

Tallies

Since the histories are random, x also is a random variable. It does not in general coincide with the random variables that are sampled in producing the histories: the scattering angles, positions, and distances between collisions. Rather, x most often is related to scalar flux, current distribution, escape probability, or one of the other dependent variables that are sought from the solution of the transport equation. Our task then is to ask which of the properties that we have available from the simulation of random particle histories should be tallied in order to calculate the scalar flux, current, or other parameters of interest.

For scalar flux the two most widely used tallies result from the relationship between collision density and scalar flux and from the definition of scalar flux in terms of total neutron track length, both discussed in Chapter 1. Suppose that we want to calculate the average scalar flux $\bar{\phi}$ in some volume \bar{V} where the total cross section is $\bar{\sigma}$. Then since $\bar{\sigma}\bar{\phi}$ is the collision density; \bar{c} , the mean number of collisions in V per unit time, is

$$\bar{c} = \bar{V}\bar{\sigma}\bar{\phi}. \quad (7-48)$$

Hence for the Monte Carlo simulation we may write

$$\bar{\phi} = \frac{1}{\bar{V}\bar{\sigma}} \bar{c}, \quad (7-49)$$

where \bar{c} is the mean number of collisions, normalized to one source particle. The random variable whose mean we want to calculate is thus \bar{c} , the mean number of collisions per neutron history in \bar{V} . If we normalize our calculation to a source strength of one neutron, we then have a sample estimate of \hat{c} :

$$\hat{c} = \frac{1}{N} \sum_n c_n, \quad (7-50)$$

where c_n is the number of collisions made in \bar{V} during the n th history. Our sample estimate of the scalar flux is then

$$\hat{\phi} = \frac{1}{\bar{V}\bar{\sigma}} \frac{1}{N} \sum_n c_n. \quad (7-51)$$

A shortcoming of this estimate of the scalar flux lies in the fact that only particles that collide in \bar{V} will contribute to the collision estimator $\hat{\phi}$. We

next discuss the path length estimator for which every particle that passes through \bar{V} contributes, whether or not a collision occurs. Recall from Chapter 1 that the scalar flux may be defined as the total track length traversed by all particles per unit volume per unit time. Hence

$$\bar{\phi} = \frac{1}{\bar{V}} \bar{l}, \quad (7-52)$$

where \bar{l} is the mean track length normalized to one source particle. If we have a Monte Carlo simulation of N particles, we therefore estimate the mean value \bar{l} of the random variable l by

$$\hat{l} = \frac{1}{N} \sum_n l_n, \quad (7-53)$$

where l_n is the track length in \bar{V} of the n th particle. Note that l_n may consist of more than one contribution since a single particle may pass through the volume \bar{V} more than once. From Eqs. 7-52 and 7-53 we then have as our path length flux estimator

$$\hat{\phi} = \frac{1}{\bar{V}} \frac{1}{N} \sum_n l_n. \quad (7-54)$$

We would also like to be able to estimate particle currents, for if currents can be determined, escape probabilities and other particle balance properties follow immediately. Suppose we want to calculate the mean value of the current crossing surface \bar{A} in the \hat{n} direction,

$$\bar{A}\bar{J} = \bar{A}(\bar{J}_+ - \bar{J}_-), \quad (7-55)$$

where \bar{J}_+ and \bar{J}_- are the mean values of the partial currents in the positive and negative directions. We may write

$$\bar{A}\bar{J}_+ = \bar{p}^+ \quad \text{and} \quad \bar{A} \cdot \bar{J} = \bar{p}^-, \quad (7-56)$$

where \bar{p}^\pm are the mean numbers of particles passing through the surface per second in the positive and negative directions respectively. These quantities can be estimated from our Monte Carlo sample as

$$\hat{p}^\pm = \frac{1}{N} \sum_n p_n^\pm \quad (7-57)$$

where p_n^+ and p_n^- are the number of passages through the surface \bar{A} made

by the n th particle history in the positive and negative direction respectively. We have

$$\hat{J}_+ = \frac{1}{A} \frac{1}{N} \sum_n p_n^+, \quad \hat{J}_- = \frac{1}{A} \frac{1}{N} \sum_n p_n^-, \quad (7-58)$$

and

$$\hat{J} = \hat{J}_+ - \hat{J}_- \quad (7-59)$$

is an approximation to the net current.

It is also possible to calculate the average scalar flux over a surface by using the relationship among angular flux, scalar flux, and current, which is given in Chapter 1. It may be shown that the value of $\bar{\phi}$ on A may be estimated from

$$\hat{\phi} = \frac{1}{A} \frac{1}{N} \sum_n \zeta_n \quad (7-60)$$

where ζ_n is the number of crossings of the n th neutron, each weighted by $|1/\mu|$, where $\mu = \hat{\Omega} \cdot \hat{n}$ is the direction cosine of the particle with respect to the positive normal to the surface. Thus if there were I crossings in the n th history,

$$\zeta_n = \sum_{i=1}^I \left| \frac{1}{\mu_i} \right|. \quad (7-61)$$

A difficulty arises if one must calculate the flux over a very small volume or surface, as is the case, for example, when it is desired to determine the response of a "point" detector in a system. The foregoing tallies become useless, since if the volume is very small no histories are likely to collide in it, or even to pass through it. In such circumstances there are two alternatives. One may use an adjoint Monte Carlo calculation in which particles are emitted from the detector volume,^{2,13} or one may resort to one of the more subtle tallying techniques for the estimate of the flux at a point.^{7,14-16} We defer discussion of the use of the adjoint equation until Section 7-6; estimates of the flux at a point and some of the tallies are treated in Section 7-7.

Before proceeding, it is important to note that it is common practice to normalize Monte Carlo results to a source of one particle, while in steady-state deterministic transport calculations the source is normally given in terms of particles per second. Thus the foregoing tallies have units of cm^{-2}

rather than particles/cm²/sec as in deterministic calculations. For steady-state calculations, however, the correspondence is clear. The results of the Monte Carlo calculation are just multiplied by the number of particles produced per second; the magnitudes of the tallies are then correct, and the units become particles/cm²/sec.

7-4 ERROR ESTIMATES

In the preceding section we indicated how to use a number of random variables to estimate the scalar flux and current in analog Monte Carlo calculations. The question now arises as to how much error the sample estimate $\hat{\phi}$ or \hat{J} is likely to have in relation to the true values of the mean $\bar{\phi}$ or \bar{J} . To make an estimation of the statistical uncertainty of our results, we must go back to the properties of a random variable, introduce the concepts of expectation values and variance, and utilize the central limit theorem to arrive at an error estimate.

In the following discussion we designate the random variables c , l , p^+ , p^- , ξ used in the preceding section to estimate flux or current as x . For a particular simulation in principle there exists a probability density function $f(x)$ for each of these estimators. Of course we can never determine this function exactly unless the problem is so simple that it can be solved analytically; otherwise an infinite number of particle histories would be required. Estimating the properties of $f(x)$, however, leads in turn to an estimate of the error in \hat{x} .

The functional dependence of $f(x)$ on x may have different forms depending on which of the estimators is under consideration. For example, the collision and surface crossing estimators c_n and p_n^+ and p_n^- can take on only integer values. Hence the probability density function has the form

$$f(x) = \sum_i p_i \delta(x - i), \quad (7-62)$$

where

$$\sum_i p_i = 1, \quad (7-63)$$

while the coefficients p_i determine the distribution. A special case of Eq. 7-62 is the binomial estimator

$$f(x) = p_0 \delta(x) + [1 - p_0] \delta(x - 1), \quad (7-64)$$

where the estimator can take on only values of zero and one. This would be