Chapter 8

Particle Transport in Matter

8.1 Introduction

Simulation of particle transport in matter became of increasing importance in recent years. Basics have been developed in the late 1960s and early 1970s in connection with the development of better nuclear reactors, and, of course, in connection with many atomic weapons programs. But with ever increasing computer capacity and cheaper computing, simulation of particle transport is nowadays of great importance in:

- Radiation therapy in cancer treatment: γ-knife, γ and X-ray radiation treatment planning, electron radiation treatment, hadron-radiation treatment (protons and neutrons), and the most recent application: light ion radiation therapy. It is the aim here to improve energy deposition in malignant tissue and to reduce radiation hazards for healthy tissue.

- Simulation of the properties of radiation detectors. Research centers like CERN, DESY, etc. make increasingly use of simulation techniques to improve detector performance in their experimental setups.

- Design of particle sources, like spallation neutron sources. Design of accelerators.

- Design of biological shields in high intensity radiation areas. This helps to improve the radiation protection for the personnel.

Simulation of particle transport covers a huge variety of particles like electrons, protons, neutrons, α-particles, photons (γ-radiation), muons, etc;

particle energies start from some TeV to parts of meV (ultra cold neutrons). There are two major techniques:

1. Description of the particle transport using the BOLTZMANN transport equation:

$$
\begin{aligned}
\frac{1}{v_i}\frac{\partial \varphi_i}{\partial t} \quad = \quad & -\mathbf{\Omega}\,\mathrm{grad}\varphi_i \\
& + \sum_j \left[\int d^3\Omega' dE_B\, \sigma_{ij}(\mathbf{x}, E_B \to E, \mathbf{\Omega} \to \mathbf{\Omega}')\varphi_j \right. \\
& \left. - \int d^3\Omega' dE_B\, \sigma_{ij}(\mathbf{x}, E \to E_B, \mathbf{\Omega} \to \mathbf{\Omega}')\varphi_j \right] \sigma_i(\mathbf{x}, E)\varphi_i \\
& + \left(\frac{\partial}{\partial E}\varphi_i S\right) \\
& - \frac{1}{\lambda_i}\varphi_i \\
& + Y_i(\mathbf{x}, E, \mathbf{\Omega}, t). \qquad (8.1)
\end{aligned}
$$

Here, $\varphi_i(\mathbf{x}, E, \mathbf{\Omega}, t)$ is the angular flux of a particle if type i in the volume $dx\, dy\, dz$ around the space point **x**, in the energy interval dE around E and in the space angle interval $d\mathbf{\Omega}$ around $\mathbf{\Omega}$ multiplied by the particle velocity v_i. The first term of Eq. (8.1) describes the translation of the particle, the second the change in energy, flight angle, and particle type due to interaction between the transported particle with matter. $\sigma_{ij}(\ldots)$ is a cross-section and describes the probability to generate a particle of type i from a particle of type j at the phase space coordinates $(\mathbf{x}, E_B, \mathbf{\Omega}', t)$ due to some interaction process. This term contains two contributions:

   (a) $\sigma_{ij}(\mathbf{x}, E_B \to E, \mathbf{\Omega} \to \mathbf{\Omega}')$: Particles with energies (E) less than the initial energy (E_B) are generated.
   (b) $\sigma_{ij}(\mathbf{x}, E \to E_B, \mathbf{\Omega} \to \mathbf{\Omega}')$: Particles with energies (E) greater than the initial energy (E_B) are generated.

   The third term of Eq. (8.1) describes the continuous deceleration of particles which results in a reduction of the particle energy. S is the *stopping power*. The fourth term describes the annihilation of particles, and, finally, the fifth term allows generation of particles by external sources.

   There are numerous techniques to solve the BOLTZMANN equation. Approximations allow analytic solutions but most of the time such an approach is not feasible in practical applications. Thus, Monte Carlo methods are applied to solve the BOLTZMANN equation for practical purposes. In particle transport, the BOLTZMANN equation is applied to describe mainly neutron transport in matter. The appropriate energy range is $130\,\mathrm{MeV}$ to a few meV.

2. The other approach to solving the problem of particle transport is to involve so-called *Analogue Monte Carlo* techniques. This method tries to simulate the transport process as close to the "real" process as possible. Such an approach will also give insight into (maybe) significant fluctuations which can be expected in a real system and which cannot be described using the BOLTZMANN equation because of its statistical nature.

Common to both techniques is a minimum of necessary steps which a simulation will have to follow:

1. The geometrical setup of the space area to be investigated is to be defined an all necessary detail. This setup consists of a description of the geometrical shape of the various elements and their relative position as well as of the materials used to build the elements.

2. Definition of the type i of the particle to be traced on its path through matter. This is the source particle.

3. Given a certain material, the mean free path of the source particle in this material is to be determined. This mean free path defines the next point in space at which the source particle will undergo an interaction.

4. Is this point of interaction within the geometry to be investigated and are there no internal boundaries to be crossed on the way to this interaction point, then it will be possible to determine the interaction type which usually depends on the material in which the particle moves. This interaction could result in secondary particles which are stored on a stack for later use. After the interaction the source particle has a new energy and a new velocity as a result of the interaction process.

5. Is this point of interaction outside the geometry the trace of the source particle is finished and the first particle on stack (a secondary particle as a result of one of the interactions) is 'popped' and becomes the source particle for tracing.

6. If an internal boundary is crossed on the way to the interaction point the particle moves on a straight line until it reaches the internal boundary. A new mean free path is determined if there is a material change at this boundary and this defines a new interaction point. The simulation moves to point 4 of this list.

This description shows that book keeping is a major task in particle transport simulation. Nevertheless, we see that the simulation, in particular if we concentrate on Analogue Monte Carlo, consists of two basic elements:

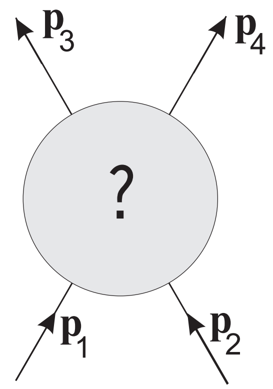

Figure 8.1: An elementary process.

- Description of the interaction processes, the *elementary processes*.
- The particle transport simulation, *i.e.:* how does the particle move from one interaction point to the next?

8.2 Particle Transport in Analogue Monte Carlo

8.2.1 Elementary Processes

The elementary process is the interaction of the source particle with a building element of the material within which the source particle moves. Such a process is described by the relativistic law of impact which requires the conservation of four-momentum (Fig. 8.1):

$$p_1^\mu + p_2^\mu = p_3^\mu + p_4^\mu. \tag{8.2}$$

The four-momentum is defined as

$$p^\mu = (m_0 c, m_0 \mathbf{v}),$$

with m_0 the particle's rest mass. Thus, Eq. (8.2) results in the following two laws of conservation:

$$\begin{aligned} m_0^{(1)} + m_0^{(2)} &= m_0^{(3)} + m_0^{(4)} && (8.3)\\ m_0^{(1)}\mathbf{v}^{(1)} + m_0^{(2)}\mathbf{v}^{(3)} &= m_0^{(3)}\mathbf{v}^{(3)} + m_0^{(4)}\mathbf{v}^{(4)}. && (8.4) \end{aligned}$$

The conservation of total mass (8.3) and the conservation of kinetic energy (8.4). Only this relativistic expansion of the classical laws of impact made it possible to describe particle type transformation due to interaction processes. We also see that these equations are not sufficient to determine the finals states p_3^μ and p_4^μ from the sole knowledge of the initial states p_1^μ and

p_2^μ. The required additional information is derived from the physical properties of the particular interaction process (indicated by the question mark in Fig. 8.1). This information is contained in the *interaction cross-section*.

The important observable is the *particle flux* Φ which is defined as particle velocity per unit volume (units: $\mathrm{m}^{-2}\mathrm{s}^{-1}$). We assume the material foil to be very thin and we can assume that the particle flux is only little perturbed. Thus, we assume the number C of interactions which will take place in unit time and unit volume within the foil to be proportional to the number N of atoms per unit volume and to be proportional to the particle flux which hits the foil:

$$C \propto N\Phi.$$

The constant of proportionality is the *microscopic cross-section* and it is, in general, dependent on matter, particle type and particle energy. Thus, we write:

$$C = \sigma N \Phi,$$

or

$$\sigma = \frac{C}{N\Phi}.$$

According to this relation, the cross-section is the number of interactions in unit area which can occur per number of atoms and source particles. It is better to write

$$\Sigma = N\sigma = \frac{C}{\Phi}$$

(unit: barn = 10^{-24} cm^2). Thus, $N\sigma$ is of dimension area and σ is the active cross-section of an atom for possible interactions. Σ is the *macroscopic cross-section*.

The cross-section describes quantum mechanical processes and one has to apply Quantum Field Theory to describe cross-sections theoretically. For instance, Quantum Electrodynamics describes the interaction of photons (γ-particles), electrons or positrons with matter, the so-called electrodynamic shower. Hadron and high energy interaction is described by Quantum Chromodynamics. Because of the quantum mechanical nature of all those processes, the cross-section describes the probability that some particular process can indeed happen within given matter for a given particle type and energy. Of course, cross-sections can also be acquired using various experimental techniques and these data, together with theoretical models are the backbone of the description of elementary processes particles undergo in their ‘travel’ through matter.

If we investigate the elementary interaction processes a source particle can undergo with matter we have to decide which of all the possible processes will indeed take place at a given interaction point. Each process is described by a cross-section and we may have, for instance, cross-sections for elastic, inelastic scattering, particle capture, particle fission, particle fusion, etc. Thus, we have a problem of ‘probability mixing’ of P possible processes numbered by an index i. The numbers $i = 1, \ldots, P$ are possible values of a random variable I and their distribution is described by the PDF

$$p(i) = \frac{\sum_{j=1}^{i} \sigma_j}{\sigma_t}, \qquad \sigma_t = \sum_{i=1}^{P} \sigma_i,$$

with σ_t the *total cross-section*. σ_i is the microscopic cross section of the process of type i. The random variable is sampled using a equally distributed random number $r \in [0, 1)$ and the condition

$$p(i-1) < r < p(i), \qquad p(0) = 0 \tag{8.5}$$

defines the process type i and, thus the PDF σ_i which determines the physics. [p(0) stands for the possibility that nothing happens.] It is the final job to calculate the final state of the particles after the interaction using the conservation laws (8.3) and (8.4).

In general, the final state of the interaction process is given by, say, n parameters $\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_n)$ and the *differential cross-section* is of the form

$$\frac{d^n\sigma}{d\mu^n} = g(\boldsymbol{\mu}).$$

Using

$$\sigma = \int d^n\mu \, g(\boldsymbol{\mu})$$

reproduces the microscopic cross-section. For instance,

$$\frac{d^2\sigma_i}{d\varepsilon d\Omega}$$

is the probability in a process of type i to find a particular particle in the energy interval $[\varepsilon, \varepsilon + d\varepsilon]$ and in the space angle element $d\Omega$ around the final velocity direction Ω.

The function

$$P(\boldsymbol{\mu}) = \frac{g(\boldsymbol{\mu})}{\sigma} \tag{8.6}$$

is, obviously normalized to one and has the properties of a PDF. This PDF is sampled to determine a random variable M which determines the final state of the interaction. This determines the number of particles generated during the interaction together with the four-momentum of one final-state particle. The conservation law (8.2) allows to determine the final states of all other particles involved. Is one of the final-state particles of the source particle's type then this particle becomes the new source particle. All other particles are put on stack.

Thus we have the following procedure:

1. An equally distributed random number $r \in [0, 1)$ is sampled. This determines the type of interaction according to Eq. (8.5).

2. A random number is sampled from PDF (8.6) which describes interaction process i. This determines the final state of one particle and the number of particles of the final state. The final states of all other particles are calculated using the conservation law (8.2).

This procedure ascertains that all possible processes will be considered according to their probability.

8.2.2 Particle Transport

Particle transport can be regarded as Brown's motion of a particle in matter with the difference that the stochastic force is replaced by quantum mechanical interactions of the traced particle with the elements matter consists of. Non charged particles do not experience the equivalence of the viscosity term, charged particles experience *Bremsstrahlung* as the equivalence of a viscosity term.

In simulations of Brown's motion the distance between interaction points (where the stochastic force hits) is just the mean free path and the particle moves 'freely' between two interaction points. In particle transport we also assume that particles move freely between two interaction points, *i.e.:* non-charged particles move along a straight line, charged particles under the influence of the Bremsstrahlung. The interval between two interactions is in principle determined by the mean free path

$$\lambda = \frac{1}{\Sigma_t} = \frac{M}{N_A \rho \sigma_t}.$$

Here, M is the molecular weight of matter, N_A LOSCHMIDT's number (AVOGADRO's number), ρ the matter's density, and σ_t the total cross-section of one molecule. The probability of an interaction to take place in the interval $[x, x + dx]$ is then determined by

$$P(dx) = \frac{dx}{\lambda}.$$

In general, the mean free path is not a constant along the trajectory of a particle through matter. The material may change but the particle may also loose energy which changes σ_t which depends on particle energy. We introduce the 'number of mean free paths' a particle traverses in its way from x_0 to the next interaction point x

$$N_\lambda = \int_{x_0}^{x} dx \, \lambda^{-1}(x)$$

because, in contrast to Brown's motion and to BOLTZMANN's equation the particle must not necessarily experience an interaction after traveling precisely one mean free path. The mean free path is a statistical information and can only be used as a basis in our simulation of a purely stochastic process. Let N be a random variable which gives the (non integer) number of mean free paths traveled by the particle from x_0 to the next interaction point x. We have to determine the probability $P(N|\mathcal{B})$ which is the basis for the PDF which determines the random variable N. Let $P(x|\lambda, \mathcal{B})$ be the probability for x to be the next interaction point for a given value of λ which is assumed to follow a POISSON distribution

$$P(x|\lambda, \mathcal{B}) = \frac{1}{\lambda} \exp\{-x/\lambda\}.$$

We find using the marginalization theorem:

$$\begin{aligned}
P(N_\lambda|\mathcal{B}) &= \int_0^\infty d\tilde{\lambda}\, P(N\tilde{\lambda}|\mathcal{B}) \\
&= \int_0^\infty d\tilde{\lambda}\, P(N_\lambda|\tilde{\lambda}\mathcal{B})P(\tilde{\lambda}|\mathcal{B}) \\
P(N_\lambda|\tilde{\lambda}\mathcal{B}) &= \int_0^\infty dx\, \underbrace{P(N|x)}_{=\delta(N_\lambda - \frac{x}{\tilde{\lambda}})} P(x|\tilde{\lambda}\mathcal{B}) \\
&= \int_0^\infty dx\, \underbrace{\delta(N_\lambda - \frac{x}{\tilde{\lambda}})}_{=\tilde{\lambda}\delta(\tilde{\lambda}N_\lambda - x)} \frac{1}{\tilde{\lambda}} \exp\left\{-x/\tilde{\lambda}\right\} \\
&= \int_0^\infty dx\, \tilde{\lambda}\delta(\tilde{\lambda}N_\lambda - x)\frac{1}{\tilde{\lambda}} \exp\left\{-x/\tilde{\lambda}\right\} \\
&= \exp\{-N_\lambda\}, \\
P(N_\lambda|\mathcal{B}) &= \int_0^\infty d\tilde{\lambda}\, e^{-N_\lambda} P(\tilde{\lambda}|\mathcal{B}) \\
&= e^{-N_\lambda} \underbrace{\int_0^\infty d\tilde{\lambda}\, P(\tilde{\lambda}|\mathcal{B})}_{=1} \\
&= e^{-N_\lambda}.
\end{aligned}$$

This results in the CDF

$$F(N) = P(N < N_\lambda) = 1 - \exp\{-N_\lambda\}, \quad N_\lambda > 0$$

which ensures that we have with certainty an interaction as $N_\lambda \to \infty$ while the probability for an interaction becomes very unlikely as $N_\lambda \to 0$.

This CDF defines the number of traversed mean free paths traveled by the source particle from one interaction point to the next one. To calculate this number we generate an equally distributed random number $r \in [1, 0)$. The random number $r' = 1 - r$ is also equally distributed and N_λ is calculated using the inverse transformation method (see Sec. 1.2.2):

$$N_\lambda = -\ln(r), \qquad r \in (0, 1]. \tag{8.7}$$

As flight direction and momentum of all particles generated in the final state of the interaction are known it is possible to determine the next interaction point for the source particle:

1. Calculate the mean free path at the momentary position of the source particle.

2. Generate a random number $r_1 \in (0, 1]$ which determines N_λ according to Eq. (8.7). $\ell_1 = \lambda N_\lambda$ corresponds to the (fictuous) position of the next interaction.

3. Calculate the distance d_1 along the flight path to the next internal boundary.

4. Let $\ell_2 = \min(\ell_1, d_1)$ and the particle moves the distance ℓ_2.

5. For $\ell_2 = \ell_1$ the particle reached the next interaction point and this loop is terminated.

6. For $\ell_2 = d_1$ an internal boundary has been reached. Is there a new material, the loop starts at point 1, otherwise we proceed at point two. If the boundary is an outer boundary the particle is going to leave the geometry and it will not be traced any longer. A new particle is popped from the stack and treated as a new source particle. The loop starts at point 1.