Chapter 19

MATHEMATICAL FORMULATION OF PARTICLE TRANSPORT IN MONTE CARLO THEORY

10/30/2013

19.1 INTRODUCTION

A mathematical formulation of particle transport using the Monte Carlo method is exposed. It is recognized that the Monte Carlo method being primarily a numerical integration methods is best applied within the context of an integral formulation of the transport equation rather than an integro-differential form. The term *particle* is general and refers to neutral or charged particles, gas or fluid molecules or photons. Even though Monte Carlo can treat non-linear systems, we consider here the linear form of the Boltzmann's transport equation for ease of exposition. Introducing nonlinearity can be done in the course of the simulation process.

19.2 THE BOLTZMANN EQUATION FOR PARTICLE TRANSPORT

The Boltzmann equation is used to describe the motion of the following particles or pseudo particles: neutrons, photons, fluid or gas molecules, ions and electrons, phonons, and even motor cars in a traffic situation. The underlying assumptions for its use in neutron and gamma rays transport will be discussed here.

The equation was first published in 1872 by Boltzmann as a particle balance for the distribution function:

$$n(\bar{v}, \bar{r}, t)$$

where:

$$n(\bar{v}, \bar{r}, t) d\bar{v} d\bar{r}$$

is the average number of particles in the volume element $d\bar{r}$ about $\bar{r}$ with velocities in the range $(\bar{v}, \bar{v} + d\bar{v})$, at time t:

$$\frac{\partial n}{\partial t} + \bar{v}.\nabla_r n + \bar{a}.\nabla_v n = C(n,n) \qquad (1)$$

where: $\bar{a} = \frac{\bar{F}}{m}$ is the acceleration vector due to the force $\bar{F}$,

The left hand side represents losses from a unit volume of phase space due to the applied forces and gradients in density. The right hand side is a term whose presence attempts to restore the thermal equilibrium destroyed by the loss terms in the left hand side.

C(n, n) is a collision term which is nonlinear in n and assumes that the molecular chaos hypothesis or Stosszahlansatz is valid. This means that there exists no correlation between the velocities and positions at collisions. This consequently reduces the equation to the consideration of "mean values" only.

In general, several particles are interacting and there will be a particle distribution function for each species, which leads to a set of coupled equations:

$$\frac{\partial n_i}{\partial t} + \bar{v}.\nabla_r n_i + \bar{a}.\nabla_v n_i = \sum_{j=1}^{N} C_{ij}(n_i, n_j) + \sum_{j=1}^{N} S_{ij}(n_i, n_j),\ i = 1, 2, \ldots, N \qquad (2)$$

where: $C_{ij}(n_i, n_j)$ is the collision term between particles i and j,

$S_{ij}(n_i, n_j)$ accouts for sources and sinks of particles.

This equation is general, but is normally simplified for the different situations at hand. As a special case for nuclear applications we can make the following assumptions:

a. We regard the neutrons and the nuclei of the medium with which they interact as a mixture of two gases.
b. The force terms which could be magnetic, electrical, gravitational or inertial are considered negligible for the problems under consideration.

These simplifications lead to the equations:

$$\begin{aligned} &\frac{\partial n}{\partial t} + \bar{v}.\nabla n = C_{nn}(n,n) + C_{nM}(n,M) + S_{nn}(n,n) + S_{nM}(n,M) \\ &\frac{\partial M}{\partial t} + \bar{V}.\nabla M = C_{MM}(M,M) + C_{nM}(n,M) + S_{MM}(M,M) + S_{nM}(n,M) \end{aligned} \qquad (3)$$

where: n refers to the neutron density function,

M refers to the medium density function.

If we further consider that:

c. The neutron particle density n is about 10^{10} [particles/cm^3] which is much smaller than the medium atomic density M= 10^{22} [nuclei/cm^3], so that we can neglect n with respect to M.

Thus:

$$\frac{\partial n}{\partial t} + \bar{\mathrm{v}}.\nabla n = C_{nM}(n,M) + S_{nM}(n,M)$$
$$\frac{\partial M}{\partial t} + \bar{V}.\nabla M = C_{MM}(M,M) + S_{MM}(M,M) \qquad (4)$$

19.3 INTEGRO-DIFFERENTIAL FORM OF THE BOLTZMANN EQUATION

Still further simplification can be achieved if we consider that:

c. The atoms of the medium are in thermal equilibrium, or that their distribution function M is known,

then we can accept the neutron density equation as a linear equation in n.

The collision term $C_{nM}(n,M)$ which represents the scattering in and out of the velocity range $(\bar{\mathrm{v}}, \bar{\mathrm{v}} + d\bar{\mathrm{v}})$ can be written as:

$$C_{nM}(n,M) = \int K(\bar{\mathrm{v}}' \to \bar{\mathrm{v}}) n(\bar{\mathrm{v}}', \bar{r}, t) d\bar{\mathrm{v}}' - \mathrm{v}\sum\nolimits_s(\mathrm{v}) n(\bar{\mathrm{v}}, \bar{r}, t) \qquad (5)$$

where: $K(\bar{\mathrm{v}}' \to \bar{\mathrm{v}})$ is the neutron-nucleus scattering kernel,
$\sum_s(\mathrm{v})$ is the total scattering cross section defined as:

$$\mathrm{v}\sum\nolimits_s(\mathrm{v}) = \int K(\bar{\mathrm{v}}' \to \bar{\mathrm{v}}) d\bar{\mathrm{v}}' \qquad (6)$$

The source term $S_{nM}(n,M)$ can be written as:

$$S_{nM}(n,M) = Q + S_f + S_a \qquad (7)$$

where: Q is an external source term,
S_a is a negative source term representing absorptions:

$$S_a = -\mathrm{v}\sum\nolimits_a(\mathrm{v}) n(\bar{\mathrm{v}}, \bar{r}, t),$$

S_f is a fission source term:

$$S_f = (1-\beta)\frac{\chi_p(\mathrm{v})}{4\pi}\int \bar{\nu}\,\mathrm{v}\sum\nolimits_f(\mathrm{v}) n(\bar{\mathrm{v}}, \bar{r}, t) d\bar{\mathrm{v}} + \frac{1}{4\pi}\sum_i \lambda_i \Lambda_i(\bar{r}, t)\chi_i(\mathrm{v}) \qquad (8)$$

$\sum_f(\mathrm{v})$ is the fission cross section,

λ_i is the decay constant for the delayed neutrons whose precursor concentration is $\Lambda_i(\bar{r},t)$,

$\bar{\nu}$ is the mean number of neutrons per fission,

$\chi_p(\mathrm{v})$ is the fission spectrum of prompt neutrons,

$\chi_i(\mathrm{v})$ is the fission spectrum of the i-th delayed neutron group, with:

$$\frac{d\Lambda_i(\bar{r},t)}{dt} = -\lambda_i\Lambda_i(\bar{r},t) + \beta_i \int \bar{\nu}\mathrm{v}\sum\nolimits_f(\mathrm{v})n(\bar{\mathrm{v}},\bar{r},t)d\bar{\nu}, \qquad (9)$$

$$\beta = \sum_i \beta_i ,$$

where: β_i is the fraction in the i-th delayed group from fission.

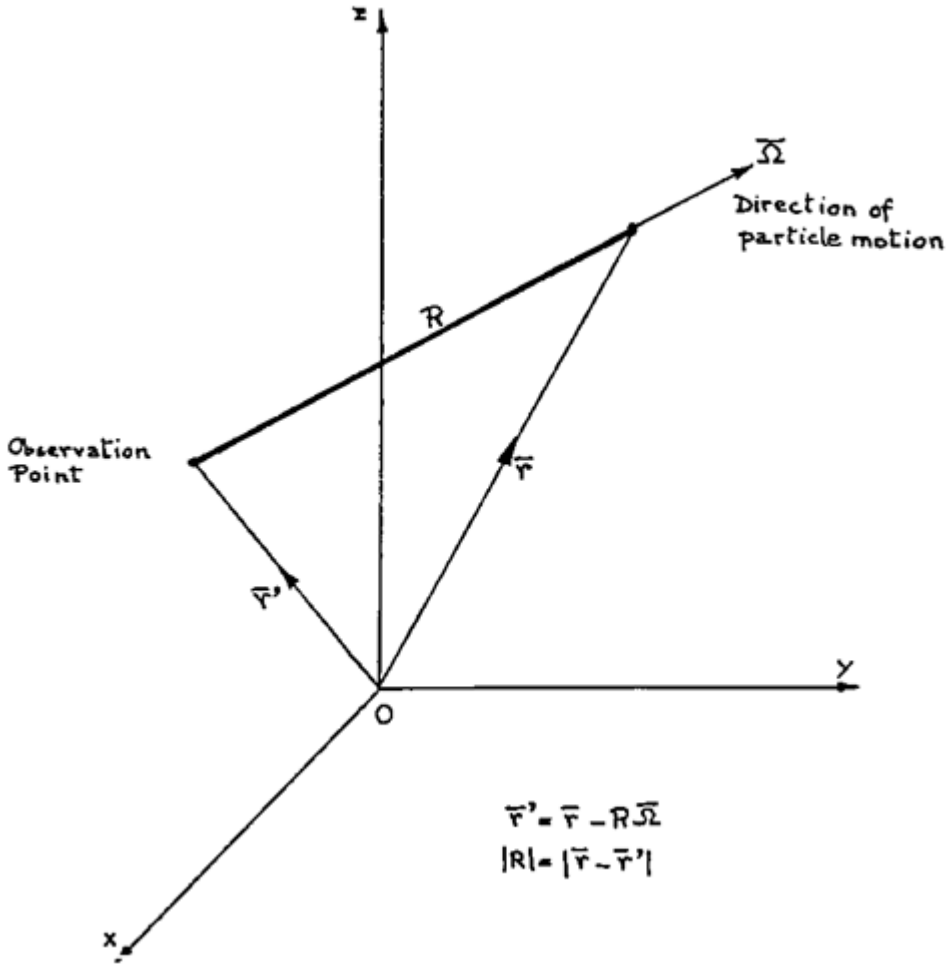

Figure 1. Coordinate System for particle transport.

It is noticed that the moderator atom distribution M is included in the definition of the macroscopic cross sections $\sum_a(\mathrm{v})$ and $\sum_f(\mathrm{v})$:

$$\begin{aligned} \mathrm{v}\sum\nolimits_f(\mathrm{v}) &= \int M(V)\left|\bar{\mathrm{v}}-\bar{V}\right|\sigma_f(\left|\bar{\mathrm{v}}-\bar{V}\right|)d\bar{\mathrm{v}}, \\ \mathrm{v}\sum\nolimits_a(\mathrm{v}) &= \int M(V)\left|\bar{\mathrm{v}}-\bar{V}\right|\sigma_a(\left|\bar{\mathrm{v}}-\bar{V}\right|)d\bar{\mathrm{v}}. \end{aligned} \qquad (10)$$

This leads to Doppler broadening in the case of a resonance-type cross section.

With some further manipulations, the time independent integro-differential form of the transport equation for the neutron density can be written; as a function of particle energy, rather than velocity:

$$\hat{\Omega}.\nabla\phi(\bar{r},\bar{E})\sum\nolimits_T(\bar{r},E)\phi(\bar{r},\bar{E}) = S(\bar{r},\bar{E}) + \int\sum\nolimits_s(\bar{r},\bar{E}'\to\bar{E})\phi(\bar{r},\bar{E}')d\bar{E}' \qquad (11)$$

where: $\phi(\bar{r},\bar{E}) = \mathrm{v}n(\bar{r},\bar{\mathrm{v}},t)$ is the particle angular flux,

$\sum_T(\bar{r},E) = \sum_s(\bar{r},E) + \sum_a(\bar{r},E)$ is the total macroscopic cross section, including fission,

Σ_s, Σ_a are the scattering and absorption macroscopic cross sections, respectively,

$\bar{E}$ is the shorthand for $(E,\hat{\Omega})$

$d\bar{E}$ denotes $dEd\hat{\Omega}$,

$\hat{\Omega}$ is a unit vector in the direction in the direction of particle motion,

$S(\bar{r},\bar{E}) = Q + S_f$ is an external Q and fission S_f source density.

The geometry of the system is shown in Fig. 1.

19.4 INTEGRAL FORM OFTHE BOLTZMANN EQUATION FOR PARTICLE TRANSPORT

The integro-differential form of the Boltzmann equation can be converted to an integral form that is more suitable for Monte Carlo simulations as:

$$\begin{aligned} \phi(\bar{r},\bar{E}) &= \int_0^\infty e^{-\int_0^R\sum_T(\bar{r}-R'\hat{\Omega},E)dR'}\,dR.[S(\bar{r}-R\hat{\Omega},E) + \int\sum\nolimits_s(\bar{r}-R\hat{\Omega},\bar{E}'\to\bar{E})\phi(\bar{r}-R\hat{\Omega},\bar{E}')d\bar{E}' \\ \bar{r}' &= \bar{r} - R\hat{\Omega} \\ R &= \left|\bar{r}-\bar{r}'\right| \end{aligned} \qquad (12)$$

This integral form recognizes the Monte Carlo method as a numerical integration method, and is the most suitable for such an analysis.

19.5 COLLISION RATE DENSITY FORMS OF THE BOLTMANN EQUATION

We define the optical distance, or distance in number of mean free paths as:

$$\beta(\bar{r}, R, \bar{E}) = \int_0^R \sum\nolimits_T (\bar{r} - R'\hat{\Omega}, E) dR' \tag{13}$$

and two types of collision densities:

a. The density of particles entering a collision per unit time at $\bar{r}$ with *incoming* velocity $\bar{E}$; thus it is referred to as the "collision rate density" :

$$\psi(\bar{r}, \bar{E}) = \sum\nolimits_T (\bar{r}, \bar{E}).\phi(\bar{r}, \bar{E}) \tag{14}$$

b. The density of particles leaving a collision per unit time or a source at $\bar{r}$ with *outgoing* velocity $\bar{E}$:

$$\chi(\bar{r}, \bar{E}) = S(\bar{r}, \bar{E}) + \int \sum\nolimits_s (\bar{r}, \bar{E}' \to \bar{E}).\phi(\bar{r}, \bar{E}')d\bar{E}' \tag{15}$$

From Eqn. 12 for $\phi(\bar{r}, \bar{E})$ we get the integral forms for the ingoing and the outgoing collision rate densities as:

$$\psi(r, E) = \int \sum\nolimits_T (\bar{r}, \bar{E}) e^{-\beta(\bar{r}, R, \bar{E}')} dR.[S(\bar{r} - R\hat{\Omega}, \hat{E}) + \int \frac{\sum_s (\bar{r} - R\hat{\Omega}, \bar{E}' \to \bar{E})}{\sum_T (\bar{r} - R\hat{\Omega}, \bar{E}')} \psi(\bar{r} - R\hat{\Omega}, \bar{E}')d\bar{E}' \tag{16}$$

$$\chi(r, E) = S(\bar{r}, \bar{E}) + \int \frac{\sum_s (\bar{r} - R\hat{\Omega}, \bar{E}' \to \bar{E})}{\sum_T (\bar{r} - R\hat{\Omega}, \bar{E}')} d\bar{E}'.\int e^{-\beta(\bar{r}, R, \bar{E}')} \sum\nolimits_T (\bar{r}, \bar{E}')\chi(\bar{r} - R\hat{\Omega}, \bar{E}')dR \tag{17}$$

19.6 KERNEL FORMS OF THE INTEGRAL TRANSPORT EQUATIONS

By transforming the transport equation into a three dimensional form, setting:

$$R\hat{\Omega} = \bar{r} - \bar{r}' \quad , \quad R = |\bar{r} - \bar{r}'|$$

$$d\bar{r}' = R^2 dR d\hat{\Omega} \quad , \quad \hat{\Omega}'.\hat{\Omega} = \frac{\bar{r} - \bar{r}'}{|\bar{r} - \bar{r}'|}.\hat{\Omega}$$

and introducing the *transport kernel*:

$$T(\bar{r}',\bar{r}\mid\bar{E})=\sum\nolimits_T(\bar{r},E).e^{\int_{\bar{r}'\to\bar{r}}\sum_T(\bar{r}'',E)ds}.\frac{\delta(\hat{\Omega}.\frac{(\bar{r}-\bar{r}')}{|\bar{r}-\bar{r}'|}-1)}{|\bar{r}-\bar{r}'|^2}, \tag{18}$$

and the *collision kernel*:

$$C(\bar{E}',\bar{E}\mid R)=\frac{\sum_s(\bar{r},\bar{E}'\to\bar{E})}{\sum_T(\bar{r},\bar{E}')} \tag{19}$$

where: $\int_{\bar{r}'\to\bar{r}}\sum_T(\bar{r}'',E)ds$, is the integral of Σ_T along the line from $\bar{r}'$ to $\bar{r}$.

The ingoing collision rate density can be written in the following simple form:

$$\psi=S_c+(TC)\psi \tag{20}$$

where:

$$S_c(\bar{r},\bar{E})=\int T(\bar{r}',\bar{r}\mid E)S(\bar{r}',\bar{E})dr'=TS \tag{21}$$

is the first collision source, or a source whose particles have been transported once but not yet collided.

The outgoing collision rate density can be written in the simple form:

$$\chi=S+(CT)\chi \tag{22}$$

The flux equation is expressed in a more complicated manner:

$$\phi(\bar{r},\bar{E})=\frac{S_c(\bar{r},\bar{E})}{\sum_T(\bar{r},E)}+\iint\frac{\sum_T(\bar{r}',E')}{\sum_T(\bar{r},E)}T(\bar{r}',\bar{r}\mid E).C(\bar{E}',\bar{E}\mid r').\phi(\bar{r}',\bar{E}')d\bar{r}'d\bar{E}' \tag{23}$$

It can be observed that Monte Carlo simulations fundamentally estimate collision rate densities either outgoing or ingoing, and that the flux is an estimated derived quantity where the ingoing collision density is divided into the total cross section.

19.7 NEUMANN SERIES SOLUTION FOR THE INGOING COLLISION RATE DENSITY

Using matrix notation for Eqn. 20, and considering the transport operator T and collision operator C as matrix operators and rearranging, we get:

$$\begin{aligned} \psi &= S_c + (TC)\psi, \\ \psi - (TC)\psi &= S_c, \\ [I - (TC)]\psi &= S_c \end{aligned} \tag{24}$$

where I is a unit matrix operator.

Premultiplying by the inverse in Eqn. 24 we get:

$$\begin{aligned} [I - (TC)]^{-1}.[I - (TC)]\psi &= [I - (TC)]^{-1}.S_c \\ I.\psi &= \frac{I}{I - (TC)}.S_c \end{aligned} \tag{25}$$

Using the expansion:

$$\frac{1}{1-x} = 1 + x^2 + x^3 + \ldots \quad , \quad \forall x < 1, \tag{26}$$

Eqn. 25 yields the Neumann series expansion for the ingoing collision density:

$$\begin{aligned} \psi &= [I + (TC) + (TC)^2 + \ldots \ ].S_c \\ &= S_c + (TC)S_c + (TC)^2 S_c + \ldots \quad , \quad \forall \ \rho(TC) < 1. \end{aligned} \tag{27}$$

where the spectral radius of (TC) is less than unity.

19.8 NEUMANN SERIES SOLUTION FOR THE OUTGOING COLLISION RATE DENSITY

Using matrix notation for Eqn. 22, and considering the transport operator T and collision operator C as matrix operators and rearranging, we get:

$$\begin{aligned} \chi &= S + (CT)\chi, \\ \chi - (CT)\chi &= S, \\ [I - (CT)]\chi &= S \end{aligned} \tag{28}$$

where I is a unit matrix operator.

Premultiplying by the inverse in Eqn. 28 we get:

$$\begin{aligned} [I - (TC)]^{-1}.[I - (TC)]\psi &= [I - (TC)]^{-1}.S_c \\ I.\psi &= \frac{I}{I - (TC)}.S_c \end{aligned} \tag{29}$$

Using the expansion of Eqn. 26, Eqn. 25 yields the Neumann series expansion for the outgoing collision rate density:

$$\chi = [I + (CT) + (CT)^2 + \ldots \ ].S$$
$$= S + (CT)S + (CT)^2 S + \ldots \quad , \quad \forall \ \rho(CT) < 1. \tag{30}$$

Notice the actual physical source S appears in the solution for the outgoing collision density, whereas the first transported source S_c = (TS) appears in the solution for the ingoing collision density. Also notice the order of the transport operator as (CT) in the outgoing collision density solution, and (TC) in the ingoing collision density solution.

19.9 PROCEDURE FOR MONTE CARLO SIMULATION OF THE BOLTZMANN EQUATION: COLLISION RATE DENSITY ESTIMATION

The following flow chart shown in Fig. 2 outlines the procedure for the Monte Carlo simulation of the Boltzmann equation. This procedure actually corresponds to the calculation of estimates for the Neumann series terms for the integral form of the transport equation.

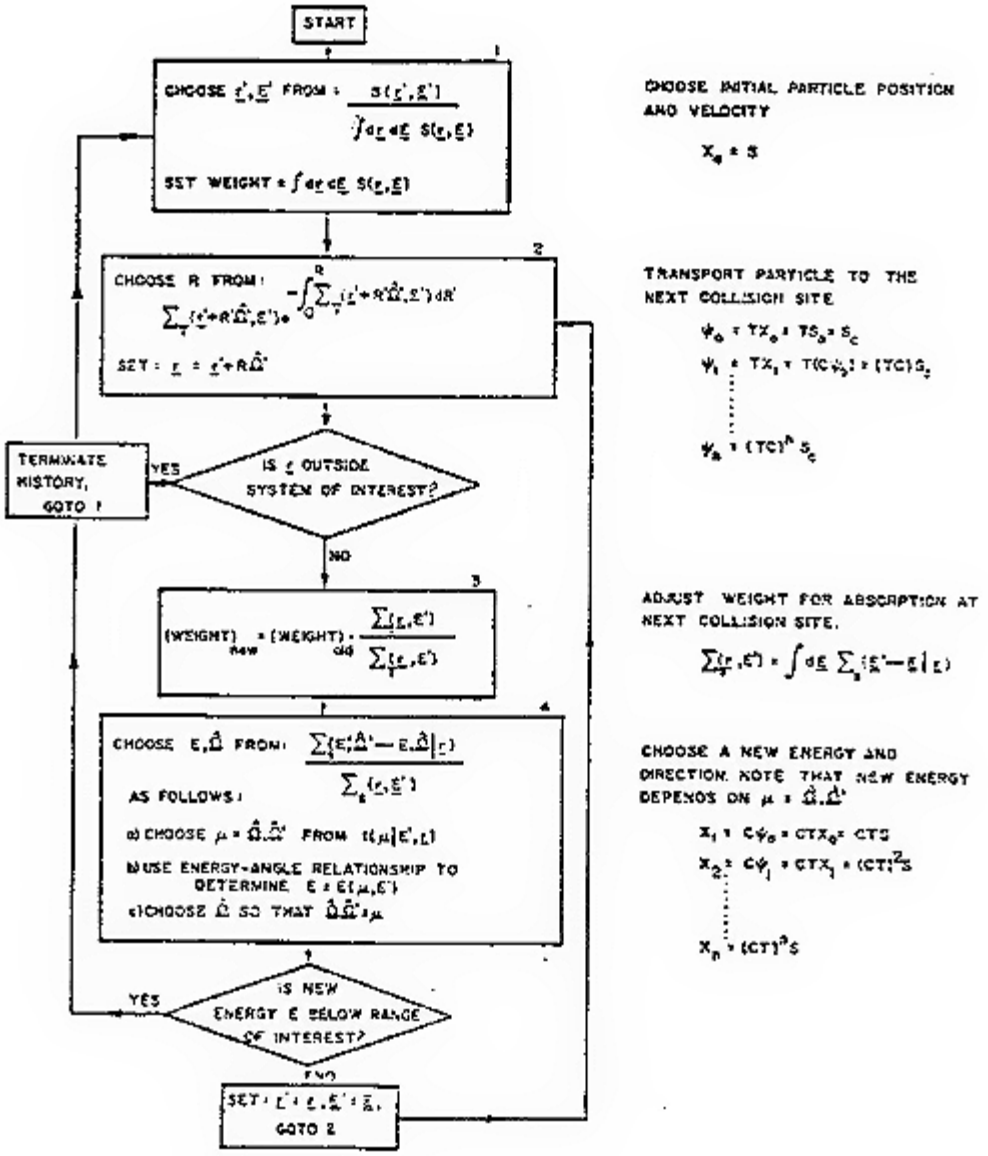

Figure 2. Procedure for estimation of ingoing and outgoing collision densities. Source: Oak Ridge National Laboratory (ORNL).

Step 1 yields: $\chi_0 = S$,

which corresponds to sampling the actual physical source.

Step 2 yields: $\psi_0 = T\chi_0 = TS$,

which corresponds to transporting the physical source one step, or generating the first transported source.

There is no statistical weight factor adjustment during the transport process, which moves the particle from one point to another according to the sampling of the transport

kernel T. This is so because both the source and the transport kernel are normalized to unity. In fact, for a finite size system, the transport kernel is normalized to less than unity, but this is accounted for by the termination of those particle histories which escape from the system. An alternative approach worth investigating is to prohibit escape from the system and use a weight factor.

A method of terminating the particle histories such as Russian Roulette would then need to be used to terminate the particle histories.

Step 3 and 4 yield: $\chi_1 = C\psi_0$

We return iteratively to step 2 to calculate:

Step 2 yields: $\psi_n = T\chi_n$,

Step 3 and 4 yield: $\chi_{n+1} = C\psi_n$.

Final estimates of the solution can be obtained as follows:

a. By summing all particle statistical weights at the beginning of step 2, we obtain:

$$\chi = S + \sum_{i=1}^{N} \chi_n \tag{31}$$

where N is the number of collisions undergone by the particle in the medium, or the number of Neumann series terms generated in a given history.

b. By summing all particle statistical weights at the beginning of step 3, we get:

$$\psi = S_c + \sum_{i=1}^{N} \psi_n \tag{32}$$

c. An estimate of the flux can be obtained by dividing the ingoing collision density by the total macroscopic cross section as:

$$\phi = \frac{\psi}{\Sigma_T} = \frac{S_c}{\Sigma_T} + \frac{1}{\Sigma_T} \sum_{i=1}^{N} \psi_n \tag{33}$$

19.10 THE VALUE OR IMPORTANCE EQUATION FOR COLLISION RATE DENSITIES AND RECIPROCITY RELATIONS

We define $\psi^{\dagger}(\bar{r}, \bar{E})$ to be the *value* of an event or collision at point $\bar{r}$ for a particle *entering* the collision with energy $\bar{E}$. We can write the following equation, which is adjoint to the collision density Eqn. 20:

$$\begin{aligned}\psi^{\dagger} &= S^{\dagger} + (TC)^{\dagger}\psi^{\dagger} \\ &= S^{\dagger} + (C^{\dagger}T^{\dagger})\psi^{\dagger}\end{aligned} \tag{34}$$

where: $S^{\dagger}$ is the immediate payoff at entering a collision.

If F is some linear functional:

$$F = <\psi, S^{\dagger}> \tag{35}$$

where: < , > denotes an inner product, we also have:

$$F = <\psi^{\dagger}, S_c>. \tag{36}$$

We similarly can define the value or importance at leaving a collision, which yields an equation adjoint to that for χ:

$$\begin{aligned}\chi^{\dagger} &= S_c{}^{\dagger} + (CT)^{\dagger}\chi^{\dagger} \\ &= S_c{}^{\dagger} + (T^{\dagger}C^{\dagger})\chi^{\dagger} \\ &where:\ S_c{}^{\dagger} = T^{\dagger}S^{\dagger}\end{aligned} \tag{37}$$

We thus have two additional equations for the functional F, which are equivalent to those already obtained; yielding the following reciprocity relations:

$$F = <\psi, S^{\dagger}> = <\psi^{\dagger}, S_c> = <\chi, S_c{}^{\dagger}> = <\chi^{\dagger}, S> \tag{38}$$

This is the quantity that is normally estimated in Monte Carlo simulations describing detector responses or reaction rates.

19.11 DISCUSSION

We use position, energy, direction and time to specify the random walk that describes successive observations of particles or radiation interacting with matter. The linear Boltzmann equation in its integral form represents this process and is in fact a Fredholm equation of the second type.

Any average quantity of interest that derives from particle transport can be obtained by an inner product or average:

$$F = <\psi, S^{\dagger}> = \iiint S^{\dagger}(\bar{r}, \bar{E}, t)\psi(\bar{r}, \bar{E}, t)d\bar{r}d\bar{E}dt \tag{39}$$

where the detector $S^{\dagger}$ response is related to both the medium and the nature of the quantity to be determined.

A great deal of effort is spent in the formulation of the detector response $S^{\dagger}$ that allows results of practical scientific and engineering interest to be computed efficiently.