Chapter 7 Function-based Particle Transport

7.1 Application of Dirac delta approximation to the forward transport equation

NOTE: Throughout this section, to simplify the notation, I DO NOT use any vector symbols. You need to remember that $r \equiv \bar{r}$ and $\Omega \equiv \bar{\Omega}$ are position and direction, respectively.

We begin with the integral transport equation:

$$\phi(r,\Omega,E) = \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r-R'\Omega,E)} \Big[S(r-R\Omega,\Omega,E)$$

$$+ \int d\Omega' \int dE'\, \Sigma_s(\bar{r}-R\Omega,\Omega' \to \Omega, E' \to E)\phi(\bar{r}-R\Omega,\Omega',E') \Big] \tag{7-1}$$

NOTE: I have breezily skimmed over the mathematical difficulty of r and Ω being vectors (i.e., 3 dimensions and 2 dimensions, respectively), so the Dirac deltas for these variables would really consist of 3 Dirac deltas for space and 2 for direction. But, since the integration rules are the same—1 if inside the domain of integration and 0 if outside—the complexity (that the 1 is really a product of 1's and the 0 a product including at least one zero) is not worth the extra notation.

The physical meaning of this is that the flux is found from exponential transport (using the total number of mean free paths in the distance R that lies between r and r' at energy E) from all source particles and scattered particles to all of the points in the system.

We start by changing the equation to one that is more appropriate for comparing to event-based Monte Carlo. This is because "flux" is not an event that occurs at a specific place; it involves particles moving from one place to another. So, we take the term in the brackets in (7-1) and give it the name "emerging particles density," i.e., the spatial, energy, and directional density of particles "emerging"—either directly from the source or from scattering events. (These occur with specific values of position, energy, and direction, so fit an "event-based" point of view.

$$\chi(r,\Omega,E) = S(r,\Omega,E) + \int d\Omega' \int dE'\, \Sigma_s(\bar{r},\Omega' \to \Omega, E' \to E)\phi(\bar{r},\Omega',E') \tag{7-2}$$

(It is unfortunate that the traditional symbol for this is the same as the traditional symbol for the fission neutron energy distribution, but we have to keep up with the differences.)

The flux equation can then be written (by substituting (7-2) into (7-1)) as:

$$\phi(r,\Omega,E) = \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r-R'\Omega,E)} \chi(r-R\Omega,\Omega,E) \tag{7-3}$$

And then substituting (7-3) into (7-2) gives us an integral equation for the emerging particle density:

$$\chi(r,\Omega,E) = S(r,\Omega,E) +$$

$$\int d\Omega' \int dE'\, \Sigma_s(\bar{r},\Omega' \to \Omega, E' \to E) \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r-R'\Omega',E')} \chi(r-R\Omega',\Omega',E') \tag{7-4}$$

We apply the Neumann procedure to deal with the flux appearing on both sides:

$$\chi(r,\Omega,E) = \sum_{j=0}^\infty \chi_j(r,\Omega,E) \tag{7-5}$$

where the 0th order equation is given by:

$$\chi_0(r,\Omega,E) = S(r,\Omega,E) \tag{7-6}$$

and the higher order terms are given by:

$$\chi_{\ell+1}(r,\Omega,E) = \int d\Omega' \int dE'\, \Sigma_s(\bar{r},\Omega' \to \Omega, E' \to E) \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r-R'\Omega',E')} \chi_\ell(r-R\Omega',\Omega',E') \tag{7-7}$$

We can apply the stochastic approximations to the integrals of 7-6 and 7-7 to get what we have been calling a "general" Monte Carlo algorithms (those with one or more PDF's unspecified. (Once all of the PDF's are specified, we have a "specific" algorithm that is ready to be coded into a computer program.)

0th order term

Starting with equation 7-4, we simply sample the source, giving us:

$$\chi_0(r,\Omega,E) \cong \frac{S(\hat{r}_0,\hat{\Omega}_0,\hat{E}_0)}{\pi(\hat{r}_0,\hat{\Omega}_0,\hat{E}_0)} \delta(r-\hat{r}_0)\delta(\Omega-\hat{\Omega}_0)\delta(E-\hat{E}_0)$$
$$= w_0 \delta(r-\hat{r}_0)\delta(\Omega-\hat{\Omega}_0)\delta(E-\hat{E}_0) \tag{7-8}$$

where

$$w_0 = \frac{S\left(\hat{r}_0, \hat{\Omega}_0, \hat{E}_0\right)}{\pi\left(\hat{r}_0, \hat{\Omega}_0, \hat{E}_0\right)} \qquad (7\text{-}9)$$

(j+1)st order term

We now proceed inductively. Given that the jth order term can be approximated using:

$$\chi_j\left(r,\Omega,E\right) \cong w_j \delta\left(r - \hat{r}_j\right)\delta\left(\Omega - \hat{\Omega}_j\right)\delta\left(E - \hat{E}_j\right) \qquad (7\text{-}10)$$

the $(j+1)^{st}$ term can be found. We begin by substituting 7-10 into 7-7 to get:

$$\chi_{\ell+1}\left(r,\Omega,E\right) = \int d\Omega' \int dE' \Sigma_s\left(\bar{r},\Omega' \to \Omega, E' \to E\right) \times$$

$$\int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r - R'\Omega',E')}\left[w_\ell \delta\left(r - R\Omega' - \hat{r}_j\right)\delta\left(\Omega' - \hat{\Omega}_j\right)\delta\left(E' - \hat{E}_j\right)\right] \qquad (7\text{-}11)$$

Noting that the equivalence

$$f(x)\delta\left(x - \hat{x}_0\right) = f(\hat{x}_0)\delta\left(x - \hat{x}_0\right)$$

allows us to replace continuous variables (i.e., x in the previous equation) with the values that make the Dirac delta go to zero, we can convert 7-11 into:

$$\chi_{\ell+1}\left(r,\Omega,E\right) = w_\ell\, \Sigma_s\left(\bar{r},\hat{\Omega}_j \to \Omega, \hat{E}_j \to E\right) \times \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t\left(r - R'\hat{\Omega}_j,\hat{E}_j\right)}\delta\left(r - R\hat{\Omega}_j - \hat{r}_j\right) \qquad (7\text{-}12)$$

We deal with the integral by sampling R get:

$$\chi_{\ell+1}\left(r,\Omega,E\right) = w_\ell\, \Sigma_s\left(\bar{r},\hat{\Omega}_\ell \to \Omega, \hat{E}_\ell \to E\right)\frac{e^{-\int_0^{\hat{R}_\ell} dR'\, \Sigma_t\left(r - R'\hat{\Omega}_\ell,\hat{E}_\ell\right)}}{\pi\left(\hat{R}_\ell\right)}\delta\left(r - \hat{R}_\ell\hat{\Omega}_\ell - \hat{r}_\ell\right) \qquad (7\text{-}13)$$

We now deal with the two remaining continuous variables (and) by sampling them and simplifying to get:

$$\chi_{\ell+1}\left(r,\Omega,E\right) \cong w_\ell\, \frac{\Sigma_s\left(\bar{r},\hat{\Omega}_\ell \to \hat{\Omega}_{\ell+1}, \hat{E}_\ell \to \hat{E}_{\ell+1}\right)}{\pi\left(\hat{\Omega}_{\ell+1},\hat{E}_{\ell+1}\right)}\frac{e^{-\int_0^{\hat{R}_\ell} dR'\, \Sigma_t\left(\hat{r}_\ell + \hat{R}_\ell\hat{\Omega}_\ell - R'\hat{\Omega}_\ell,\hat{E}_\ell\right)}}{\pi\left(\hat{R}_\ell\right)}\delta\left(r - \hat{R}_\ell\hat{\Omega}_\ell - \hat{r}_\ell\right)\delta\left(\Omega - \hat{\Omega}_{\ell+1}\right)\delta\left(E - \hat{E}_{\ell+1}\right.$$

$$(7\text{-}14)$$

We complete the inductive development by writing this as:

$$\chi_{\ell+1}(r,\Omega,E) \cong w_{\ell+1}\, \delta(r-\hat{r}_{\ell+1})\delta(\Omega-\hat{\Omega}_{\ell+1})\delta(E-\hat{E}_{\ell+1}) \qquad (7\text{-}15)$$

where

$$w_{j+1} \equiv w_j \frac{\Sigma_s\left(\hat{r}_j,\hat{\Omega}_j \to \hat{\Omega}_{j+1}, \hat{E}_j \to \hat{E}_{j+1}\right)e^{-\int_0^{\hat{R}_{j+1}} dR'\, \Sigma_t\left(\hat{r}_{j+1}-R'\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)}}{\pi_{j+1}\left(\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)\pi_{j+1}\left(\hat{R}_{j+1}\right)}$$

$$\hat{r}_{j+1} \equiv \hat{r}_j + \hat{\Omega}_{j+1}\hat{R}_{j+1} \qquad (7\text{-}16)$$

Putting it together: Flux approximation

Combining the previous results into equation 7-5 gives us our final Monte Carlo estimate of the emerging particle density:

$$\chi(r,\Omega,E) = \sum_{j=0}^{\infty}\chi_j(r,\Omega,E)$$

$$\cong \sum_{j=0}^{\infty}w_j\delta(r-\hat{r}_j)\delta(\Omega-\hat{\Omega}_j)\delta(E-\hat{E}_j) \qquad (7\text{-}17)$$

which is interpreted to mean:

$$\chi(r,\Omega,E) = \lim_{I\to\infty}\frac{1}{I}\sum_{i=1}^{I}\ \sum_{j=0}^{\infty}w_{ji}\delta(r-\hat{r}_{ji})\delta(\Omega-\hat{\Omega}_{ji})\delta(E-\hat{E}_{ji}) \qquad (7\text{-}18)$$

where I have added an *i* index to count the histories; remember that j counts Neumann (scattering) steps.

Because of the two infinity occurrences, this does not look very useful for implementation on a computer. We take care of the first one by just resigning ourselves to the fact that limiting I to a finite value will leave us with an approximation to $\chi(r,\Omega,E)$:

$$\chi(r,\Omega,E) \approx \chi_I(r,\Omega,E) \equiv \frac{1}{I}\sum_{i=1}^{I}\ \sum_{j=0}^{\infty}w_{ji}\delta(r-\hat{r}_{ji})\delta(\Omega-\hat{\Omega}_{ji})\delta(E-\hat{E}_{ji}) \qquad (7\text{-}19)$$

More surprising is the fact that the second infinity does not have to be approximated. Equation 7-16 tells us that the sequence of w_{ji} values build on each other multiplicatively; this means that, once a given w_{ji} becomes zero, all the weights for larger values of j) will also be zero, so do not have to be approximated.

Therefore, dealing with the infinity can be accomplished by designing the algorithm so that the weights will always (eventually at least) go to zero. This is usually done in one of two ways:

1. Choose one or more PDF's so that a value of the random variable resulting in $w_{ji} = 0$ can be chosen. (This sometimes happens "naturally" in analog algorithms.)

2. ("Russian roulette") Introduce a statistically equivalent transformation of one or more w_{ji} values:

$$w'_{ji} = \begin{cases} \dfrac{w_{ji}}{p} \text{ with probability } p \\ 0 \text{ with probability } 1-p \end{cases}$$

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:

$$\phi(r,\Omega,E) \cong \int_0^\infty dR\, e^{-\int_0^R dR'\,\Sigma_t(r-R'\Omega,E)} \left[\sum_{j=0}^\infty w_j \delta\left(r-R\Omega-\hat{r}_j\right)\delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right) \right]$$

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

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:

$$\phi(r,\Omega,E) \cong \begin{cases} \sum_{j=0}^\infty w_j\, e^{-\int_0^u dR'\,\Sigma_t\left(\hat{r}_j+(u-R')\hat{\Omega}_j,\hat{E}_j\right)} \delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right)\delta(v)\delta(w) \text{ for } 0<u<\infty \\ 0 \hspace{8cm} \text{for } u<0 \end{cases} \quad (7\text{-}22)$$

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 $\hat{r}_\phi = \hat{r}_{j+1}$.

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7.2 General to specific forward algorithm

We will continue using the Equations from the previous section. The general Monte Carlo algorithm of equations 7-9, 7-16, and 7-18 is turned into a specific algorithm by the selection of particular PDF's to use. Each PDF used must obey three rules:

1. The PDF must be non-negative for all points.

2. The integral of the PDF over its selection domain must be 1. (Integration of a function over the complete problem domain will be denoted as $\langle f(x, y, \ldots) \rangle$.)

3. The PDF must be non-zero for all values of its selection domain for which a non-zero contribution to any tally is possible.

Analog algorithm

The simplest of these uses the natural PDFs, which leads to the "analog" algorithm. The PDF's associated with the analog algorithm are:

$$\pi_s(\hat{r}', \hat{\Omega}, \hat{E}) = \frac{S(\hat{r}', \hat{\Omega}, \hat{E})}{\left\langle S(\hat{r}', \hat{\Omega}, \hat{E}) \right\rangle}$$

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

$$\pi_{j+1}\left(\hat{\Omega}, \hat{E}\right) = \frac{\Sigma_s\left(\hat{r}_j, \hat{\Omega}_j \to \hat{\Omega}, \hat{E}_j \to \hat{E}\right)}{\Sigma_s\left(\hat{r}_j, \hat{E}_j\right)}$$

$$\pi_{j+1}\left(\hat{R}\right) = \Sigma_t\left(\hat{r}_j + \hat{R}\,\hat{\Omega}_{j+1}, \hat{E}_{j+1}\right) e^{-\int_0^{\hat{R}} dR'\,\Sigma_t\left(\hat{r}_j + R'\hat{\Omega}_{j+1}, \hat{E}_{j+1}\right)}$$

(7-20)

Substituting these PDF's into equations 7-9 and 7-16 give Dirac weights of:

$$w_{0i} = \left\langle S(\hat{r}', \hat{\Omega}, \hat{E}) \right\rangle \left(1 - e^{-\int_0^{\hat{R}_{boundary}} dR'\,\Sigma_t\left(\hat{r}_0' + R'\hat{\Omega}_0, \hat{E}_0\right)} \right)$$

(7-21)

and

$$w_{j+1} = w_j \frac{\Sigma_s\left(\hat{r}_j, \hat{E}_j\right) \left(1 - e^{-\int_0^{\hat{R}_{boundary}} dR'\,\Sigma_t\left(\hat{r}_j + R'\hat{\Omega}_j, \hat{E}_j\right)} \right)}{\Sigma_t\left(\hat{r}_j, \hat{E}_j\right)}$$

(7-22)

In most "analog" methods, the random walk is modified to keep the flux weights equal to the inverse of the total cross section at the latest collision. Modifying the weight streams given by equations 7-21 and 7-22 is accomplished in these algorithms with the following modifications (to get rid of the numerator terms):

1. The total source strength term, $\left\langle S(\hat{r}', \hat{\Omega}, \hat{E}) \right\rangle$, is just set to 1 and the user is required to know that the reported tallies are on a "per emitted source particle" basis (or the code multiplies the tallies by a user-specified constant equal to the source strength).

2. The $\left(1 - e^{-\int_0^{\hat{R}_{boundary}} dR'\,\Sigma_t\left(\hat{r}_0' + R'\hat{\Omega}_0, \hat{E}_0\right)} \right)$ and $\left(1 - e^{-\int_0^{\hat{R}_{boundary}} dR'\,\Sigma_t\left(\hat{r}_j + R'\hat{\Omega}_j, \hat{E}_j\right)} \right)$ terms are replaced with

    Russian roulette games with these survival probabilities, p. The resulting weight is then either 1 or 0, corresponding physically to a test of whether or not the particle escapes the problem geometry.

3. The $\Sigma_s\left(\hat{r}_j,\hat{E}_j\right)\big/\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)$ term is replaced with a Russian roulette game with this survival probability. The resulting weight is then either 1 or 0, corresponding physically to a test of whether the particle is scattered or is absorbed (ending the particle history).

7.3 Flux tallies using Dirac deltas

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

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

(7-23)

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:

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

(7-24)

Substituting the flux approximation gives us:

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

(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 $R_x(r,\Omega,E)$ 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:

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

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.

7.4 Application to adjoint transport equation

We begin with the integral transport equation that you derived in the previous section:

$$\phi^*\left(r,\Omega,E\right) = \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t(r+R'\Omega,E)} \left[S^*\left(r+R\Omega,\Omega,E\right) \right.$$
$$\left. + \int d\Omega' \int dE'\, \Sigma_s\left(\vec{r}+R\Omega,\Omega \to \Omega', E \to E'\right)\phi^*\left(\vec{r}+R\Omega,\Omega',E'\right) \right) \tag{7-27}$$

We apply the Neumann procedure to deal with the flux appearing on both sides:

$$\phi^*\left(r,\Omega,E\right) = \sum_{j=0}^\infty \phi_j^*\left(r,\Omega,E\right) \tag{7-28}$$

where the 0th order equation is given by:

$$\phi_0^*\left(r,\Omega,E\right) = \int_0^\infty dR\, e^{-\int_0^R dR''\, \Sigma_t(r+R''\Omega,E)} S^*\left(r+R\Omega,\Omega,E\right) \tag{7-29}$$

and the higher order terms are given by:

$$\phi_{j+1}^*\left(r,\Omega,E\right) = \int_0^\infty dR\, e^{-\int_0^R dR''\, \Sigma_t(r+R''\Omega,E)} \int d\Omega' \int dE'\, \Sigma_s\left(r+R\Omega,\Omega \to \Omega', E \to E'\right)$$
$$\cdot \phi_j^*\left(r+R\Omega,\Omega',E'\right) \;,\; j=0,1,\ldots,\infty \tag{7-30}$$

We can apply the stochastic approximations to the integrals of 7-29 and 7-30 to get what we have been calling a "general" Monte Carlo algorithms (those with one or more PDF's

unspecified. (Once all of the PDF's are specified, we have a "specific" algorithm that is ready to be coded into a computer program.)

0th order term

Starting with equation 7-28, we first rewrite it with the changes of variable:

$$r' = r + R\Omega$$
$$R' = R - R'' \tag{7-31}$$

to get:

$$\phi_0^*\left(r' - R\Omega, \Omega, E\right) = \int_0^\infty dR\, e^{-\int_0^R dR'\, \Sigma_t\left(r' - R'\Omega, E\right)} S^*\left(r', \Omega, E\right) \tag{7-32}$$

We next apply the Dirac Monte Carlo approximation to each of the variables on the right-hand-side of 7-32:

$$S^*(r', \Omega, E) \cong \frac{S^*(\hat{r}_s, \hat{\Omega}_0, \hat{E}_0)}{\pi_s(\hat{r}_s, \hat{\Omega}_0, \hat{E}_0)} \delta(r' - \hat{r}_0')\delta\left(\Omega - \hat{\Omega}_0\right)\delta\left(E - \hat{E}_0\right)$$

$$e^{-\int_0^R dR'\, \Sigma_t\left(r' - R'\Omega, E\right)} \cong \frac{e^{-\int_0^{\hat{R}_0} dR'\, \Sigma_t\left(\hat{r}_0' - R'\hat{\Omega}_0, \hat{E}_0\right)}}{\pi_0\left(\hat{R}_0\right)} \delta\left(R - \hat{R}_0\right) \tag{7-33}$$

and substitute these into 7-32 to give:

$$\phi_0^*\left(r' + R\Omega, \Omega, E\right) \cong \frac{w_0^*}{\Sigma_t\left(\hat{r}_s + \hat{R}_0\hat{\Omega}_0, \hat{E}_0\right)} \delta(r' - \hat{r}_s)\delta\left(\Omega - \hat{\Omega}_0\right)\delta\left(E - \hat{E}_0\right) \tag{7-34}$$

where

$$w_0^* = \frac{S^*(\hat{r}_s, \hat{\Omega}_0, \hat{E}_0)\Sigma_t\left(\hat{r}_s + \hat{R}_0\hat{\Omega}_0, \hat{E}_0\right)e^{-\int_0^{\hat{R}_0} dR'\, \Sigma_t\left(\hat{r}_0' - R'\hat{\Omega}_0, \hat{E}_0\right)}}{\pi_s(\hat{r}_s, \hat{\Omega}_0, \hat{E}_0)\pi_0\left(\hat{R}_0\right)} \tag{7-35}$$

Using equation 7-31, this becomes:

$$\phi_0^*\left(r, \Omega, E\right) \cong \frac{w_0^*}{\Sigma_t\left(\hat{r}_0, \hat{E}_0\right)} \delta(r - \hat{r}_0)\delta\left(\Omega - \hat{\Omega}_0\right)\delta\left(E - \hat{E}_0\right) \tag{7-36}$$

where:

$$\hat{r}_0 \equiv \hat{r}_s + \hat{R}_0\hat{\Omega}_0 \tag{7-37}$$

(j+1)ˢᵗ order term

Given that the jth order term can be approximated using:

$$\phi_j^*(r,\Omega,E) \cong \frac{w_j^*}{\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)}\delta\left(r-\hat{r}_j\right)\delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right) \tag{7-38}$$

the $(j+1)^{st}$ term can be found. We begin by substituting 7-38 into 7-30 to get:

$$\phi_{j+1}^*(r,\Omega,E) \cong \int_0^\infty dR\, e^{-\int_0^R dR''\,\Sigma_t(r+R''\Omega,E)}\int d\Omega'\int dE'\,\Sigma_s\left(r+R\Omega,\Omega\to\Omega',E\to E'\right)$$

$$\cdot\frac{w_j^*}{\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)}\delta\left(r'-\hat{r}_j\right)\delta\left(\Omega'-\hat{\Omega}_j\right)\delta\left(E'-\hat{E}_j\right)$$

$$\cong w_j^*\int_0^\infty dR\, e^{-\int_0^R dR'\,\Sigma_t\left(\hat{r}_j-R'\Omega,E\right)}\frac{\Sigma_s\left(\hat{r}_j,\Omega\to\hat{\Omega}_j,E\to\hat{E}_j\right)}{\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)}\delta\left(\vec{r}+\Omega R-\hat{r}_j\right) \tag{7-39}$$

(where I have again applied the changes of variable from 7-31).

If we again apply the Dirac Monte Carlo approximation, we get:

$$\Sigma_s\left(\hat{r}_j,\Omega\to\hat{\Omega}_j,E\to\hat{E}_j\right)$$

$$\cong\frac{\Sigma_s\left(\hat{r}_j,\hat{\Omega}_{j+1}\to\hat{\Omega}_j,\hat{E}_{j+1}\to\hat{E}_j\right)}{\pi_{j+1}\left(\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)}\delta\left(\Omega-\hat{\Omega}_{j+1}\right)\delta\left(E-\hat{E}_{j+1}\right)$$

$$e^{-\int_0^R dR'\,\Sigma_t\left(\hat{r}_j-R'\Omega,E\right)}\cong\frac{e^{-\int_0^{\hat{R}_{j+1}} dR'\,\Sigma_t\left(\hat{r}_j-R'\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)}}{\pi_{j+1}\left(\hat{R}_{j+1}\right)}\delta\left(R-\hat{R}_{j+1}\right) \tag{7-40}$$

we can substitute these into Equation 7-39 to get:

$$\phi_{j+1}^*(\vec{r},\Omega,E) \cong \frac{w_{j+1}^*}{\Sigma_t\left(\hat{r}_{j+1},\hat{E}_{j+1}\right)}\delta\left(\Omega-\hat{\Omega}_{j+1}\right)\delta\left(E-\hat{E}_{j+1}\right)\delta\left(r-\hat{r}_{j+1}\right) \tag{7-41}$$

where:

$$w_{j+1}^* \equiv w_j^* \; \frac{\Sigma_s\left(\hat{r}_j,\hat{\Omega}_{j+1}\to\hat{\Omega}_j,\hat{E}_{j+1}\to\hat{E}_j\right)}{\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)} \; \frac{e^{-\int_0^{\hat{R}_{j+1,i}} dR'\,\Sigma_t\left(\hat{r}_j-R'\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)}}{\pi_{j+1}\left(\hat{\Omega}_{j+1},\hat{E}_{j+1}\right)\pi_{j+1}\left(\hat{R}_{j+1}\right)}$$

$$\hat{r}_{j+1} \equiv \hat{r}_j + \hat{\Omega}_{j+1}\hat{R}_{j+1} \tag{7-42}$$

Putting it together: Flux approximation

Combining the previous results into equation 7-28 gives us our final Monte Carlo adjoint flux approximation:

$$\phi^*\left(r,\Omega,E\right) = \sum_{j=0}^{\infty}\phi_j^*\left(r,\Omega,E\right)$$

$$\cong \sum_{j=0}^{\infty}\frac{w_j^*}{\Sigma_t\left(\hat{r}_j,\hat{E}_j\right)}\delta\left(r-\hat{r}_j\right)\delta\left(\Omega-\hat{\Omega}_j\right)\delta\left(E-\hat{E}_j\right) \tag{7-43}$$

which is interpreted to mean:

$$\phi^*\left(r,\Omega,E\right) = \lim_{I\to\infty}\frac{1}{I}\sum_{i=1}^{I}\ \sum_{j=0}^{\infty}\frac{w_{ji}^*}{\Sigma_t\left(\hat{r}_{ji},\hat{E}_{ji}\right)}\delta\left(r-\hat{r}_{ji}\right)\delta\left(\Omega-\hat{\Omega}_{ji}\right)\delta\left(E-\hat{E}_{ji}\right) \tag{7-44}$$

(where I have added an *i* index to count the histories.)

Because of the two infinity occurrences, this does not look very useful for implementation on a computer. We take care of the first one by just resigning ourselves to the fact that limiting I to a finite value will leave us with an approximation to $\phi^*\left(r,\Omega,E\right)$:

$$\phi^*\left(r,\Omega,E\right) \approx \phi_I^*\left(r,\Omega,E\right) \equiv \frac{1}{I}\sum_{i=1}^{I}\ \sum_{j=0}^{\infty}\frac{w_{ji}^*}{\Sigma_t\left(\hat{r}_{ji},\hat{E}_{ji}\right)}\delta\left(r-\hat{r}_{ji}\right)\delta\left(\Omega-\hat{\Omega}_{ji}\right)\delta\left(E-\hat{E}_{ji}\right) \tag{7-45}$$

More surprising is the fact that the second infinity does not have to be approximated. Equation 7-42 tells us that the sequence of w_{ji}^* values build on each other multiplicatively; this means that, once a given w_{ji}^* becomes zero, all the weights for larger values of j) will also be zero, so do not have to be approximated.

The algorithm has to be designed so that the weights will always go to zero. This is usually done in one of two ways:

1. Choose one or more PDF's so that a value of the random variable resulting in $w_{ji}^* = 0$ can be chosen. (This sometimes happens "naturally" in analog algorithms.)

2. ("Russian roulette") Introduce a statistically equivalent transformation of one or more w_{ji}^* values:

$$
w_{ji}'^* = \begin{cases} \dfrac{w_{ji}}{p} & \text{with probability } p \\ 0 & \text{with probability } 1-p \end{cases}
$$

7.5 Specific adjoint algorithm

As for the forward equation, the general Monte Carlo algorithm of equations 7-35, 7-42, and 7-44 is turned into a specific algorithm by the selection of particular PDF's to use. Some of the considerations explored Section 7.2 apply to the adjoint flux as well (e.g., escape), but, unfortunately, the way that the total cross section in the transport PDF combined nicely with the total scattering cross section in the denominator of the scattering PDF does not happen in adjoint. This has the effect of making the weights in the adjoint formulation jump around much more than in the forward algorithm.

I will give you the opportunity to explore this in the homework problem 7-2.

7.6 Adjoint tallies

Adjoint tallies are simple Monte Carlo estimates of integrals, just like in the forward. For the most part, though, adjoint tallies are restricted to flux profiles and k-effective eigenvalues.

Chapter 7 Exercises

7-1. 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:

$$r' = r - R\Omega$$
$$R' = R - R''$$

(7-5)

to get:

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

(7-6)

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:

$$r = r' + R\Omega$$

(7-6a)

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, $\delta(x - \hat{x}_0)$, 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 $f(x)\delta(x - \hat{x}_0)$ and the results of integrating $f(\hat{x}_0)\delta(x - \hat{x}_0)$.

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

$$S(r',\Omega,E) \cong \frac{S(\hat{r}_s,\hat{\Omega}_0,\hat{E}_0)}{\pi_s(\hat{r}_s,\hat{\Omega}_0,\hat{E}_0)} \delta(r'-\hat{r}_s)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right)$$

$$= w_s \delta(r'-\hat{r}_s)\delta\left(\Omega-\hat{\Omega}_0\right)\delta\left(E-\hat{E}_0\right)$$

(7-6b)

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

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

(7-7)

To deal with the integral over R, we approximate:

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

and substitute this into 7-6 to give:

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

(7-8)

where

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

(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:

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

(7-10)

where:

$$\hat{r}_0 \equiv \hat{r}_0' + \hat{R}_0\hat{\Omega}_0$$

(7-11)