uncertainty of $\bar{Q}$ can be estimated by its variance.

- Q> Why is the normal distribution commonly encountered in practice?

  A> *By the central limit theorem, under certain conditions the sum of a number of random variables with finite means and variances approaches a normal distribution as the number of variables increases.*

- Central Limit Theorem
  - Let $X_1, X_2, X_3, \ldots X_n$ be a sequence of ***n*** **independent and identically distributed (i.i.d)** random variables each having finite values of expectation μ and variance $\sigma^2 > 0$.
  - The central limit theorem states that as the sample size *n* increases, the distribution of the sample average of these random variables approaches the normal distribution with a mean μ and variance σ^2 / n irrespective of the shape of the original distribution.

➡ $$\sigma^2\left[\bar{Q}\right] = \frac{1}{N(N-1)}\sum_{i=1}^{N}\left(Q_i - \bar{Q}\right)^2$$

Track Length Estimator

- In a vacuum region, physical quantities cannot be estimated by the collision estimator. In addition, the estimation with the collision estimator is less accurate in a region where the number of collisions is small.
- The track length estimator overcomes these drawbacks of the collision estimator.
- By the track length estimator, the reaction rate from the *j*-th track of history *i* is scored as follows:

$$Q_{i,j} = \Sigma(L_{i,j})W_{i,j}L_{i,j}\delta_{V_T}(\mathbf{P}_{i,j})$$

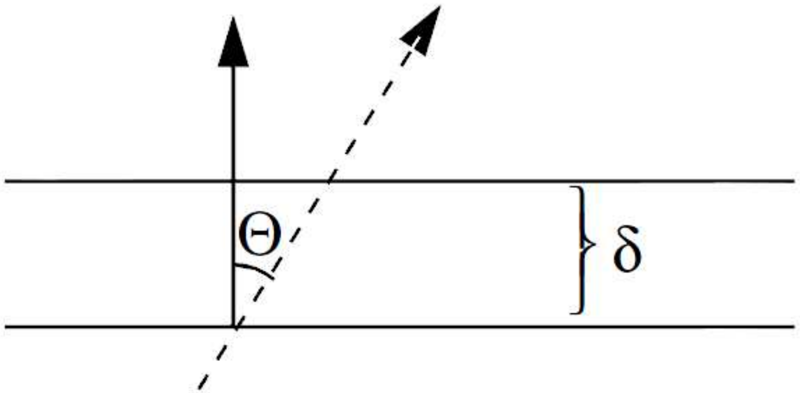
$L_{i,j}$ is the *j*-th track (path) length of history *i*.

$\Sigma(L_{i,j})$ means that the reaction cross sections are assumed to be constant in space and time along the path $L_{i,j}$.

Surface Crossing Estimator

- The surface crossing estimator estimates physical quantities when particles pass through a surface in space.
  - The particle current is defined by the number of particles that pass through a surface per unit area.
  - The particle flux is defined by the number of particles that pass through a surface along the normal direction per unit area.

- The surface flux is a surface estimator but can be thought of as the limiting case of the cell flux or track length estimator when the cell becomes infinitely thin.



$$Q_{i,j} = \lim_{\delta \to 0} \frac{W_{i,j} L_{i,j} \delta_{V_T}(\mathbf{P}_{i,j})}{V_T}$$
$$= \lim_{\delta \to 0} \frac{W_{i,j} \left(\not{\delta} / \cos\theta \right) \delta_{V_T}(\mathbf{P}_{i,j})}{A \not{\delta}}$$
$$= \frac{\left(W_{i,j} / \cos\theta \right) \delta_{V_T}(\mathbf{P}_{i,j})}{A}$$

- In MCNP or McCARD, $|\mu|$ is set to 0.05 when $|\mu|<0.1$.

Standard Approach for the Surface Flux Tallies

- When a particle grazes the surface, the cosine of the surface-crossing angle is small, and the particle's score can be huge, leading to infinite variances.
- To circumvent this problem, Clark [3] recommended "excluding grazing fluxes from the stochastic estimate."
  - The standard estimate of the contribution from grazing angles, which can be inferred from Clark's theoretical analysis, is as follows.
  - Let μ represent the cosine of the surface-crossing angle and ε where $|\mu|<\varepsilon$ the "grazing band."
  - When $|\mu|>\varepsilon$ score $1/|\mu|$ as normal, but $|\mu|<\varepsilon$ score $2/\varepsilon$.
  - For example in MCNP, whenever $|\mu|$ is less than 0.1, $2/\varepsilon$=20 is scored instead.
  - In Ref [4], ε=0.01 is suggested.

[3] F. H. Clark, "Variance of Certain Flux Estimators Used in Monte Carlo Calculations," *Nucl. Sci. Eng.*, **27**, 235 (1967).

[4] S. A. Dupree and S. K. Fraley, *A Monte Carlo Primer: A Practical Approach to Radiation Transport*, Chapter 7, Kluwer Academic/Plenum Publishers, NY (2002).

Recent Works on the Surface Flux Tallies

- For years, the standard estimate has been considered accurate if the angular flux on the surface is isotropic or linearly anisotropic. This assumption is due to Clark [3], who expanded the surface flux as $\phi(\mu)=g_0+g_1\mu$.
- Recently [5,6], however, the accuracy of the standard estimate was found to require a very isotropic flux on external surfaces, not a linearly anisotropic flux.

[5] J. A. Favorite, A. D. Thomas, and T. E. Booth, "On the Accuracy of a Common Monte Carlo Surface Flux Grazing Approximation," *Nucl. Sci. Eng.*, **168**, (2011).

[6] J. A. Favorite, "Monte Carlo Surface Flux Tallies," M&C 2011, Rio de Janeiro, Brazil, May 8-12 (2011).

Net Multiplication Factor

- In a fixed source problem, the net multiplication factor M is defined to be unity plus the gain G_f in neutrons from fission plus the gain G_x from nonfission multiplicative reactions.

$$M = 1 + G_f + G_x$$