

CHAPTER 3 BOLTZMANN TRANSPORT EQUATION

The Boltzmann transport equation is a conservation equation of particles in space. It is simply a bookkeeping process of particles in the phase space. One of the forms of this equation is the "integral emergent particle density equation", which is best suited for use in the random walk process. This equation is expressed as:

$$\chi(\mathbf{r}, E, \Omega, t) = S_g(\mathbf{r}, E, \Omega, t) + C(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) T(\mathbf{r}' \rightarrow \mathbf{r}, E, \Omega) \chi(\mathbf{r}', E', \Omega', t)$$

where $\chi(\mathbf{r}, E, \Omega, t)$ is the density of particles leaving a source or emerging from a collision at phase space coordinates \mathbf{r} in direction Ω at time t with energy E , $S_g(\mathbf{r}, E, \Omega, t)$ is the density of particles generated by an external source, $T(\mathbf{r}' \rightarrow \mathbf{r}, E, \Omega)$ is a transport integral operator (kernel) and $C(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega)$ is collision integral operator.

Eq. (3.1) can be approximated by the sum:

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

$$\chi_0(\mathbf{r}, E, \Omega, t) = S_g(\mathbf{r}, E, \Omega, t)$$

and

$$\chi_n(\mathbf{r}, E, \Omega, t) = C(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) T(\mathbf{r}' \rightarrow \mathbf{r}, E, \Omega) \chi_{n-1}(\mathbf{r}', E', \Omega', t)$$

Thus, the random walk can be described as follows. The source coordinates $(\mathbf{r}_0, E_0, \Omega_0, t_0)$ are selected from $S_g(\mathbf{r}, E, \Omega, t)$ and a flight distance R is picked using the transport kernel, $T(\mathbf{r}' \rightarrow \mathbf{r}, E, \Omega)$, to determine the site of the first collision, $\mathbf{r}_1 = \mathbf{r}_0 + R\Omega_0$, and the particle's age, $T_1 = t_0 + R/v_0$, where v_0 is the particle's speed corresponding to energy E_0 .

The probability of scattering at the new site is $\Sigma_s(\mathbf{r}_1, E_0) / \Sigma_t(\mathbf{r}_1, E_0)$, where Σ is the macroscopic cross section of the material at position \mathbf{r}_1 and the subscripts s and t designate respectively the scattering and total cross sections.

Usually, no particle absorption is allowed, to allow the random walk to continue. This is a form of biasing aimed at avoiding early termination of the random walk. This biasing is compensated for by originally assigning the source particle a weight Ω_0 , typically equal to unity, and modifying it by the non-absorption probability, $1 - \Sigma_s(\mathbf{r}_1, E_0) / \Sigma_t(\mathbf{r}_1, E_0)$ following a collision.

A new particle energy, E_1 is selected according to the distribution

$$\int_{4\pi} d\Omega \Sigma_s(\mathbf{r}_1, E_0 \rightarrow E_1, \Omega_0 \rightarrow \Omega_1) / \Sigma_s(\mathbf{r}_1, E_0)$$

and a new direction is sampled from $\Sigma_s(\mathbf{r}_1, E_0 \rightarrow E_1, \Omega_0 \rightarrow \Omega_1) / \Sigma_s(\mathbf{r}_1, E_0)$.

The above process is repeated until the particle is terminated by escaping the system (to an artificially created external void), reaching a pre-assigned age, energy or weight cut-off.

Contributions to the quantity of interest are estimated at appropriate points or regions in the random walk phase space and the particle's weight and the appropriate response function are tallied.

In summary, the random walk is controlled by the transport and collision kernels. The distance of flight is sampled from a distribution described by the transport kernel, while the status of the particle after collision is governed by a distribution defined by the collision kernel. Both kernels are defined by the material's cross sections presented in the form of probability tables.

Throughout the transport process, a particle encounters different geometrical configurations and materials. Some biasing techniques may also be applied to discard particles that are unlikely to significantly contribute to the particle of interest and promote particles of importance. Eventually, of course, estimates of the quantity of interest must be obtained, otherwise the entire exercise is fruitless. One has however to start with a source. The next chapters describe the parameters MCNP uses to define the geometry, source, material, estimates of quantity of interest (tallies), importance sampling (biasing techniques), error analysis and criticality calculations.

3.1 Work Problem

Starting from the conventional integro-differential Boltzmann particle-transport equation

$$(1/v)\partial \Phi(\mathbf{r}, E, \Omega, t) / \partial t + \Sigma_t \Phi(\mathbf{r}, E, \Omega, t) = \int \int dE' d\Omega' \Sigma_s(\mathbf{r}, E, \Omega, t) \Phi(\mathbf{r}, E', \Omega', t) + S(\mathbf{r}, E, \Omega, t)$$

derive the "integral emergent particle density equation", Eq. (3.1)). Hint:

Introduce the integral operators; $T(\mathbf{r}' \rightarrow \mathbf{r}, E, \Omega) = \int_0^\infty dR \Sigma_t(\mathbf{r}, E) \exp[-\beta(\mathbf{r}, R, \Omega)]$,

$$C(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) = \int_{E'=E}^\infty \int d\Omega' \Sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) / \Sigma_t(\mathbf{r}, E')$$

with $b(\mathbf{r}, R, \Omega) = \int_0^\infty \Sigma_t(\mathbf{r}-R'\Omega) dR'$, into the effect of interest equation:

$$\lambda(E) = \int \int \int P^\chi(\mathbf{r}, E, \Omega, t) \chi(\mathbf{r}, E, \Omega, t) d\mathbf{r} d\Omega dt$$

where the response function $\chi(\mathbf{r}, E, \Omega, t)$ is obtained by particle which emerges from a collision at \mathbf{r} with phase space coordinates E, Ω and t .
