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THE ADJOINT BOLTZMANN EQUATION AND ITS SIMULATION BY MONTE CARLO*

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The Boltzmann equation for neutron transport is discussed in both integro-differential and integral form. The "value" or "importance" equation is derived and shown to be equivalent, in the integral form, to the adjoint of the collision density. However, the value is also equivalent to the adjoint of the flux when the adjoint operation is carried out on the integro-differential equation. Possible ways of simulating both the forward and adjoint equations by Monte Carlo are discussed. Because the value equation is a "flux-like" equation, direct simulation of it proves to be unwieldly. Instead, a "collision density" for adjoint particles, equal to the value or adjoint flux times the total cross section, is introduced. The equation for this adjuncton collision density may be simulated by the same routines as were used for the forward calculation and only the cross sections need to be changed. The extension of this to problems involving multiplying media is also included.

1. Introduction

1.1. *General comments*

Solutions to adjoint equations have been commonplace in finite difference method calculations for many years. However, it is only in the last few years that attention has been turned to adjoint calculations in Monte Carlo programs. In the course of attempts to simulate adjoint equations much confusion has arisen. Much of this stems from the fact that the processes of converting from integro-differential form to integral form and of converting to adjoint do not commute.*** In fact, the "value" or "importance" equation which is adjoint to the integral collision density equation is also the integral form of the adjoint integro-differential flux equation. Since the value equation is flux-like in nature, attempts to simulate it by Monte Carlo prove to be unwieldly. If the value is multiplied by the total cross section, the adjoint equation is converted to a form similar to that for the collision density. In fact, this equation can be simulated by Monte Carlo using the same subroutines as used in the forward solution. Only the cross sections used need to be changed for the adjoint.

The following derivations then cover the various forms of the forward and the adjoint Boltzmann equation and show clearly the flux-like nature of the value equation. Several sections outline the simulation of the forward and adjoint equations by Monte Carlo. The difficulties involved in simulating directly a flux equation are discussed. A final section describes the Monte Carlo solution of the Boltzmann equation for problems involving multiplying media.

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*** This fact was realized many years ago by Robkin and Clark [1], but this work was apparently not widely known. I did not learn of it until long after completing the derivations given in this paper. For an alternate interpretation of this problem see the recent article by Nelson [2].

1.2. *The "forward" or "direct" equation in integro-differential and integral form*

Let us start with the integro-differential form of the Boltzmann equation:

$$\hat{\Omega}\cdot\nabla\varphi(\mathbf{r},\mathbf{E}) + \Sigma_T(\mathbf{r},E)\,\varphi(\mathbf{r},\mathbf{E}) = S(\mathbf{r},\mathbf{E}) + \int d\mathbf{E}'\,\Sigma_s(\mathbf{r},\mathbf{E}'\to\mathbf{E})\,\varphi(\mathbf{r},\mathbf{E}')\,. \tag{1.1}$$

Here $\varphi(\mathbf{r},\mathbf{E})$ is the flux of particles and $S(\mathbf{r},\mathbf{E})$ is the source density. Throughout this paper $\mathbf{E}$ is used as shorthand for $(E,\hat{\Omega})$, thus $d\mathbf{E}$ denotes $dE\,d\hat{\Omega}$, etc. Vectors denoted by "^", such as $\hat{\Omega}$, will be unit vectors.

The first step is to convert this equation to its integral form. We let $\mathbf{r}$ be a fixed point and consider $\mathbf{r}' = \mathbf{r} - R\hat{\Omega}$ where R is a variable. Then

$$\frac{d\varphi(\mathbf{r}',\mathbf{E})}{dR} = \frac{dx'}{dR}\frac{\partial\varphi}{\partial x'} + \frac{dy'}{dR}\frac{\partial\varphi}{\partial y'} + \frac{dz'}{dR}\frac{\partial\varphi}{\partial z'} = -\Omega_{x'}\frac{\partial\varphi}{\partial x'} - \Omega_{y'}\frac{\partial\varphi}{\partial y'} - \Omega_{z'}\frac{\partial\varphi}{\partial z'} = -\hat{\Omega}\cdot\nabla\varphi(\mathbf{r}',\mathbf{E})$$

and, introducing the integrating factor $\exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]$,

$$-\frac{d}{dR}\left\{\varphi(\mathbf{r}',\mathbf{E})\exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]\right\}$$

$$= -\frac{d\varphi(\mathbf{r}',\mathbf{E})}{dR}\exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right] + \Sigma_T(\mathbf{r}',E)\,\varphi(\mathbf{r}',\mathbf{E})\exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]$$

$$= \exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]\left[-\frac{d\varphi(\mathbf{r}',\mathbf{E})}{dR} + \Sigma_T(\mathbf{r}',E)\,\varphi(\mathbf{r}',\mathbf{E})\right]$$

$$= \exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]\left[\hat{\Omega}\cdot\nabla\varphi(\mathbf{r}',\mathbf{E}) + \Sigma_T(\mathbf{r}',E)\,\varphi(\mathbf{r}',\mathbf{E})\right]$$

$$= \exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]\left[S(\mathbf{r}',\mathbf{E}) + \int d\mathbf{E}'\,\Sigma_s(\mathbf{r}',\mathbf{E}'\to\mathbf{E})\,\varphi(\mathbf{r}',\mathbf{E}')\right].$$

Now we integrate this last equation from $R = 0$ to $R = \infty$ and assume that the bracketed quantity on the left vanishes at $R = \infty$. This gives the integral form of the Boltzmann equation for the flux:

$$\varphi(\mathbf{r},\mathbf{E}) = \int_0^\infty dR\,\exp\left[-\int_0^R \Sigma_T(\mathbf{r}-R'\hat{\Omega},E)\,dR'\right]\{S(\mathbf{r}-R\hat{\Omega},\mathbf{E}) + \int d\mathbf{E}'\,\Sigma_s(\mathbf{r}-R'\hat{\Omega},\mathbf{E}'\to\mathbf{E})$$

$$\times\,\varphi(\mathbf{r}-R\hat{\Omega},\mathbf{E}')\}\,. \tag{1.2}$$

To simplify these equations we shall from time to time use

$$\beta(\mathbf{r}, R, \mathbf{E}) = \int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}, E)\, dR' . \tag{1.3}$$

$\beta(\mathbf{r}, R, \mathbf{E})$ is the optical distance or distance in number of mean free paths.

There are two kinds of collision densities which may be introduced,

$$\psi(\mathbf{r}, \mathbf{E}) = \Sigma_T(\mathbf{r}, E)\, \varphi(\mathbf{r}, \mathbf{E}) , \tag{1.4}$$

which is the density of particles *entering* a collision at $\mathbf{r}$ with *incoming* velocity $\mathbf{E}$, and is usually referred to as simply "the collision density", and

$$\chi(\mathbf{r}, \mathbf{E}) = S(\mathbf{r}, \mathbf{E}) + \int d\mathbf{E}' \Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})\, \varphi(\mathbf{r}, \mathbf{E}') , \tag{1.5}$$

which is the density of particles *leaving* a real collision or a source at $\mathbf{r}$ with *outgoing* velocity $\mathbf{E}$.

By multiplying eq. (1.2) by $\Sigma_T(\mathbf{r}, E)$ we derive the integral equation for the collision density:

$$\psi(\mathbf{r}, \mathbf{E}) = \int_0^\infty dR\, \Sigma_T(\mathbf{r}, E) \exp\left[- \int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}, E)\, dR' \right]$$

$$\times \left\{ S(\mathbf{r} - R\hat{\Omega}, \mathbf{E}) + \int d\mathbf{E}' \frac{\Sigma_s(\mathbf{r} - R\hat{\Omega}, \mathbf{E}' \to \mathbf{E})}{\Sigma_T(\mathbf{r} - R\hat{\Omega}, E')}\, \psi(\mathbf{r} - R\hat{\Omega}, \mathbf{E}') \right\} . \tag{1.6}$$

The integral equation for the density leaving collision is obtained by substituting eq. (1.5) into the bracketed part of eq. (1.2) and substituting the equation for φ back into eq. (1.5).

$$\chi(\mathbf{r}, \mathbf{E}) = S(\mathbf{r}, \mathbf{E}) + \int d\mathbf{E}' \Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E}) \int_0^\infty dR\, e^{-\beta(\mathbf{r}, R, \mathbf{E}')}\, \chi(\mathbf{r} - R\hat{\Omega}', \mathbf{E}')$$

$$= S(\mathbf{r}, \mathbf{E}) + \int d\mathbf{E}' \frac{\Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})}{\Sigma_T(\mathbf{r}, E')} \int_0^\infty dR\, \Sigma_T(\mathbf{r}, E')\, e^{-\beta(\mathbf{r}, R, \mathbf{E}')} \chi(\mathbf{r} - R\hat{\Omega}', \mathbf{E}') . \tag{1.7}$$

2. The integral equations in kernel form

The integral equations can all be expressed in a kernel form. To do this we must first transform the transport portion into a three-dimensional form

$$\psi(\mathbf{r}, \mathbf{E}) = \int_0^\infty dR\, \Sigma_T(\mathbf{r}, E)\, e^{-\beta(\mathbf{r}, R, \mathbf{E})}\, \chi(\mathbf{r} - R\hat{\Omega}, \mathbf{E})$$

$$= \int d\hat{\Omega}' \int_0^\infty R^2\, dR\, \frac{\delta(\hat{\Omega}' \cdot \hat{\Omega} - 1)}{R^2}\, \Sigma_T(\mathbf{r}, E) \exp\left[- \int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}', E)\, dR' \right] \chi(\mathbf{r} - R\hat{\Omega}', E) .$$

We set

$$\mathbf{r}' = \mathbf{r} - R\hat{\Omega}'$$

or

$$R\hat{\Omega}' = \mathbf{r} - \mathbf{r}'$$

and

$$\hat{\Omega}' \cdot \hat{\Omega} = \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \cdot \hat{\Omega} .$$

Also

$$\mathrm{d}\mathbf{r}' = R^2 \mathrm{d}R \, \mathrm{d}\hat{\Omega}' .$$

Thus

$$\psi(\mathbf{r}, \mathbf{E}) = \int \mathrm{d}\mathbf{r}' \, \Sigma_T(\mathbf{r}, E) \exp\left[- \int_{\mathbf{r}' \to \mathbf{r}} \Sigma_T(\mathbf{r}'', E) \, \mathrm{d}s \right] \frac{\delta\left(\hat{\Omega} \cdot \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - 1 \right)}{|\mathbf{r} - \mathbf{r}'|^2} \chi(\mathbf{r}', \mathbf{E}) ,$$

where

$$\int_{\mathbf{r}' \to \mathbf{r}} \Sigma_T(\mathbf{r}'', E) \, \mathrm{d}s$$

is the integral of Σ_T along the line from $\mathbf{r}'$ to $\mathbf{r}$.

In this form we can introduce the transport kernel

$$T(\mathbf{r}', \mathbf{r}|\mathbf{E}) = \Sigma_T(\mathbf{r}, E) \exp\left[- \int_{\mathbf{r}' \to \mathbf{r}} \Sigma_T(\mathbf{r}'', E) \, \mathrm{d}s \right] \frac{\delta\left(\hat{\Omega} \cdot \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - 1 \right)}{|\mathbf{r} - \mathbf{r}'|^2} \tag{2.1}$$

and the collision kernel

$$C(\mathbf{E}', \mathbf{E}|\mathbf{r}) = \frac{\Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})}{\Sigma_T(\mathbf{r}, E')} . \tag{2.2}$$

In this form the collision density equation is

$$\begin{aligned} \psi(\mathbf{r}, \mathbf{E}) &= \int \mathrm{d}\mathbf{r}' \, T(\mathbf{r}', \mathbf{r}|\mathbf{E}) \{ S(\mathbf{r}', \mathbf{E}) + \int \mathrm{d}\mathbf{E}' \, C(\mathbf{E}', \mathbf{E}|\mathbf{r}') \, \psi(\mathbf{r}', \mathbf{E}') \} \\ &= S_c(\mathbf{r}, \mathbf{E}) + \iint \mathrm{d}\mathbf{r}' \, \mathrm{d}\mathbf{E}' \, T(\mathbf{r}', \mathbf{r}|\mathbf{E}) \, C(\mathbf{E}', \mathbf{E}|\mathbf{r}') \, \psi(\mathbf{r}', \mathbf{E}') , \end{aligned} \tag{2.3}$$

where we have introduced the first-collision source,

$$S_c(\mathbf{r}, \mathbf{E}) = \int d\mathbf{r}'\, T(\mathbf{r}', \mathbf{r}|\mathbf{E})\, S(\mathbf{r}', \mathbf{E}) . \tag{2.4}$$

Likewise the equation for the density leaving is becomes

$$\chi(\mathbf{r}, \mathbf{E}) = S(\mathbf{r}, \mathbf{E}) + \iint d\mathbf{E}'\, d\mathbf{r}'\, C(\mathbf{E}', \mathbf{E}|\mathbf{r})\, T(\mathbf{r}', \mathbf{r}|\mathbf{E}')\, \chi(\mathbf{r}', \mathbf{E}') . \tag{2.5}$$

However, the flux equation is not expressed quite so simply in terms of the kernels. Thus we have

$$\begin{aligned}\varphi(\mathbf{r}, \mathbf{E}) &= \int d\mathbf{r}' \frac{T(\mathbf{r}', \mathbf{r}|\mathbf{E})}{\Sigma_T(\mathbf{r}, E)} \{S(\mathbf{r}', \mathbf{E}) + \int d\mathbf{E}'\, \Sigma_T(\mathbf{r}', E')\, C(\mathbf{E}', \mathbf{E}|\mathbf{r}')\, \varphi(\mathbf{r}', \mathbf{E}')\} \\ &= \frac{S_c(\mathbf{r}, \mathbf{E})}{\Sigma_T(\mathbf{r}, E)} + \iint d\mathbf{r}'\, d\mathbf{E}' \frac{\Sigma_T(\mathbf{r}', E')}{\Sigma_T(\mathbf{r}, E)} T(\mathbf{r}', \mathbf{r}|\mathbf{E})\, C(\mathbf{E}', \mathbf{E}|\mathbf{r}')\, \varphi(\mathbf{r}', E') . \end{aligned} \tag{2.6}$$

3. Monte Carlo simulation of the Boltzmann equation

The following is a somewhat simplified outline of the usual procedure followed in choosing Monte Carlo histories.

Step 1: An initial position and energy are chosen and weight assigned:
Choose $\mathbf{r}', \mathbf{E}'$ from $S(\mathbf{r}', \mathbf{E}')/\int d\mathbf{r}\, d\mathbf{E}\, S(\mathbf{r}, \mathbf{E})$.
Set weight $= \int d\mathbf{r}\, d\mathbf{E}\, S(\mathbf{r}, \mathbf{E})$.

Step 2: Next the particle is transported to the next collision site:
Choose R from

$$\Sigma_T(\mathbf{r}' + R\hat{\Omega}', E') \exp\left[-\int_0^R \Sigma_T(\mathbf{r}' + R'\hat{\Omega}', E')\, dR'\right] .$$

Set $\mathbf{r} = \mathbf{r}' + R\hat{\Omega}'$.
If $\mathbf{r}$ is outside the system of interest, the particle has escaped and the history is terminated.

Step 3: At the new collision site the particle weight is adjusted for absorption:

$$\text{Weight} = \begin{pmatrix}\text{previous} \\ \text{weight}\end{pmatrix} \frac{\Sigma_s(\mathbf{r}, E')}{\Sigma_T(\mathbf{r}, E')} .$$

Step 4: Finally a new energy and direction are chosen.
Choose $E, \hat{\Omega}$ from

$$\frac{\Sigma_s(E', \hat{\Omega}' \to E, \hat{\Omega}|\mathbf{r})}{\Sigma_s(\mathbf{r}, E')}$$

as follows:
Choose μ from $f(\mu|E', \mathbf{r})$.
Use energy-angle relationship to determine $E = E(\mu, E')$.
Choose $\hat{\Omega}$ so that $\hat{\Omega}\cdot\hat{\Omega}' = \mu$.

Step 5: If the new energy, E, is below the energy range of interest, the history is terminated, otherwise we set $\mathbf{r}' = \mathbf{r}$ and $\mathbf{E}' = \mathbf{E}$ and go back to step 2.

This procedure corresponds to the calculation of estimates for the Von Neumann series for the transport equation. We begin with $\chi_0(\mathbf{r}', \mathbf{E}') = S(\mathbf{r}', \mathbf{E}')$ at step 1. Step 2 then produces

$$\psi_0(\mathbf{r}, \mathbf{E}') = \int d\mathbf{r}'\, T(\mathbf{r}', \mathbf{r}|\mathbf{E}')\, \chi_0(\mathbf{r}', \mathbf{E}') .$$

[Note that there is no weight factor at this step. This is because the transport kernel is properly normalized. Actually, in a finite system, the transport kernel is normalized to less than one, but this is taken care of by terminating those histories which escape from the system. Alternatively one could prohibit escapes and use a weight factor.]

Steps 3 and 4 correspond to calculating

$$\chi_1(\mathbf{r}, \mathbf{E}) = \int d\mathbf{E}'\, C(\mathbf{E}', \mathbf{E}|\mathbf{r})\, \psi_0(\mathbf{r}, \mathbf{E}')$$

where we have used

$$\Sigma_s(\mathbf{r}, E') = \int d\mathbf{E}\, \Sigma_s(\mathbf{E}' \to \mathbf{E}|\mathbf{r})$$

and

$$f(\mathbf{E}' \to \mathbf{E}|\mathbf{r}) = \frac{\Sigma_s(\mathbf{E}' \to \mathbf{E}|\mathbf{r})}{\Sigma_s(\mathbf{r}, E')} .$$

Then the process returns iteratively to step 2 to calculate

$$\psi_n(\mathbf{r}, \mathbf{E}') = \int d\mathbf{r}'\, T(\mathbf{r}', \mathbf{r}|\mathbf{E}')\, \chi_n(\mathbf{r}', \mathbf{E}')$$

and to steps 3 and 4 to calculate

$$\chi_{n+1}(\mathbf{r}, \mathbf{E}) = \int d\mathbf{E}'\, C(\mathbf{E}', \mathbf{E}|\mathbf{r})\, \psi_n(\mathbf{r}, \mathbf{E}') .$$

At the termination of all the histories we may sum the Von Neumann series to obtain the collision densities:

$$\chi(\mathbf{r}, \mathbf{E}) = \sum_{n=0}^{\infty} \chi_n(\mathbf{r}, \mathbf{E}) .$$

This is estimated by summing all particle weights at the beginning of step 2, and

$$\psi(\mathbf{r}, \mathbf{E}) = \sum_{n=0}^{\infty} \psi_n(\mathbf{r}, \mathbf{E}) ,$$

this is estimated by summing all particle weights at the beginning of step 3. An estimate for the flux may be obtained from the estimate for ψ by dividing it by Σ_T.

The usual Monte Carlo transport calculation is properly a calculation of the collision density, not the flux. It is possible, however, to consider simulating the flux equation directly. The procedure would be as follows:

Step 1: Choose $\mathbf{r}', \mathbf{E}'$ from

$$\frac{S_c(\mathbf{r}', \mathbf{E}')}{\Sigma_T(\mathbf{r}', E')} \Big/ \int d\mathbf{r}\, d\mathbf{E} \frac{S_c(\mathbf{r}, \mathbf{E})}{\Sigma_T(\mathbf{r}, E)} .$$

Step 2: Multiply the particle weight by

$$\frac{\Sigma_s(\mathbf{r}', E)}{\Sigma_T(\mathbf{r}', E')} .$$

Step 3: Choose $\mathbf{E}$ from $f(\mathbf{E}' \to \mathbf{E}|\mathbf{r}')$.
Terminate if E is out of desired range.
Step 4: Choose $\mathbf{r}$ from $T(\mathbf{r}', \mathbf{r}|\mathbf{E})$.
Terminate if particle escapes.
Step 5: Multiply the particle weight by

$$\frac{\Sigma_T(\mathbf{r}', E')}{\Sigma_T(\mathbf{r}, E)} .$$

Return to step 2, setting $\mathbf{r}' = \mathbf{r}$, $\mathbf{E}' = \mathbf{E}$.

This procedure is the same as for calculating ψ except for the additional weight factor in step 5. Since this extra weight factor is likely to increase the variance of the calculation, the collision density, rather than the flux, is the quantity which is usually simulated directly by a Monte Carlo procedure.

4. The value equation and the adjoint equation

We turn our attention now from the direct equation to the various forms of adjoint equations. One such form that is frequently encountered is the "value" or "importance" equation. Its derivation is as follows.

Let us define a function, $W(\mathbf{r}, \mathbf{E})$, to be the value of an event or collision at the point $\mathbf{r}$. (It should be noted that this "value" is for a particle entering the collision with energy $\mathbf{E}$.) The "value" is the sum of two factors, the immediate payoff, $P(\mathbf{r}, \mathbf{E})$, and the payoff that may be expected to result from all future collisions. The future payoff is the expected value ($\iint d\mathbf{E}'\, dR \ldots$) of the probability of emerging from this event with the outgoing energy $\mathbf{E}'(\Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')/ \Sigma_T(\mathbf{r}, E))$ times the probability of going from $\mathbf{r}$ to another point $\mathbf{r} + R\hat{\Omega}'$ and having an event there

$$\Sigma_T(\mathbf{r} + R\hat{\Omega}', E') \exp\left[- \int_0^R \Sigma_T(\mathbf{r} + R'\hat{\Omega}', E')\, dR' \right] ,$$

times the value of having an event at $\mathbf{r} + R\hat{\Omega}'$ with incoming energy $\mathbf{E}'(W(\mathbf{r} + R\hat{\Omega}', \mathbf{E}))$. This leads to the following equation for the value

$$W(\mathbf{r}, \mathbf{E}) = P(\mathbf{r}, \mathbf{E}) + \int dE' \frac{\Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')}{\Sigma_T(\mathbf{r}, E)} \int dR\, \Sigma_T(\mathbf{r} + R\hat{\Omega}', E')$$

$$\times \exp\left[- \int_0^R \Sigma_T(\mathbf{r} + R'\hat{\Omega}', E')\, dR' \right] W(\mathbf{r} + R\hat{\Omega}, \mathbf{E}') . \tag{4.1}$$

To compare this equation with the direct equation, we will convert it into a kernel form. The first step is the transformation of the transport portion into a three-dimensional form

$$\int_0^\infty dR\, \Sigma_T(\mathbf{r}+R\hat{\Omega}', E') \exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}', E')\, dR'\right] W(\mathbf{r}+R\hat{\Omega}', \mathbf{E}')$$

$$= \iint d\hat{\Omega}''\, R^2 dR\, \frac{\delta(\hat{\Omega}''\cdot\hat{\Omega}'-1)}{R^2}\, \Sigma_T(\mathbf{r}+R\hat{\Omega}'', E') \exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}'', E')\, dR'\right] W(\mathbf{r}+R\Omega'', \mathbf{E}')$$

Set

$$\mathbf{r}' = \mathbf{r} + R\hat{\Omega}''$$

or

$$R\hat{\Omega}'' = \mathbf{r}' - \mathbf{r}\,.$$

Then

$$\hat{\Omega}''\cdot\hat{\Omega}' = \frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|}\cdot\hat{\Omega}'$$

and

$$d\mathbf{r}' = R^2 dR\, d\hat{\Omega}''\,.$$

Our transport term becomes

$$\int d\mathbf{r}' \frac{\delta\left(\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|}\cdot\hat{\Omega}'-1\right)}{|\mathbf{r}'-\mathbf{r}|^2}\, \Sigma_T(\mathbf{r}', E') \exp\left[-\int_{\mathbf{r}\to\mathbf{r}'} \Sigma_T(\mathbf{r}'', E)\, ds\right] W(\mathbf{r}', \mathbf{E}') = \int d\mathbf{r}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E}')\, W(\mathbf{r}', \mathbf{E}')\,,$$

where the transport kernel is the same function introduced in eq. (2.1), only now we note that $\mathbf{r}$ and $\mathbf{r}'$ are interchanged.

To complete the conversion we note that the collision term in the value equation is identical to the collision kernel in eq. (2.2) except that $\mathbf{E}$ and $\mathbf{E}'$ have been interchanged. Thus the value equation may be written

$$W(\mathbf{r}, \mathbf{E}) = P(\mathbf{r}, \mathbf{E}) + \iint d\mathbf{E}'\, d\mathbf{r}'\, C(\mathbf{E}, \mathbf{E}'|\mathbf{r})\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E}')\, W(\mathbf{r}', \mathbf{E}')\,. \tag{4.2}$$

We may compare this equation with the collision density equation (2.3). Since the transpose of $T(\mathbf{r}', \mathbf{r}|\mathbf{E})\, C(\mathbf{E}', \mathbf{E}|\mathbf{r}')$ is $C(\mathbf{E}, \mathbf{E}'|\mathbf{r})\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E}')$, the value equation is adjoint to the collision density equation. We can now specify our "payoff" function, P. If λ is some quantity of interest and

$$\lambda = \int d\mathbf{r}\, d\mathbf{E}\, \psi(\mathbf{r}, \mathbf{E}) P(\mathbf{r}, \mathbf{E})\,, \tag{4.3}$$

then we also have that

$$\lambda = \int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{E}\, W(\mathbf{r}, \mathbf{E}) S_c(\mathbf{r}, \mathbf{E}) . \tag{4.4}$$

[The equality of these two equations is proved rather trivially by multiplying eq. (2.3) by W and eq. (4.2) by ψ and integrating over $\mathbf{r}$ and $\mathbf{E}$.]

Just as there were two collision densities, the density of particles entering a collision and the density leaving a collision, so, too, we can speak of the value of entering a collision and the value of leaving a collision. We define the value of leaving a collision to be

$$\chi^*(\mathbf{r}, \mathbf{E}) = \int \mathrm{d}\mathbf{r}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\, W(\mathbf{r}', \mathbf{E})$$

$$= \int \mathrm{d}R\, \Sigma_T(\mathbf{r} + R\hat{\Omega}, E) \exp\left[- \int_0^R \Sigma_T(\mathbf{r} + R'\hat{\Omega}, E)\, \mathrm{d}R' \right] W(\mathbf{r} + R\hat{\Omega}, \mathbf{E}) . \tag{4.5}$$

This can be interpreted as the expected value of the probability of traveling from $\mathbf{r}$ to $\mathbf{r} + R\hat{\Omega}$ and having an event there times the value of having a collision at $\mathbf{r} + R\hat{\Omega}$ with incoming energy $\mathbf{E}$, and is thus the value of leaving a collision at $\mathbf{r}$ with outgoing energy $\mathbf{E}$.

By substituting χ^* into eq. (4.2) and substituting the results in eq. (4.5), we can obtain the equation for χ^*

$$\chi^*(\mathbf{r}, \mathbf{E}) = \int \mathrm{d}\mathbf{r}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E}) \{ P(\mathbf{r}', \mathbf{E}) + \int \mathrm{d}\mathbf{E}'\, C(\mathbf{E}, \mathbf{E}'|\mathbf{r}')\, \chi^*(\mathbf{r}', \mathbf{E}') \}$$

$$= P_c(\mathbf{r}, \mathbf{E}) + \int \mathrm{d}\mathbf{r}'\, \mathrm{d}\mathbf{E}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\, C(\mathbf{E}, \mathbf{E}'|\mathbf{r}')\, \chi^*(\mathbf{r}', \mathbf{E}') \tag{4.6}$$

where we have introduced

$$P_c(\mathbf{r}, \mathbf{E}) = \int \mathrm{d}\mathbf{r}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\, P(\mathbf{r}', \mathbf{E})$$

in analogy to S_c, the first-collision source.

By inspection of eqs. (4.6) and (2.5), we can see that χ and χ^* are adjoint to each other just as ψ and W are. Then we also have two additional equations for λ, the quantity of interest.

$$\lambda = \int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{E}\, \chi(\mathbf{r}, \mathbf{E}) P_c(\mathbf{r}, \mathbf{E}) , \tag{4.7}$$

$$\lambda = \int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{E}\, \chi^*(\mathbf{r}, \mathbf{E}) S(\mathbf{r}, \mathbf{E}) . \tag{4.8}$$

(The equivalence of these two equations to eqs. (4.3) and (4.4) is shown in Appendix 4.)

5. The adjoint flux equation

Let us digress for a moment and derive the adjoint equation in a different manner. We will start again with the integro-differential form of the direct Boltzmann eq. (1.1). The adjoint to this is

$$-\hat{\Omega} \cdot \nabla \varphi^*(\mathbf{r}, \mathbf{E}) + \Sigma_T(\mathbf{r}, E)\, \varphi^*(\mathbf{r}, \mathbf{E}) = S^*(\mathbf{r}, \mathbf{E}) + \int \mathrm{d}\mathbf{E}'\, \Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')\, \varphi^*(\mathbf{r}, \mathbf{E}') . \tag{5.1}$$

To convert this to an integral equation we follow the same steps as were used in Sect. 1 for the direct equation. We again let $\mathbf{r}$ be a fixed point but we consider $\mathbf{r}' = \mathbf{r} + R\hat{\Omega}$. Then

$$\frac{\mathrm{d}\varphi^*(\mathbf{r}', \mathbf{E})}{\mathrm{d}R} = \hat{\Omega}\cdot\nabla\,\varphi^*(\mathbf{r}', \mathbf{E})$$

and

$$-\frac{\mathrm{d}}{\mathrm{d}R}\left\{\varphi^*(\mathbf{r}', \mathbf{E})\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]\right\} = -\frac{\mathrm{d}\varphi^*(\mathbf{r}', \mathbf{E})}{\mathrm{d}R}\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]$$

$$+\Sigma_T(\mathbf{r}', E)\,\varphi^*(\mathbf{r}', \mathbf{E})\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]$$

$$=\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]\left[-\hat{\Omega}\cdot\nabla\,\varphi^*(\mathbf{r}', \mathbf{E}) + \Sigma_T(\mathbf{r}', E)\,\varphi^*(\mathbf{r}', \mathbf{E})\right]$$

$$=\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]\left[S^*(\mathbf{r}', \mathbf{E}) + \int \mathrm{d}\mathbf{E}'\,\Sigma_s(\mathbf{r}', \mathbf{E}\to\mathbf{E}')\,\varphi^*(\mathbf{r}', \mathbf{E}')\right].$$

As before we integrate from $R = 0$ to $R = \infty$ and assume that the bracketed quantity on the left vanishes at $R = \infty$. This leads to

$$\varphi^*(\mathbf{r}, \mathbf{E}) = \int_0^\infty \mathrm{d}R\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]\{S^*(\mathbf{r}+R\hat{\Omega}, \mathbf{E}) + \int \mathrm{d}\mathbf{E}'\,\Sigma_s(\mathbf{r}+R\hat{\Omega}, \mathbf{E}\to\mathbf{E}')$$

$$\times\,\varphi^*(\mathbf{r}+R\hat{\Omega}, \mathbf{E}')\} = \int_0^\infty \mathrm{d}R\,\Sigma_T(\mathbf{r}+R\hat{\Omega}, E)\exp\left[-\int_0^R \Sigma_T(\mathbf{r}+R'\hat{\Omega}, E)\,\mathrm{d}R'\right]$$

$$\times\left\{\frac{S^*(\mathbf{r}+R\hat{\Omega}, \mathbf{E})}{\Sigma_T(\mathbf{r}+R\hat{\Omega}, E)} + \int \mathrm{d}\mathbf{E}'\,\frac{\Sigma_s(\mathbf{r}+R\hat{\Omega}, \mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r}+R\hat{\Omega}, E)}\,\varphi^*(\mathbf{r}+R\hat{\Omega}, \mathbf{E}')\right\}. \tag{5.2}$$

In kernel form this becomes

$$\varphi^*(\mathbf{r}, \mathbf{E}) = \int \mathrm{d}\mathbf{r}'\,T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\left\{\frac{S^*(\mathbf{r}', \mathbf{E})}{\Sigma_T(\mathbf{r}', E)} + \int \mathrm{d}\mathbf{E}'\,C(\mathbf{E}, \mathbf{E}'|\mathbf{r}')\,\varphi^*(\mathbf{r}', \mathbf{E}')\right\}$$

$$= S_c^*(\mathbf{r}, \mathbf{E}) + \int \mathrm{d}\mathbf{r}'\,\mathrm{d}\mathbf{E}'\,T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\,C(\mathbf{E}, \mathbf{E}'|\mathbf{r}')\,\varphi^*(\mathbf{r}', \mathbf{E}') \tag{5.3}$$

where

$$S_c^* = \int \mathrm{d}\mathbf{r}'\,T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\,\frac{S^*(\mathbf{r}', \mathbf{E})}{\Sigma_T(\mathbf{r}', E)}.$$

By comparison of eqs. (5.3) and (4.6) we see that if we equate $S^*(\mathbf{r}, \mathbf{E})$ to $\Sigma_T(\mathbf{r}, E) P(\mathbf{r}, \mathbf{E})$ then

$$\varphi^*(\mathbf{r}, \mathbf{E}) \equiv \chi^*(\mathbf{r}, \mathbf{E}) .$$

Therefore, the adjoint flux is the value of a particle leaving a collision.

To further justify the equality of value and adjoint flux let us consider a large number, N, of particles of energy $\mathbf{E}$ moving an infinitesimal distance from $\mathbf{r}$ to $\mathbf{r} + dR\hat{\Omega}$. In this distance $N \Sigma_T(\mathbf{r}, E)\, dR$ collisions will occur. There will be a loss of value of $N \Sigma_T(\mathbf{r}, E)\, dR\, \chi^*(\mathbf{r}, \mathbf{E})$ due to the removal of the colliding particles from the group. The immediate payoff from these collisions will be $N \Sigma_T(\mathbf{r}, E)\, dR\, P(\mathbf{r}, \mathbf{E})$. In addition there will be $N \Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')\, dR\, d\mathbf{E}'$ particles scattered to a new energy in $d\mathbf{E}'$ about $\mathbf{E}'$ where they will have a value $\chi^*(\mathbf{r}, \mathbf{E}')$. This will contribute $N dR \int d\mathbf{E}'\, \Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')\, \chi^*(\mathbf{r}', \mathbf{E}')$ to the value. For the particles which do not collide (all the particles except an infinitesimal number), they will experience a change in value due to a change in position. This value change will be $N(\chi^*(\mathbf{r}, \mathbf{E}) - \chi^*(\mathbf{r} + dR\hat{\Omega}, \mathbf{E}))$. Now from the definition of the value function we should have a law of conservation of value, that is, the change in value (initial-final) as particles move from point to point should equal the immediate payoff. Thus we should have

$$N dR \cdot \Sigma_T(\mathbf{r}, E)\, P(\mathbf{r}, \mathbf{E}) = N dR \left[+ \Sigma_T(\mathbf{r}, E)\, \chi^*(\mathbf{r}, \mathbf{E}) - \int d\mathbf{E}'\, \Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')\, \chi^*(\mathbf{r}, \mathbf{E}') + \frac{\chi^*(\mathbf{r}, \mathbf{E}) - \chi^*(\mathbf{r} + dR\hat{\Omega}, \mathbf{E})}{dR} \right],$$

or

$$\Sigma_T(\mathbf{r}, E)\, P(\mathbf{r}, \mathbf{E}) = \Sigma_T(\mathbf{r}, E)\, \chi^*(\mathbf{r}, \mathbf{E}) - \int d\mathbf{E}'\, \Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')\, \chi^*(\mathbf{r}, \mathbf{E}') - \hat{\Omega} \cdot \nabla \chi^*(\mathbf{r}, \mathbf{E}) .$$

This, however, is the eq. (5.1) satisfied by the adjoint flux, showing again that $\chi^* = \varphi^*$ and $\Sigma_T P = S^*$.

6. Simulation of the adjoint equations by Monte Carlo

We will start with the value equation (4.1) and try to devise a simulation procedure working analogously to simulation of the direct equation. The ficticious particles which will be transported in the adjoint solution will be called adjunctons. The first step is obviously to choose a source position and energy from $P(\mathbf{r}, \mathbf{E})$.

Step 1: Choose $\mathbf{r}', \mathbf{E}'$ from $P(\mathbf{r}', \mathbf{E}') / \int d\mathbf{r}\, d\mathbf{E} P(\mathbf{r}, \mathbf{E})$.

Set weight $= \int d\mathbf{r}\, d\mathbf{E} P(\mathbf{r}, \mathbf{E})$.

The next step is to transport the adjuncton to the next collision site. Now we begin to run into some problems. We need to choose an R from

$$\Sigma_T(\mathbf{r}', E') \exp\left[- \int_0^R \Sigma_T(\mathbf{r}' - R'\hat{\Omega}', E')\, dR' \right]$$

and then set $\mathbf{r} = \mathbf{r}' - R\hat{\Omega}'$. This means that our particles will be travelling in the opposite direction to their velocity but that is merely a minor curiosity. The real snag is that the transposed transport kernel is not normalized. To pick from it we will have to normalize it and then use a weight factor.† This leads to:

† An alternative, suggested by M.H.Kalos, is to determine the normalization of the adjoint kernel, (continued on next page.)

Step 2: Choose R from

$$\Sigma_T(\mathbf{r}' - R\hat{\Omega}', E') \exp\left[- \int_0^R \Sigma_T(\mathbf{r}' - R'\hat{\Omega}', E')\, dR' \right].$$

$$\text{Set weight} = \begin{pmatrix}\text{previous}\\ \text{weight}\end{pmatrix} \frac{\Sigma_T(\mathbf{r}', E')}{\Sigma_T(\mathbf{r}, E')}.$$

The history will terminate here if the adjuncton has escaped from the system of interest.

In trying to choose the new energy for the particle following the collision we run into similar problems with normalization. In the direct equation the collision kernel is easily factored:

$$\frac{\Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})}{\Sigma_T(\mathbf{r}, \mathbf{E}')} = f(\mathbf{E}' \to \mathbf{E}|\mathbf{r}) \cdot \frac{\Sigma_s(\mathbf{r}, E')}{\Sigma_T(\mathbf{r}, E')},$$

where $f(\mathbf{E}' - \mathbf{E}|\mathbf{r})$ is the normalized distribution function

$$f(\mathbf{E}' \to \mathbf{E}|\mathbf{r}) = \frac{\Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})}{\int d\mathbf{E}''\, \Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E}'')} = \frac{\Sigma_s(\mathbf{r}, \mathbf{E}' \to \mathbf{E})}{\Sigma_s(\mathbf{r}, E')}$$

and the weight factor is the familiar non-absorption probability

$$\frac{\Sigma_s(\mathbf{r}, E')}{\Sigma_T(\mathbf{r}, E')} \leqslant 1 .$$

For the value equation we must still obtain a normalized distribution

$$f^*(\mathbf{E} \to \mathbf{E}'|\mathbf{r}) = \frac{\Sigma_s(\mathbf{r}, \mathbf{E} \to \mathbf{E}')}{\int d\mathbf{E}''\, \Sigma_s(\mathbf{r}, \mathbf{E}'' \to \mathbf{E}')}$$

but now the weight factor,

$$\frac{\int d\mathbf{E}''\, \Sigma_s(\mathbf{r}, \mathbf{E}'' \to \mathbf{E}')}{\Sigma_T(\mathbf{r}, E)}$$

(Continued from preceding page)

$$U = \int_0^\infty dR\, \Sigma_T(\mathbf{r}', E') \exp\left[- \int_0^R \Sigma_T(\mathbf{r}' - R'\hat{\Omega}', E')\, dR' \right].$$

U is broken into its integral, $[U]$, and fractional, $\{U\}$ parts. We then choose $[U]$ times from the normalized kernel and start off $[U]$ separate adjunctons from these collision points. With probability $\{U\}$ we also have one more adjuncton.

For any but the simplest geometries this procedure is undesirable. In order to determine U, the geometric tracking must trace the particle ray out to the edge of the system. This could greatly increase the computing time spent in the geometry portion of the calculation and easily negate the advantage in variance reduction gained by avoiding a weight factor.

is not so simple and may even be greater than one.† In addition it contains $\Sigma_T(\mathbf{r}, E)$ and not $\Sigma_T(\mathbf{r}, E')$ and so must be determined after choosing the outgoing energy. Thus:

Step 3: Choose $E, \hat{\Omega}$ from $f^*(E, \hat{\Omega} \to E', \hat{\Omega}'|\mathbf{r})$.

If E is *above* the range of interest, the history is terminated.

Step 4:

$$\text{Set weight} = \text{weight} \cdot \frac{\int \mathrm{d}\mathbf{E}''\, \Sigma_s(\mathbf{r}, \mathbf{E}'' \to \mathbf{E}')}{\Sigma_T(\mathbf{r}, E)} .$$

Step 5: Set $\mathbf{r}' = \mathbf{r}$,

$\mathbf{E}' = \mathbf{E}$.

Go back to step 2.

However, the value equation is actually a flux-like equation, the φ^* equation. The additional weight factor that appears in the transport process is similar to that which appears in the direct simulation of the flux equation in sect. 3. It will disappear if we treat the adjoint equation as a flux equation and multiply by the total cross section to get a collision density. That is, we introduce

$$H(\mathbf{r}, \mathbf{E}) = \Sigma_T(\mathbf{r}, E)\, \varphi^*(\mathbf{r}, -\mathbf{E}) . \tag{6.1}$$

(The $-\mathbf{E}$ will make our adjoint particles, or adjunctons, travel in the direction of their velocity rather than opposed to it.) From 5.2 we can obtain the equation for H

$$H(\mathbf{r}, \mathbf{E}) = \int_0^R \mathrm{d}R\, \Sigma_T(\mathbf{r}, E) \exp\left[-\int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}, E)\, \mathrm{d}R'\right]$$

$$\left\{\Sigma_T(\mathbf{r} - R\hat{\Omega}, E)\, P(\mathbf{r} - R\hat{\Omega}, -\mathbf{E}) + \int \mathrm{d}\mathbf{E}' \frac{\Sigma_s(\mathbf{r} - R\hat{\Omega}, -\mathbf{E} \to \mathbf{E}')}{\Sigma_T(\mathbf{r} - R\hat{\Omega}, E')} H(\mathbf{r} - R\hat{\Omega}, -\mathbf{E}')\right\} .$$

If we set $\mathbf{E}'' = -\mathbf{E}'$ and note that $\Sigma_s(\mathbf{r}, -\mathbf{E} \to -\mathbf{E}'') = \Sigma_s(\mathbf{r}'\, \mathbf{E} \to \mathbf{E}'')$ we get

$$H(\mathbf{r}, \mathbf{E}) = \int_0^\infty \mathrm{d}R\, \Sigma_T(\mathbf{r}, E) \exp\left[-\int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}, E)\, \mathrm{d}R'\right]$$

$$\times \left\{A(\mathbf{r} - R\hat{\Omega}, \mathbf{E}) + \int \mathrm{d}\mathbf{E}'' \frac{\Sigma_s(\mathbf{r} - R\hat{\Omega}, \mathbf{E} \to \mathbf{E}'')}{\Sigma_T(\mathbf{r} - R\hat{\Omega}, E'')} H(\mathbf{r} - R\hat{\Omega}, \mathbf{E}'')\right\} , \tag{6.2}$$

where we have set

$$A(\mathbf{r}, \mathbf{E}) = \Sigma_T(\mathbf{r}, E)\, P(\mathbf{r}, -\mathbf{E}) ; \tag{6.3}$$

$A(\mathbf{r}, \mathbf{E})$ is our adjuncton source density. The simulation of H would proceed as follows:

Step 1: Choose $\mathbf{r}', \mathbf{E}'$ from $A(\mathbf{r}', \mathbf{E}')/\int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{E} A(\mathbf{r}, \mathbf{E})$.

Set weight = $\int \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{E} A(\mathbf{r}, \mathbf{E})$.

† This means that there is no such thing as "analogue" scattering for adjunctons and we will always treat the non-absorption factor as a weight factor. Adjuncton weights may increase at some collisions.

Step 2: Choose R from

$$\Sigma_T(\mathbf{r}'+R\hat{\Omega}', E') \exp\left[-\int_0^R \Sigma_T(\mathbf{r}'+R'\hat{\Omega}', E')\, dR'\right].$$

Set $\mathbf{r}=\mathbf{r}'+R\hat{\Omega}'$.

Terminate history if adjuncton escapes.

Step 3:

$$\text{Set weight} = \text{weight} \cdot \frac{\int \Sigma_s(\mathbf{r}, \mathbf{E}''\to\mathbf{E}')\, d\mathbf{E}''}{\Sigma_T(\mathbf{r}, E')}.$$

Step 4: Choose $E, \hat{\Omega}$ from $f(\mathbf{E}\to\mathbf{E}'|\mathbf{r})$.

If E is outside the energy range of interest, terminate the history, otherwise, set $\mathbf{r}'=\mathbf{r}$ and $\mathbf{E}'=\mathbf{E}$ and return to step 2.

Notice that this formulation not only eliminates the unwanted weight factor at the transport step but also is exactly parallel to the simulation of the direct equation. This means that except for the cross sections used, the adjunctons can be transported by the same program as was developed for the simulation of the direct equation.

7. Monte Carlo simulation in problems involving multiplying media

In a fissioning system, the source of neutrons for one generation, n, comes from the fissions occuring in the previous generation.

$$S_n(\mathbf{r}, \mathbf{E}) = \frac{f(E)}{4\pi}\int d\mathbf{E}'\, \nu\Sigma_f(\mathbf{r}, E')\, \varphi_{n-1}(\mathbf{r}, \mathbf{E}') = \frac{f(E)}{4\pi}\int d\mathbf{E}' \frac{\nu\Sigma_f(\mathbf{r}, E')}{\Sigma_T(\mathbf{r}, E')}\, \psi_{n-1}(\mathbf{r}, \mathbf{E}'), \tag{7.1}$$

where $f(E)$ is the fission distribution and we have written $\nu(\mathbf{r}, E)\,\Sigma_f(\mathbf{r}, E)$ as a single quantity. This neutron source then gives rise to a collision density for that generation.

$$\psi_n(\mathbf{r}, \mathbf{E}) = \int dR\, \Sigma_T(\mathbf{r}, E)\, e^{-\beta(\mathbf{r}, R, \mathbf{E})} \left\{S_n(\mathbf{r}-R\hat{\Omega}, \mathbf{E}) + \int d\mathbf{E}' \frac{\Sigma_s(\mathbf{r}-R\hat{\Omega}, \mathbf{E}'\to\mathbf{E})}{\Sigma_T(\mathbf{r}-R\hat{\Omega}, \mathbf{E}')}\, \psi(\mathbf{r}-R\hat{\Omega}, \mathbf{E}')\right\}. \tag{7.2}$$

We may combine these two equations and write this as an eigenvalue equation

$$\psi(\mathbf{r}, \mathbf{E}) = \int dR\, \Sigma_T(\mathbf{r}, E)\, e^{-\beta(\mathbf{r}, R, E)} \left\{\frac{1}{k}\frac{f(E)}{4\pi}\int d\mathbf{E}' \frac{\nu\Sigma_f(\mathbf{r}-R\hat{\Omega}, E')}{\Sigma_T(\mathbf{r}-R\hat{\Omega}, E')}\right.$$

$$\left. \times\, \psi(\mathbf{r}-R\hat{\Omega}, \mathbf{E}') + \int d\mathbf{E}' \frac{\Sigma_s(\mathbf{r}-R\hat{\Omega}, \mathbf{E}'\to\mathbf{E})}{\Sigma_T(\mathbf{r}-R\hat{\Omega}, E')}\, \psi(\mathbf{r}-R\hat{\Omega}, \mathbf{E}')\right\}. \tag{7.3}$$

The purpose of a "reactor" calculation is then to find the eigenfunction, $\psi(\mathbf{r}, \mathbf{E})$, and the eigenvalue, k.

In the 05R neutron transport code [3], this problem is solved iteratively, each batch being one iteration. The source for the first batch, S_1, is chosen arbitrarily. From this source an estimate of the resulting collision density, ψ_1, is calculated from (7.2). The source for the next batch is S_2 as obtained from (7.1). To keep the number of

neutrons in each batch from multiplying or decreasing indefinitely, a normalization condition is imposed on each source.

$$\int S_n(\mathbf{r}, \mathbf{E})\, d\mathbf{r}\, d\mathbf{E} = \int S_1(\mathbf{r}, \mathbf{E})\, d\mathbf{r}\, d\mathbf{E} = N\,. \tag{7.4}$$

The weights of the source neutrons for batch 2 are adjusted to satisfy (7.4) and then an estimate of ψ_2 is obtained After several batches it is assumed that the source has "converged" and that from this point on ψ_n is an estimate of the eigenfunction ψ in (7.3). There are various methods which may be used to determine when "convergence" has been reached.

Once the eigenfunction has been obtained, an estimate of the criticality of the system,

$$k_n = \frac{\int \frac{\nu\Sigma_f(\mathbf{r}, E)}{\Sigma_T(\mathbf{r}, E)} \psi_n(\mathbf{r}, \mathbf{E})\, d\mathbf{r}\, d\mathbf{E}}{\int S_n(\mathbf{r}, \mathbf{E})\, d\mathbf{r}\, d\mathbf{E}}\,, \tag{7.5}$$

is calculated at the end of each batch. The final criticality factor is the mean value of k_n averaged over all batches calculated after convergence was achieved.

Eq. (7.2) is calculated by 05R in the same manner as it would be for non-fissioning systems. Here the fission cross section is treated as absorption in the scattering process and the neutron weights are reduced accordingly. k_n is estimated by summing a contribution

$$\frac{\nu\Sigma_f(\mathbf{r}, E)}{\Sigma_T(\mathbf{r}, E)} \cdot W_b$$

at every collision (W_b, the weight before collision, is an estimate of the collision density). Here $\nu\Sigma_f/\Sigma_T$ is a function of the *medium* in which the collision occurred and the contribution is scored regardless of whether the collision subsequently was determined to be a collision with a fissionable nuclide or not. At the end of the batch, k_n is divided by N, the total starting weight of the batch.

The source for the next batch is not obtained directly from the individual contributions $(\nu\Sigma_f/\Sigma_T)\cdot W_b$. Instead Russian Roulette and splitting are used to discretize these contributions into ones of equal value. The splitting and Russian Roulette parameters used are determined by an input quantity, FWLOW, the desired value of a single contribution. FWLOW should be set to the anticipated value of k, as this will keep the average number of pseudo-neutrons in each batch close to the initial number. At the start of the next batch, the neutron weights are renormalized so as to satisfy (7.4). Due to Russian Roulette, the renormalization factor will not be exactly equal to $1/k$.

Let us consider the eigenvalue equation (7.3) and try to write down a value equation adjoint to it. Let $W(\mathbf{r}, \mathbf{E})$ be the value of having a collision at $\mathbf{r}$ with energy $\mathbf{E}$. What is the value of this collision? First it may, with probability $[\Sigma_s(\mathbf{r}, E)/\Sigma_T(\mathbf{r}, E)]$ be a scattering. The expected number of neutrons which will emerge with energy in $d\mathbf{E}'$ about $\mathbf{E}'$ is $[\Sigma_s(\mathbf{r}, \mathbf{E}\to\mathbf{E}')/\Sigma_T(\mathbf{r}, E)]\, d\mathbf{E}'$. These neutrons will travel to $\mathbf{r}+R\hat{\Omega}'$ without collision with a probability $e^{-\beta^*(\mathbf{r}, R, \mathbf{E}')}$. The probability that they will have a collision in dR about $\mathbf{r}+R\hat{\Omega}'$ is $\Sigma_T(\mathbf{r}+R\hat{\Omega}', E')\, dR$. This collision will have a value $W(\mathbf{r}+R\hat{\Omega}', \mathbf{E}')$. The expected contribution to the value from scattering collisions is then

$$\int d\mathbf{E}' \frac{\Sigma_s(\mathbf{r}, \mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r}, E)} \int dR\, \Sigma_T(\mathbf{r}+R\hat{\Omega}', E')\, e^{-\beta^*(\mathbf{r}, R, \mathbf{E}')}\, W(\mathbf{r}+R\hat{\Omega}', \mathbf{E}')\,.$$

This is the same term as in the adjoint for a non-fissioning system. However, there is also a probability

$[\Sigma_f(\mathbf{r},E)/\Sigma_T(\mathbf{r},E)]$ that the collision will be a fission event. The expected number of neutrons emerging from fissions in $d\mathbf{E}'$ about $\mathbf{E}'$ is

$$\frac{\nu\Sigma_f(\mathbf{r},E)}{\Sigma_T(\mathbf{r},E)}\frac{f(E')}{4\pi}d\mathbf{E}'.$$

These neutrons will travel, etc. Thus the expected contribution to the value from fissions is

$$\frac{\nu\Sigma_f(\mathbf{r},E)}{\Sigma_T(\mathbf{r},E)}\int d\mathbf{E}'\frac{f(E')}{4\pi}\int dR\,\Sigma_T(\mathbf{r}+R\hat{\Omega}',E')\,e^{-\beta^*(\mathbf{r},R,\mathbf{E}')}\,W(\mathbf{r}+R\hat{\Omega}',\mathbf{E}').$$

However, these fissions produce neutrons for the succeeding generation. Due to renormalization of the source of the next generation, this term must be multiplied by a factor of $1/k$. Thus the eigenfunction equation for the value is

$$W(\mathbf{r},\mathbf{E})=\int d\mathbf{E}'\frac{\Sigma_s(\mathbf{r},\mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r},E)}\int dR\,\Sigma_T(\mathbf{r}+R\hat{\Omega}',E')\,e^{-\beta^*(\mathbf{r},R,\mathbf{E}')}W(\mathbf{r}+R\hat{\Omega}',\mathbf{E}')$$
$$+\frac{1}{k}\frac{\nu\Sigma_f(\mathbf{r},E)}{\Sigma_T(\mathbf{r},E)}\int d\mathbf{E}'\frac{f(E')}{4\pi}\int dR\,\Sigma_T(\mathbf{r}+R\hat{\Omega}',E')\,e^{-\beta^*(\mathbf{r},R,\mathbf{E}')}W(\mathbf{r}+R\hat{\Omega}',E'). \tag{7.6}$$

We can simplify somewhat by introducing

$$\chi^*(\mathbf{r},\mathbf{E})=\int dR\,\Sigma_T(\mathbf{r}+R\hat{\Omega},E)\;e^{-\beta^*(\mathbf{r},R,\mathbf{E})}\,W(\mathbf{r}+R\hat{\Omega},\mathbf{E})$$
$$=\int dR\,\Sigma_T(\mathbf{r}+R\hat{\Omega},E)\,e^{-\beta^*(\mathbf{r},R,\mathbf{E})}\left\{\int d\mathbf{E}'\frac{\Sigma_s(\mathbf{r}+R\hat{\Omega},\mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r}+R\hat{\Omega},E)}\chi^*(\mathbf{r}+R\hat{\Omega},\mathbf{E}')\right.$$
$$\left.+\frac{1}{k}\frac{\nu\Sigma_f(\mathbf{r}+R\hat{\Omega},E)}{\Sigma_T(\mathbf{r}+R\hat{\Omega},E)}\int d\mathbf{E}'\frac{f(E')}{4\pi}\chi^*(\mathbf{r}+R\hat{\Omega},\mathbf{E}')\right\}$$
$$=\int dR\,e^{-\beta^*(\mathbf{r},R,\mathbf{E})}\left\{\int d\mathbf{E}'\,\Sigma_s(\mathbf{r}+R\hat{\Omega},\mathbf{E}\to\mathbf{E}')\,\chi^*(\mathbf{r}+R\hat{\Omega},\mathbf{E}')\right.$$
$$\left.+\frac{1}{k}\nu\Sigma_f(\mathbf{r}+R\hat{\Omega},E)\int d\mathbf{E}'\frac{f(E')}{4\pi}\chi^*(\mathbf{r}+R\hat{\Omega},\mathbf{E}')\right\}.$$

This is the equation for the adjoint flux. To prepare for Monte Carlo solution we convert to the adjoint collision density

$$H(\mathbf{r},\mathbf{E})=\Sigma_T(\mathbf{r},E)\,\chi^*(\mathbf{r},-\mathbf{E}).$$

$$H(\mathbf{r},\mathbf{E})=\int dR\,\Sigma_T(\mathbf{r},E)\,e^{-\beta(\mathbf{r},R,\mathbf{E})}\left\{\int d\mathbf{E}'\frac{\Sigma_s(\mathbf{r}-R\hat{\Omega},\mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r}-R\hat{\Omega},E')}H(\mathbf{r}-R\hat{\Omega},\mathbf{E}')\right.$$
$$\left.+\frac{1}{k}\nu\Sigma_f(\mathbf{r}-R\hat{\Omega},E)\int d\mathbf{E}'\frac{f(E')}{4\pi\,\Sigma_T(\mathbf{r}-R\hat{\Omega},E')}H(\mathbf{r}-R\hat{\Omega},\mathbf{E}')\right\}. \tag{7.8}$$

The adjoint source term is

$$A(\mathbf{r},\mathbf{E}) = \frac{1}{k}\nu\Sigma_f(\mathbf{r},E)\int \mathrm{d}\mathbf{E}'\,\frac{f(E)}{4\pi\,\Sigma_T(\mathbf{r},E')}H(\mathbf{r},\mathbf{E}')$$

$$= \frac{1}{k}\,\frac{\nu\Sigma_f(\mathbf{r},E)}{4\pi\int \nu\Sigma_f(\mathbf{r},E'')\,\mathrm{d}E''}\int \mathrm{d}\mathbf{E}'\left\{\frac{f(E')\int \nu\Sigma_f(\mathbf{r},E'')\,\mathrm{d}E''}{\Sigma_T(\mathbf{r},E')}\right\}H(\mathbf{r},\mathbf{E}'), \tag{7.9}$$

where we have normalized $\nu\Sigma_f$ to make it a probability distribution for $\mathbf{E}$.

The adjoint solution is then obtained by arbitrarily choosing an initial source, $A_1(\mathbf{r},\mathbf{E})$, then cycling iteratively between

$$H(\mathbf{r},\mathbf{E}) = \int \mathrm{d}R\;\Sigma_T(\mathbf{r},E)\,\mathrm{e}^{-\beta(\mathbf{r},R,\mathbf{E})}\left\{A(\mathbf{r}-R\hat{\Omega},\mathbf{E}) + \int \mathrm{d}\mathbf{E}'\,\frac{\Sigma_s(\mathbf{r}-R\hat{\Omega},\mathbf{E}\to\mathbf{E}')}{\Sigma_T(\mathbf{r}-R\hat{\Omega},E')}H(\mathbf{r}-R\hat{\Omega},\mathbf{E}')\right\} \tag{7.10}$$

and (7.9). After several batches one assumes, as in the forward case, that the source has converged and one is estimating the eigenfunction, $H(\mathbf{r},\mathbf{E})$. At the end of each batch, one has for an estimate of k,

$$k_n = \frac{\int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{E}\,\dfrac{f(E)\int \nu\Sigma_f(\mathbf{r},E'')\,\mathrm{d}E''}{\Sigma_T(\mathbf{r},E)}H(\mathbf{r},\mathbf{E})}{\int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{E}A(\mathbf{r},\mathbf{E})}.$$

The adjoint fissioning system differs from the forward in that the scattering kernel has been reversed, i.e., we have $\Sigma_s(\mathbf{r},\mathbf{E}\to\mathbf{E}')$ instead of $\Sigma_s(\mathbf{r},\mathbf{E}'\to\mathbf{E})$, and that the fission cross section and the fission distribution have changed their roles. The adjoint-fission cross section is $f(E)\cdot\Sigma_F(\mathbf{r})$ while the energy distribution of adjunctons emerging from an adjoint-fission is $\nu\Sigma_f(\mathbf{r},E)/\Sigma_F(\mathbf{r})$ where

$$\Sigma_F(\mathbf{r}) = \int \nu\Sigma_f(\mathbf{r},E)\,\mathrm{d}E\,.$$

Other than these kernel reversals, which affect only the cross section quantities and source distribution input to the program, the 05R adjoint calculation proceeds exactly as in the forward case.

For fast reactors $[1/\Sigma_F(\mathbf{r})]\,\nu\Sigma_f(\mathbf{r},E)$ is a very poor source distribution for the adjoint. The vast majority of adjunctons will start at thermal energies and will escape before getting up in energy to a point where $f(E)$ is significantly greater than zero. The few adjunctons which do start at fast energies will cause large amounts of adjoint fissions since $[\Sigma_F(\mathbf{r})/\Sigma_T(\mathbf{r},E)]$ is a large number. This makes for extremely poor statistics. To correct it, one must bias the adjoint source distribution. Success has been achieved by using the forward power distribution as the adjoint source distribution.

8. Notation

$\varphi(\mathbf{r},\mathbf{E})\,\mathrm{d}\mathbf{E}$	= particle flux at space point $\mathbf{r}$ and in $\mathrm{d}\mathbf{E}$ about $\mathbf{E}$ (particles/cm^2-sec)
$\mathbf{E}$	= velocity variable denoting energy E and direction $\hat{\Omega}$
$\Sigma_T(\mathbf{r},E)$	= total cross section (cm^{-1})
$\Sigma_s(\mathbf{r},\mathbf{E}'\to\mathbf{E})$	= scattering cross section for change of $\mathbf{E}'$ to $\mathbf{E}$ (cm^{-1})
$S(\mathbf{r},\mathbf{E})$	= particle source density (particles/[cm^2-sec-MeV-st])
R	= length (cm)

x, y, z = Cartesian coordinates (cm)

$\beta(\mathbf{r}, R, \mathbf{E})$ = optical thickness of R (mean free paths)

$$= \int_0^R \Sigma_T(\mathbf{r} - R'\hat{\Omega}, E)\, dR'$$

$\psi(\mathbf{r}, \mathbf{E})$ = collision density of particles entering collisions at $\mathbf{r}$ and of velocity $\mathbf{E}$ (particles/[cm^3-sec-MeV-st])

$$= \Sigma_T(\mathbf{r}, E)\, \varphi(\mathbf{r}, \mathbf{E})$$

$\chi(\mathbf{r}, \mathbf{E})$ = density of emerging particles leaving a collision or a source at $\mathbf{r}$ with outgoing velocity $\mathbf{E}$

$T(\mathbf{r}', \mathbf{r}|\mathbf{E})$ = transport kernel denoting probability, given coordinates $\mathbf{r}', \mathbf{E}$ of suffering next collision at $\mathbf{r}$

$C(\mathbf{E}', \mathbf{E}|\mathbf{r})$ = collision kernel denoting probability, given a collision with coordinates $\mathbf{r}, \mathbf{E}'$, that velocity will change from $\mathbf{E}'$ to $\mathbf{E}$

$S_c(\mathbf{r}, \mathbf{E})$ = first collision source

$$= \int d\mathbf{r}'\, T(\mathbf{r}', \mathbf{r}|\mathbf{E})\, S(\mathbf{r}', \mathbf{E})$$

$f(\mu|E', \mathbf{r})$ = probability for scattering through the angle whose cosine is μ, for particles at $\mathbf{r}$ of velocity $\mathbf{E}'$

$f(\mathbf{E}' \to \mathbf{E}|\mathbf{r})$ = probability for scattering from $\mathbf{E}'$ to $\mathbf{E}$, given a collision at $\mathbf{r}$

$W(\mathbf{r}, \mathbf{E})$ = value of a particle of velocity $\mathbf{E}$ entering an event or collision at $\mathbf{r}$

$P(\mathbf{r}, \mathbf{E})$ = payoff or score for event of particle with velocity $\mathbf{E}$ at $\mathbf{r}$

λ = quantity of interest for final result of calculation

$\chi^*(\mathbf{r}, \mathbf{E})$ = value leaving a collision at $\mathbf{r}$ with outgoing velocity $\mathbf{E}$

$P_c(\mathbf{r}, \mathbf{E})$ = expected payoff for leaving a collision at $\mathbf{r}$ with outgoing velocity $\mathbf{E}$

$$= \int d\mathbf{r}'\, T(\mathbf{r}, \mathbf{r}'|\mathbf{E})\, P(\mathbf{r}', E)$$

$\varphi^*(\mathbf{r}, \mathbf{E})$ = adjoint (or adjuncton) flux

$= \chi^*(\mathbf{r}, \mathbf{E})$, value of particle leaving collision

adjunctons = fictitious particles assumed to be transported by process defined by adjoint transport equation

$H(\mathbf{r}, \mathbf{E})$ = adjuncton collision density

$$= \Sigma_T(\mathbf{r}, E)\, \varphi^*(\mathbf{r}, \mathbf{E})$$

$A(\mathbf{r}, \mathbf{E})$ = adjuncton source density

$$= \Sigma_T(\mathbf{r}, E)\, P(\mathbf{r}, E)$$

$f(E)$ = fission neutron energy distribution

ν = number of neutrons emitted per fission

$\Sigma_f(\mathbf{r}, E)$ = fission neutron cross section (cm^{-1})

k_n = criticality or multiplication factor observed for a batch of case histories, n

$f(E)\, \Sigma_F(\mathbf{r})$ = adjoint fission cross section

$\Sigma_F(\mathbf{r})$ $= \int \nu\, \Sigma_f(\mathbf{r}, E)\, dE$

Appendix 1. Recapitulation of equations for the "quantity of interest" λ

If the quantity which you desire to calculate is written, in the forward form as,

$$\lambda = \int \mathrm{dr}\,\mathrm{dE}\,P(\mathbf{r},\mathrm{E})\,\psi(\mathbf{r},\mathrm{E}) = \int \mathrm{dr}\,\mathrm{dE}\,\{P(\mathbf{r},\mathrm{E})\,\Sigma_{\mathrm{T}}(\mathbf{r},E)\}\,\varphi(\mathbf{r},\mathrm{E}) = \int \mathrm{dr}\,\mathrm{dE}\,A(\mathbf{r},-\mathrm{E})\,\varphi(\mathbf{r},\mathrm{E}).$$

Then we know that

$$\lambda = \int \mathrm{dr}\,\mathrm{dE}\,S_{\mathrm{c}}(\mathbf{r},\mathrm{E})\,W(\mathbf{r},\mathrm{E}) = \int \mathrm{dr}\,\mathrm{dE}\,S(\mathbf{r},\mathrm{E})\,\chi^{*}(\mathbf{r},\mathrm{E}) = \int \mathrm{dr}\,\mathrm{dE}\,\frac{S(\mathbf{r},\mathrm{E})}{\Sigma_{\mathrm{T}}(\mathbf{r},E)}\,H(\mathbf{r},-\mathrm{E})$$

$$= \int \mathrm{dr}\,\mathrm{dE}\left\{\frac{S(\mathbf{r},-\mathrm{E})}{\Sigma_{\mathrm{T}}(\mathbf{r},E)}\right\}H(\mathbf{r},\mathrm{E}).$$

Note: For those of you who are pleased by symmetry, please notice that

$$\lambda = \int (\text{adjuncton source})^{*}(\text{particle flux}) = \int (\text{particle source})^{*}(\text{adjuncton flux}).$$

Appendix 2. A note on the reversal of direction (equation 6.1) for adjunctons

The reversal of $\hat{\Omega}$ between particles and adjunctons is usually no problem and we just "instinctively" handle things properly. For example, if we are scoring particles as they cross a boundary going outward, then we naturally and without thinking about it start adjunctons going inward. Likewise we intuitively score adjunctons for entering a volume from which our source particles are emerging. Also, many sources and payoffs are isotropic, making the reversal of direction an academic point. However, in dealing with a case where either the source or the payoff has a complex directional behavior, intuition is likely to fail us unless the point is reiterated. Therefore, remember that the adjoint source

$$A(\mathbf{r},E,\hat{\Omega}) = \Sigma_{\mathrm{T}}(\mathbf{r},E)\,P(\mathbf{r},\mathrm{E},-\hat{\Omega})$$

and that the contribution from an adjuncton collision at $\mathbf{r}$ with incoming energy E and incident direction $\hat{\Omega}$ is

$$\frac{S(\mathbf{r},E,-\hat{\Omega})}{\Sigma_{\mathrm{T}}(\mathbf{r},E)}.$$

Appendix 3. A note on source distributions for adjunctons

Let us consider the estimation of the flux at a point, integrated over angle and over a detector response that depends on energy. Thus we are interested in

$$\lambda = \int \varphi(\mathbf{r}_0,\mathrm{E})\,\mathrm{d}(E)\,\mathrm{dE} = \int \mathrm{dE}\,\mathrm{dr}\,\{\mathrm{d}(E)\,\delta(\mathbf{r}-\mathbf{r}_0)\}\,\varphi(\mathbf{r},\mathrm{E}) = \int \mathrm{dE}\,\mathrm{dr}\left\{\frac{\mathrm{d}(E)\,\delta(\mathbf{r}-\mathbf{r}_0)}{\Sigma_{\mathrm{T}}(\mathbf{r}_0,E)}\right\}\psi(\mathbf{r},\mathrm{E}).$$

This, of course, is not the payoff we would use in solving by forward Monte Carlo. Rather than wait for a collision to occur at $\mathbf{r}_0$ and then adding a contribution of $[\mathrm{d}(E)/\Sigma_{\mathrm{T}}(\mathbf{r}_0,E)]$, we would use "statistical estimation". At each collision point, we would calculate the probability for scattering into the correct angle, $\hat{\Omega}$, that will take us to

the detector, throw in a factor of $1/R^2$ for the angle subtended by unit detector area, multiply by the probability of reaching the detector, and by the detector response. Thus our payoff would be

$$\frac{\Sigma_s(\mathbf{r}, \mathbf{E}\to \mathbf{E}_1)}{\Sigma_T(\mathbf{r}, E)} \cdot \frac{1}{|\mathbf{r}_0 - \mathbf{r}|^2} \cdot \exp\left[- \int_0^{|\mathbf{r}_0 - \mathbf{r}|} \Sigma_T(\mathbf{r} + R\hat{\Omega}_1, E_1) dR \right] d(E_1) ,$$

where $\hat{\Omega}_1$ is the direction from $\mathbf{r}$ to $\mathbf{r}_0$ and E_1 is the energy resulting from the scattering from $\hat{\Omega}$ to $\hat{\Omega}_1$. [To this we would have to add an uncollided flux contribution.] However, in solving this problem by adjoint Monte Carlo we would be wasting our time if we tried to choose our adjunctons from the source distribution

$$\frac{\Sigma_s(\mathbf{r}, -\mathbf{E}\to \mathbf{E}_1)}{|\mathbf{r}_0 - \mathbf{r}|^2} \exp\left[- \int_0^{|\mathbf{r}_0 - \mathbf{r}|} \Sigma_T(\mathbf{r} + R\hat{\Omega}_1, E_1) dR \right] d(E_1) .$$

Instead we should go back to the hypothetical payoff, $[d(E)\, \delta(\mathbf{r} - \mathbf{r}_0)/\Sigma_T(\mathbf{r}_0, E)]$, the one we would never use in a forward Monte Carlo. This would give us, as an adjuncton source, an isotropic point source with energy spectrum $d(E)$.

The reverse will happen as we consider the particle source. Monodirectional, mono-energetic point sources are the easiest sources to use in a forward Monte Carlo. They are, of course, the worst possible function to have in scoring adjoint histories. In such a case it would be necessary to use adjoint statistical estimation to calculate the result.

Appendix 4. Equivalence of equations (4.7) and (4.3)

Let

$$\lambda = \iint d\mathbf{r}\, d\mathbf{E}\, \chi(\mathbf{r}, \mathbf{E}) P_c(\mathbf{r}, \mathbf{E})$$

$$= \iint d\mathbf{r}\, d\mathbf{E}\, \chi(\mathbf{r}, \mathbf{E}) \int d\mathbf{r}' \frac{\delta\left(\frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|} \cdot \hat{\Omega} - 1 \right)}{|\mathbf{r}' - \mathbf{r}|^2} \Sigma_T(\mathbf{r}', E) \exp\left[- \int_{\mathbf{r}\to\mathbf{r}'} \Sigma_T(\mathbf{r}'', E)\, ds \right] P(\mathbf{r}', \mathbf{E}) .$$

Interchanging the order of integration

$$= \int d\mathbf{E}\, d\mathbf{r}'\, P(\mathbf{r}', \mathbf{E}) \int d\mathbf{r} \frac{\delta\left(\frac{\mathbf{r}' - \mathbf{r}}{|\mathbf{r}' - \mathbf{r}|^2} \cdot \hat{\Omega} - 1 \right)}{|\mathbf{r}' - \mathbf{r}|^2} \Sigma_T(\mathbf{r}', E) \exp\left[- \int_{\mathbf{r}-\mathbf{r}'} \Sigma_T(\mathbf{r}'', E) ds \right] \chi(\mathbf{r}, \mathbf{E}) .$$

Now we interchange the dummy variables of integration, $\mathbf{r}$ and $\mathbf{r}'$

$$= \int d\mathbf{E}\, d\mathbf{r}\, P(\mathbf{r}, \mathbf{E}) \int d\mathbf{r}' \frac{\delta(\widehat{(\mathbf{r} - \mathbf{r}')} \cdot \hat{\Omega} - 1)}{|\mathbf{r} - \mathbf{r}'|^2} \Sigma_T(\mathbf{r}, E) \exp\left[- \int_{\mathbf{r}'\to\mathbf{r}} \Sigma_T(\mathbf{r}'', E) ds \right] \chi(\mathbf{r}', \mathbf{E})$$

$$= \int d\mathbf{E}\, d\mathbf{r}\, P(\mathbf{r}, \mathbf{E})\, \psi(\mathbf{r}, \mathbf{E}) .$$

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