Chapter 8 Function-based Flux Tallies

8.1 Application of Dirac delta approximation to the forward transport equation

With those difficulties out of the way, we can proceed to translating the emerging particle density into the flux values that we really want. Returning to the point of view of a single history, we begin the process by substituting (7-17) into (7-3) to get:

$$\begin{aligned}\phi(r,\Omega,E) &\cong \int_0^\infty dR\, e^{-\int_0^R dR'\,\Sigma_t(r-R'\Omega,E)}\left[\sum_{j=0}^{\infty} w_j \delta\left(r-R\Omega-\hat{r}_j\right)\delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right)\right] \\ &\cong \sum_{j=0}^{\infty} w_j \delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right)\left[\int_0^\infty dR\, e^{-\int_0^R dR'\,\Sigma_t\left(\hat{r}_j+R\hat{\Omega}_j-R'\hat{\Omega}_j,\hat{E}_j\right)}\delta\left(r-R\hat{\Omega}_j-\hat{r}_j\right)\right]\end{aligned} \quad (7\text{-}19)$$

The term in brackets is a bit trick, since it contains two continuous variables, r and R.

The normal way to deal with this is to define the position vector r with coordinate axes with the origin at $\hat{r}_{ji}$ and one of the orthonormal direction vectors to correspond to $\hat{\Omega}_{ji}$. That is:

$$r = \hat{r}_j + u\hat{\Omega}_j + v\hat{\Omega}_v + w\hat{\Omega}_w \quad (7\text{-}20)$$

where the direction vectors $\hat{\Omega}_v$ and $\hat{\Omega}_w$ are chosen to be orthogonal to each other and to $\hat{\Omega}_j$.

This gives us:

$$\delta\left(r-R\hat{\Omega}_{ji}-\hat{r}_{ji}\right)=\delta(u-R)\,\delta(v)\,\delta(w) \quad (7\text{-}21)$$

Substituting this into (7-19) gives us:

$$\phi(r,\Omega,E)\cong\begin{cases}\sum_{j=0}^{\infty} w_j\, e^{-\int_0^u dR'\,\Sigma_t\left(\hat{r}_j+(u-R')\hat{\Omega}_j,\hat{E}_j\right)}\delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right)\delta(v)\,\delta(w) & for\ 0<u<\infty \\ 0 & for\ u<0\end{cases} \quad (7\text{-}22)$$

Examination of this reveals that the sample fixes the values of $\Omega, E, v,$ and w through the Dirac deltas, but lets u vary from 0 to infinity, so “scoring” along the ray that flows out of the point $\hat{r}_j$ in the direction $\hat{\Omega}_j$.

The simplest way to sample this is to select the variable u from 0 to infinity, giving us:

$$\phi(r,\Omega,E) \cong \sum_{j=0}^{\infty} w_j \frac{e^{-\int_0^{\hat{u}_j} dR' \Sigma_t\left(\hat{r}_j + (\hat{u}_j - R')\hat{\Omega}_j, \hat{E}_j\right)}}{\pi(\hat{u}_j)} \delta\left(\Omega - \hat{\Omega}_j\right)\delta\left(E - \hat{E}_j\right)\delta(v)\delta(w)\delta\left(u - \hat{u}_j\right) \quad (7\text{-}23)$$

In our original coordinate system, this corresponds to:

$$\phi(r,\Omega,E) \cong \sum_{j=0}^{\infty} w_j \frac{e^{-\int_0^{\hat{u}_j} dR' \Sigma_t\left(\hat{r}_j + (\hat{u}_j - R')\hat{\Omega}_j, \hat{E}_j\right)}}{\pi(\hat{u}_j)} \delta\left(\Omega - \hat{\Omega}_j\right)\delta\left(E - \hat{E}_j\right)\delta\left(r - \hat{r}_\phi\right) \quad (7\text{-}24)$$

where

$$\hat{r}_\phi = \hat{r}_j + \hat{u}_j \hat{\Omega}_j \quad (7\text{-}25)$$

Although not required by the mathematics, it is usual to use $\pi(\hat{u}_j) = \pi(\hat{R}_j)$ (i.e., the same selection as was used to find the next emerging particle site, giving us $\hat{r}_\phi = \hat{r}_{j+1}$.

(Cut and paste from before)

7.3 Flux tallies using Dirac deltas

For a given history, the flux estimate is given by equation 7-17:

$$\phi(r,\Omega,E) \cong \sum_{j=0}^{\infty} \frac{w_j}{\Sigma_t\left(\hat{r}_j, \hat{E}_j\right)} \delta\left(r - \hat{r}_j\right)\delta\left(\Omega - \hat{\Omega}_j\right)\delta\left(E - \hat{E}_j\right) \quad (7\text{-}23)$$

where the variable j counts collisions, the weight is the particle weight at the time of the collision, and the careted variables are the parameters of the particle ENTERING the collision.

With this notation laid out, the tally contributions for the history are found by just inserting this into the tally integrals.

Cell-averaged tallies

For cell-averaged, flux-based tallies, the integral for a tally of type *x* is:

$$T_x = \int_V dr \int_0^{\infty} dE \int_{4\pi} R_x(r,\Omega,E)\phi(r,\Omega,E) \quad (7\text{-}24)$$

Substituting the flux approximation gives us:

$$T_x \cong \sum_{j=0}^{\infty} \frac{R_x\left(\hat{r}_j, \hat{\Omega}_j, \hat{E}_j\right)}{\Sigma_t\left(\hat{r}_j, \hat{E}_j\right)} w_j \tag{7-25}$$

At first glance this looks a little fishy, since tallies generally are tied to a particular cell, and this formula makes it looks like EVERY collision contributes to the tally in every cell (i.e., even if not in the cell!). But, keep in mind that all spatial details of the tally (as well as energy and direction) are the responsibility of the response function. If the tally is attached to a particular cell (or group of cells), then $R_x\left(r, \Omega, E\right)$ must be equal to 0 outside the cell(s) of interest, taking care of our problem.

Also, notice that if the response is a particular reaction type x, then we would have:

$$R_x\left(\hat{r}_j, \hat{\Omega}_j, \hat{E}_j\right) = \begin{cases} \Sigma_x\left(\hat{r}_j, \hat{E}_j\right), \hat{r}_j \in \text{ Volume of interest} \\ 0 \qquad\qquad\qquad , \text{ otherwise} \end{cases} \tag{7-26}$$

When this is substituted, we see that the contribution to the tally is the particle weight times the probability of collision type x, as we would expect (knowing that a collision occurred).

> *NOTE: In case it is bothering you that the weight does not seem to be divided by the cell volume—like it did for the cell flux contribution we looked at earlier, this occurred earlier because the cell averaged flux is NOT the integrated flux over the cell, but is the AVERAGE flux, so the flux weight must be divided by the cell volume.*

(Starting over) For a given history, the flux estimate is given by equation 7-17:

$$\phi\left(r, \Omega, E\right) \cong \sum_{j=0}^{\infty} \frac{w_j}{\Sigma_t\left(\hat{r}_j, \hat{E}_j\right)} \delta\left(r - \hat{r}_j\right) \delta\left(\Omega - \hat{\Omega}_j\right) \delta\left(E - \hat{E}_j\right) \tag{7-23}$$

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Chapter 8 Exercises

8-1. Research use of the adjoint flux in Nuclear Engineering and prepare a short (< 5 page) report.

7-2. Work out the specific adjoint algorithm that comes from utilizing the forward flux as an importance function in the adjoint Monte Carlo transport solution. (I will be particularly impressed if you can explain the physical significance of doing this.)

7-3. Research and explain how k-effective estimates are combined in MCNP. (MCNP calculates k-effective 3 ways using three different flux estimators and then combines them. How does it combine them?)

7-4. Research fictitious scattering (also called delta scattering and Woodcock scattering) and prepare a short (< 5 page) report.

7-5. Research the 10 statistical tests in MCNP and prepare a short (< 5 page) report.

7-6. Research use of the Weilandt procedure for fission site convergence and prepare a short (< 5 page) report.

7-7. Research use of Shannon entropy for fission site convergence and prepare a short (< 5 page) report.

Answers to selected exercises

Chapter 7
(none)

first rewrite it with the changes of variable:

$$\begin{aligned} r' &= r - R\Omega \\ R' &= R - R'' \end{aligned} \qquad (7\text{-}5)$$

to get:

$$\phi_0\left(r,\Omega,E\right) = \int_0^\infty dR\, \mathrm{e}^{-\int_0^R dR'\, \Sigma_t\left(r'+R'\Omega,E\right)} S\left(r',\Omega,E\right) \qquad (7\text{-}6)$$

The direction and energy of the flux is identical to those variables in the source—only the position has changed. The new position relates to the position, direction, and distance through the first equation of (7-5) rearranged a bit:

$$r = r' + R\Omega \qquad (7\text{-}6a)$$

This is a bit more complicated than the examples we saw in the previous chapter, but the principles are the same: Each of the independent variables on the right hand side are approximated (even though they are not involved in the integral).

An additional notational consideration is introduced for this situation in which we do NOT immediately "integrate out" a substituted Dirac delta, we take a short cut and anticipate the effect of the impending integration by replacing the continuous variable with the selected point. That is, once we introduce a Dirac delta, $\delta\left(x-\hat{x}_0\right)$, then all occurrences of the variable *x* are replaced with $\hat{x}_0$. This is mathematically justifiable because:

1. There is nothing that can be done to translate a Dirac delta into a usable value except integration; and
2. There is no difference between the results of integrating $f(x)\delta\left(x-\hat{x}_0\right)$ and the results of integrating $f(\hat{x}_0)\delta\left(x-\hat{x}_0\right)$.

We start by applying the Dirac Monte Carlo approximation to each of the dependent variables of the source:

$$S(r',\Omega,E) \cong \frac{S(\hat{r}_s,\hat{\Omega}_0,\hat{E}_0)}{\pi_s(\hat{r}_s,\hat{\Omega}_0,\hat{E}_0)}\delta\left(r'-\hat{r}_s\right)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right)$$
$$= w_s\delta\left(r'-\hat{r}_s\right)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right) \qquad \text{(7-6b)}$$

Substituting this approximation into (7-6) to get:

$$\phi_0\left(r,\Omega,E\right) \cong w_s\int_0^\infty dR\, \mathrm{e}^{-\int_0^R dR'\,\Sigma_t\left(\hat{r}_s+R'\hat{\Omega}_0,\hat{E}_0\right)}\delta\left(r'-\hat{r}_s\right)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right) \qquad \text{(7-7)}$$

To deal with the integral over R, we approximate:

$$\mathrm{e}^{-\int_0^R dR'\,\Sigma_t\left(r'+R'\Omega,E\right)} \cong \frac{\mathrm{e}^{-\int_0^{\hat{R}_0} dR'\,\Sigma_t\left(\hat{r}_0'+R'\hat{\Omega}_0,\hat{E}_0\right)}}{\pi_0\left(\hat{R}_0\right)}\delta\left(R-\hat{R}_0\right)$$

and substitute this into 7-6 to give:

$$\phi_0\left(r,\Omega,E\right) \cong \frac{w_0}{\Sigma_t\left(\hat{r}_s+\hat{R}_0\hat{\Omega}_0,\hat{E}_0\right)}\delta\left(r'-\hat{r}_s\right)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right) \qquad \text{(7-8)}$$

where

$$w_0 = \frac{w_s\Sigma_t\left(\hat{r}_s+\hat{R}_0\hat{\Omega}_0,\hat{E}_0\right)\mathrm{e}^{-\int_0^{\hat{R}_0} dR'\,\Sigma_t\left(\hat{r}_s+R'\hat{\Omega}_0,\hat{E}_0\right)}}{\pi\left(\hat{R}_0\right)} \qquad \text{(7-9)}$$

[NOTE: The division of the weight by the total cross section in Equation 7-8 above, is traditional practice. This represents the weight of the particle BEFORE the collision at point $\hat{r}_s+\hat{R}_0\hat{\Omega}_0$; use of this factor allows the weights to remain equation to 1.000 for the traditional "analog" Monte Carlo technique.]

Using equation 7-5, this becomes:

$$\phi_0\left(r,\Omega,E\right) \cong \frac{w_0}{\Sigma_t\left(\hat{r}_0,\hat{E}_0\right)}\delta\left(r-\hat{r}_0\right)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right) \qquad \text{(7-10)}$$

where:

$$\hat{r}_0 \equiv \hat{r}_0'+\hat{R}_0\hat{\Omega}_0 \qquad \text{(7-11)}$$