7 Computer Simulation of Neutron Transport—The Monte Carlo Method

Applying the Monte Carlo (MC) method to radiation transport is analogous to modeling the principles from which the Boltzmann equation is developed. Thus, the MC method may be applied to radiation transport without reference to the Boltzmann equation. We can follow a totally different approach by simulating the particle transport directly on a computer without even referring to the transport equation.

The Monte Carlo method is well suited to solving complicated three-dimensional time-dependent problems because it does not use phase space boxes. No averaging approximation is required in space, energy, direction, and time. This is especially important in allowing detailed representation of all aspects of physical data. A main feature of the MC method is to use statistical sampling methods to simulate transport processes by developing a statistical analogue description of particle (in this book, we limit ourselves to the neutron) life history on the computer, using random sampling methods. Then by running a large number of histories, the results can be averaged to obtain estimates of the expected behavior of the particle population. MC computer codes can become quite complex. It requires modeling the relevant physics of each particle interaction event as accurately as possible by allowing the particles to stream freely between interactions.

The chapter explains the Monte Carlo (MC) method rather than delving into the mathematics of physics of collisions. Therefore, in Sect. 7.1, statistical definitions used throughout MC calculations are presented. The methodology of particle history generation is presented in Sect. 7.2. In Sect. 7.3, modeling of radiation transport parameters including source parameters such as selection randomly of the position of the initially emitted particle, its direction, and energy. Also random selection of path length before making an interaction, collision parameters after interaction, material type upon which the particle is interacting, interaction type, and parameters after collision depending on the type of interaction. Methods of variance reduction techniques such as weight and source biasing are presented in Sect. 7.4. In Sect. 7.5, criticality calculations are discussed, especially the k_{eff}

R. M. Kuridan, *Neutron Transport*, Graduate Texts in Physics,
https://doi.org/10.1007/978-3-031-26932-5_7

cycle and estimators. In Sect. 7.6, we discuss particle scoring and neutron tallies. Finally, accuracy, precision, relative error, and figure of merit are pointed out in Sect. 7.7.

7.1 Basic Statistical Definitions

The MC method has proved to be a powerful and versatile in solving particle transport problems of importance to [1]:

1. Reactor designers
2. Shield designers
3. Medical therapy
4. Complex radiation transport problems
5. Other non-nuclear engineering problems:
   - Particle physics
   - Quantum field theory
   - Astrophysics
   - Molecular modeling
   - Semiconductor devices
   - Light transport calculations
   - Traffic flow simulations
   - Environmental sciences
   - Financial market simulations
   - Optimization problems

A brief history:

- Fermi (1930): random method to calculate the properties of the newly discovered neutron.
- Manhattan project (the 1940s): simulations during the initial development of thermonuclear weapons.
- Von Neumann and Ulam coined the term "Monte Carlo".
- Metropolis (1948) first actual Monte Carlo calculations using a computer (ENIAC).
- Berger (1963): first complete coupled electron-photon transport code that became known as ETRAN.
- Exponential growth since the 1980s with the availability of digital computers.

We now present statistical definitions used in MC calculation:

1. Particle history

The history includes the birth of a particle at its source point, its random walk through the transporting medium as it undergoes various scattering interactions, and its death which terminates the history.

2. Event

An event is a physical occurrence, for example, a coin toss resulting in a head or photon assuming a specific energy E.

3. Event space

An event space or sample is the set of all possible events within the process under consideration.

Example:
A coin toss: (head, tail)
Photon energy: no. of discrete energy groups or a continuous spectrum.

4. Random variable

A variable is random (also called stochastic) if its value cannot be specified in advance of observing it, but it is possible to talk in terms of probabilities. It is defined as the mapping of an event into a real number.

Example:
A coin toss: (0 for head and 1 for tail)

5. Tally

Records of all particle parameters during simulation, e.g. flux, current, etc.

6. Mean value distribution

When values are discrete,
$\overline{x} = \mu_x = \sum_i x_i f(x_i)$; for continuous variables: $\overline{x} = \mu_x = \int_{-\infty}^{\infty} x f(x) dx$: also called the expected value of (x).

7. The expected value of $g(x)$

$\overline{g} = \sum_i g(x_i) f(x_i)$ (discrete); $\overline{g} = \int_{-\infty}^{\infty} g(x) f(x) dx$ (continuous)

Example: the mean square distance $\overline{x^2} = \sum_i x_i^2 f(x_i)$

8. Variance

The variance of a distribution function is a measure of how closely the distribution is grouped around the mean:
$\sigma_x^2 = \sum_i (x_i - \mu)^2 f(x_i)$ (discrete)
$\sigma_x^2 = \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx$ (continuous)
show that $\sigma_x^2 = \overline{x^2} - \mu_x^2$

9. Standard deviation (precision)

Is often used instead of variance as a measure of the dispersion of the mean.

$$\sigma_x = (\sigma_x^2)^{1/2}$$

10. Relative error

It is defined as the estimated standard deviation of the mean σ_x divided by the estimated mean $\overline{x}$; $R = \frac{\sigma_x}{\overline{x}}$. It is a measure of the precision of the calculation.

11. Biasing

Defined as any means of distorting the sampling technique to advantage without losing accuracy.

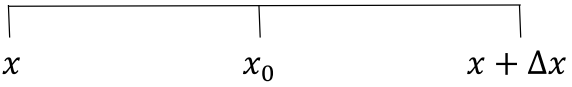
12. Probability density function (PDF)

The probability density function $f(x)$ also called probability distribution function or frequency function describes the relative frequency of occurrence of its random variable x and its domain (all possible values of x) constitutes the event space.

13. Continuous event space

Let $P(x < x_0 < x + \Delta x)$ be the probability that a random variable x_0 lies within interval $(x, x + \Delta x)$ of its event space the PDF $f(x)$ is related to this probability by the equality:

$$P(x < x_0 < x + \Delta x) = f(x)\Delta x$$



Therefore, $f(x) = \frac{P(x_0)}{\Delta x} \approx \frac{dP}{dx}$ as dx becomes vanishingly small, thus the PDF is central to the prediction problem and the knowledge of the PDF enables one to obtain the probability of occurrence of a specific event. The above equation shows that the PDF $f(x)$ gives the probability of occurrence per unit interval of the random variable x. Over larger interval PDF's are used with differentials, thus

$$P(a < x < b) = \int_a^b f(x)dx$$

14. Properties of the PDF

Since PDFs describe relative frequencies of occurrence of event within an event space, two properties of PDFs emerge,

(i) $f(x) \geq 0$
(ii) $\int_{-\infty}^{\infty} f(x)dx = 1$

The first property states that the relative frequencies (i.e. probability values) must be positive and the second property states that the property of finding a chosen event somewhere within its space must be unity.

15. Discrete event space

When the event space is discrete, the random variable can take on selected values, PDF $f(x)$ is $P(x_{i-1} < x_i < x_{i+1}) = f(x_i)$.
Properties:

(i) $f(x_i) \geq 0$
(ii) $\sum_i f(x_i) = 1$

16. Cumulative density function (CDF)

Let $P(x < x_0)$ be the probability that a random variable x has a value less than or equal to some fixed value x_0 lies within the event space then the CDF $f(x)$ is related to this probability by the equality:

17. Continuous event space

$$P(x < x_0) = F(x_0) = \int_{-\infty}^{x_0} f(x)dx$$

With the restrictions,

(i) $\lim_{x_0 \to \infty} F(x_0) = 1$
(ii) $\lim_{x_0 \to -\infty} F(x_0) = 0$

18. Discrete event space

When the event space is discrete, the random variable can take on selected values, CDF $f(x)$ is

$$P(x_i \leq x_m) = F(x_i) = \sum_{i=1}^{m} f(x_i)$$

Now the probability of finding x between a and b is

$$P(a \leq x \leq b) = \int_a^b f(x)dx = F(b) - F(a) = P(x \leq b) - P(x \leq a)$$

19. The making of a PDF:

If a given distribution does not satisfy the conditions for a PDF it can be transformed to a PDF. Suppose $q(x)$ is positive for all values of x then

$$f(x) = \frac{q(x)}{\int_{-\infty}^{+\infty} q(x)dx} \quad \text{and } F(x_0) = \frac{\int_{-\infty}^{x_0} q(x)dx}{\int_{-\infty}^{+\infty} q(x)dx}$$

Example
Suppose $q(x) = x^2$ for $2 \leq x \leq 4$ it is obvious that it does not satisfy the conditions for a PDF. According to the last procedure, the PDF is

$$f(x) = \frac{x^2}{\int_2^4 x^2 dx} = \frac{3x^2}{56} \quad \text{and } F(x_0) = \frac{\int_2^{x_0} x^2 dx}{\int_2^4 x^2 dx}$$

20. Problem solution

1. choose $f(x)$ or $F(x)$ and
2. select a random number ζ. Random numbers ζ from sequence or table of positive real numbers distributed uniformly (equally probable) on the interval [0, 1].
3. equate $F(x_0) = \zeta$ and solve for x_0 by the inverse method

21. Method of sampling from a distribution function [2]

Suppose we want to sample the random function $\cos\theta$ and $\sin\theta$. In order to do that let us consider a unit circle as shown in Fig. 7.1 and the point (x_1, x_2) is somewhere inside the circle. In general terms, we can define the coordinates as $x = -a + \zeta(2a)$ and $y = -b + \zeta(2b)$ in a rectangle $2a \times 2b$ in dimension with the origin at the center. For the square 2×2 in Fig. 7.1, x or $y = -1 + \zeta(2) = 2\zeta - 1$, however, some of the points fall outside the circle but still inside the square, therefore,

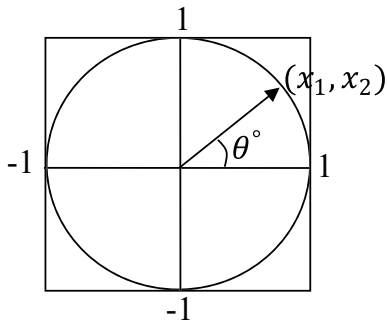


Fig. 7.1 Sampling the random function cosθ and sinθ

1. choose random numbers ζ_1 and ζ_2
2. calculate x_1, x_2 using $x_1 = 2\zeta_1 - 1$ and $x_2 = 2\zeta_2 - 1$
3. reject all points that fall outside the unit circle so that θ will be sampled uniformly between $(0, 2\pi)$
4. calculate $\cos\theta = \frac{x_1}{(x_1^2+x_2^2)^{1/2}}$ and $\sin\theta = \frac{x_2}{(x_1^2+x_2^2)^{1/2}}$
5. the efficiency of sampling is $\frac{\text{area of circle}}{\text{area of square}} = \frac{\pi}{4}$

This is the so-called rejection technique which has many applications such as the evaluation of integrals and transport kernels and many other things.

7.2 Particle History Generation

The following steps summarize the simulation of particle transport in the medium:

(1) Create a series of life histories of the source particle by using random sampling techniques.
(2) Sample the probability laws that describe the real particle's behavior.
(3) Trace out step by step the particle's "random walk" through the medium.
(4) The history of a particle is followed until it can no longer contribute information of interest to the problem in hand.
(5) Life history is then terminated and a "new" particle is started from the source.
(6) Secondary neutron and gamma photon products during collision events are tallied and also their histories are followed.

Figure 7.2 shows the possible events encountered by neutron or photon during transport in a fissionable material. The Monte Carlo approach requires the construction of case histories of travel of individual particles through the geometry and then analyzes these histories to derive the relevant data, such as flux density and dose rate. One particle history includes the birth of a particle at its source, its random walk through the transporting medium as it undergoes various scattering interactions and its death, which terminates the history. A death can occur when

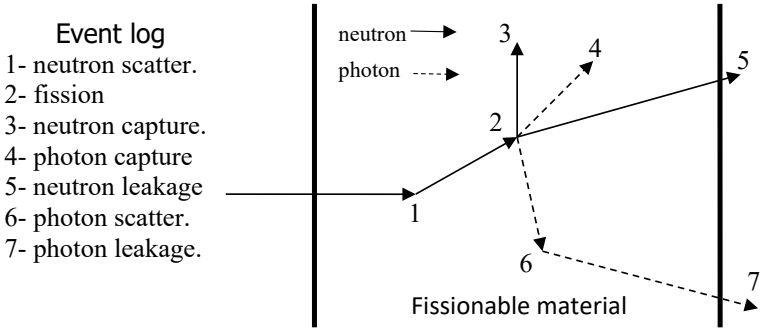


Fig. 7.2 Possible events during transport in a fissionable material

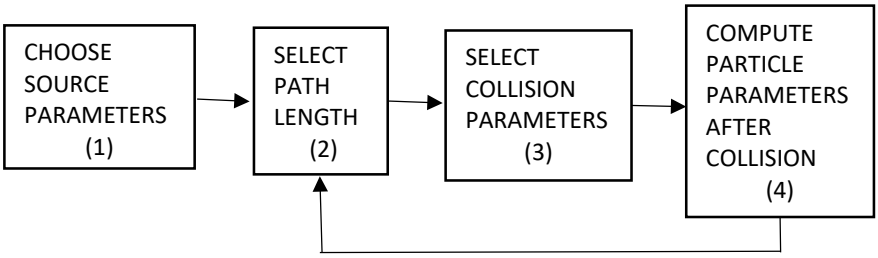


Fig. 7.3 Particle history generation

the particle becomes absorbed leaves the geometric region of interest, or loses significance owing to other factors (e.g. low energy) [3].

The major steps involved in generating a particle track history after mathematical modeling of geometry are shown in Fig. 7.3.

7.2.1 History Generator

The loop 2 through 4 is continued until the particle parameters fall outside some predetermined limit of values such as geometrical bounds, minimum energy or minimum statistical weight this process only generates particle histories. Separate provision must be made for estimating desirable output quantities such as flux density, current density, or interaction densities. The three operations in Fig. 7.3 involve the selection of parameters at random from a probability of all possible values of these parameters thus a sufficiently large number of selections of a given parameter would be distributed in the same manner as corresponding probabilities. The steps in making a random selection from such probability distributions are based on the use of numbers randomly distributed between the limits 0 and 1.

7.3 Modeling of Radiation Transport Parameters [4–6]

7.3.1 Source Parameters

The source parameters include energy, position point of origin, and direction of motion of the source particle as well as the biasing parameters. These parameters may be independent, or they may be interrelated in various ways for example, where the energy distribution is dependent on the direction of motion, the order of selection would call first for the selection of initial angle and then for the selection from energy distribution application to that angle.

1. *Selection of a spatial point*:

The problem of locating and tracking particles from point to point in material region is primarily one the geometry. The means of expressing geometric parameters depend on the choice of the coordinate system: for example, infinite medium calculation lend themselves to spherical geometry, but many shielding problems are best handled in cylindrical or rectangular geometry. Some examples of the selection of source spatial position are discussed in the following paragraphs.
Example: Selection of the initial source position from a uniformly distributed source on a disc (Fig. 7.4). The coordinates determining a point on a disc are (r, ϕ).

Firstly, we suggest the PDF $f(r) = \frac{\text{ring area}}{\text{disc area}} = \frac{2\pi r dr}{\pi R^2}$ at the radial distance r. It stands for the probability that a particle is emitted from anywhere on the ring. Check that it satisfies the two conditions for a PDF. The cumulative function is $\zeta = F(r) = \frac{2\pi \int_0^r r dr}{\pi R^2} = \frac{r^2}{R^2}$ which should be equated to the random number ζ giving a random radius: $r = R\sqrt{\zeta}$.

Secondly, the selection of the polar angle ϕ from the PDF $f(\phi) = \frac{\text{diff. angle}}{\text{total angle}} = \frac{d\phi}{2\pi}$ which represents the probability that a particle is emitted from a point at angle ϕ at the radius r. $\zeta = F(\phi) = \frac{\int_0^\varphi d\phi}{2\pi} = \frac{\phi}{2\pi}$ which gives a random angle as $\phi = 2\pi\zeta$ (a new random number should be selected for each calculation). If ϕ is measured in the range $\pm\pi$ then $\zeta = F(\phi) = \frac{\int_{-\pi}^\varphi d\phi}{2\pi} = \frac{\phi+\pi}{2\pi}$, and hence $\phi = 2\pi\zeta - \pi = (2\zeta - 1)\pi$.

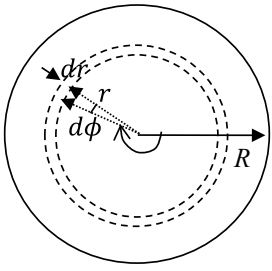


Fig. 7.4 Sampling of the emission position on a disc source

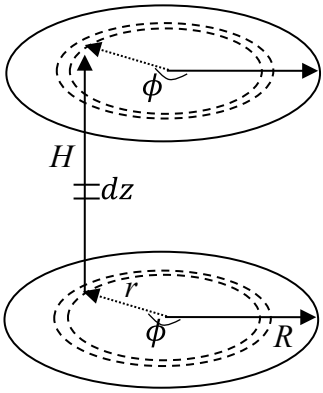


Fig. 7.5 Sampling of the position in the cylindrical source

Therefore, the coordinates (r, ϕ) are replaced by the random coordinates $\left(R\sqrt{\zeta}, (2\zeta - 1)\pi\right)$. This may be extended to cylindrical geometry by considering the third dimension z since the disc is just the base of the cylinder (Fig. 7.5). The PDF in the axial direction is just $f(z) = \frac{dz}{H}$ which is just the probability that the particle will be emitted from dz at (r, ϕ).

The CDF is

$\zeta = F(z) = \frac{\int_0^z dz}{H} = \frac{z}{H}$ and hence, $z = \zeta H$.

Therefore, the cylindrical coordinates (r, ϕ, z) are replaced by the random coordinates $\left(R\sqrt{\zeta}, (2\zeta - 1)\pi, \zeta H\right)$. Nonuniform source distribution can be considered as well.

2. *Selection from an energy distribution*:

The energy of the particles emitted from the source is sampled using the emission spectrum, $\kappa(E)$ characteristic of the source but it has to be converted to a PDF $f(E)$ first

$$f(E) = \frac{\kappa(E)}{\int_0^{E_{\max}} \kappa(E) dE}$$

where, $E_{\max}$ is the energy upper limit in the emission spectrum. The corresponding CDF $F(E)$ is

$$F(E) = \frac{\int_0^E \kappa(E) dE}{\int_0^{E_{\max}} \kappa(E) dE}$$

The function $F(E)$ will always be monotonically increasing having a maximum value of 1.0 the random choice of the energy of emitted particle is done by using a random number within the range $(0 \leq \zeta \leq 1)$ such that

$$\zeta = F(E) = \frac{\int_0^E \kappa(E) dE}{\int_0^{E_{\max}} \kappa(E) dE}$$

From this equation, the random value of E can be obtained by using any one of the root-finding techniques such as bisection method, Newton Raphson method, etc. When cumulative energy distribution is given at some energy data points, the source energy selection process is shown in Fig. 7.6.

3. *Selection of the initial direction*:

The unit vector $\underline{\Omega}$ represents the direction of a particle. Figure 7.7 shows the cylindrical volume source. $\underline{\Omega}$ is described by the two angles (θ, φ) in spherical coordinates. If isotropic emission is assumed, then it can be represented geometrically by equally probable (isotropic) vectors from the point of emission as shown in Fig. 7.8.

The calculation of the PDF proceeds for the angle θ first. The probability of emission with an angle θ in $d\theta$ is just the area of strip divided by the area of a

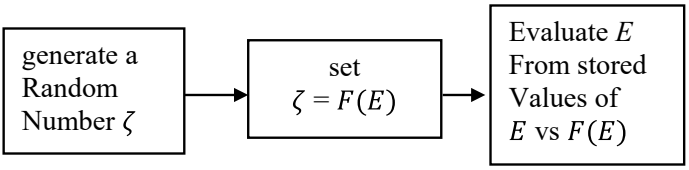


Fig. 7.6 Sampling of source energy

Fig. 7.7 Source particle coordinates in a cylinder

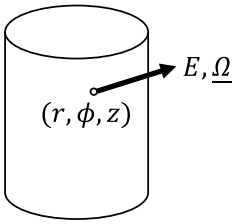
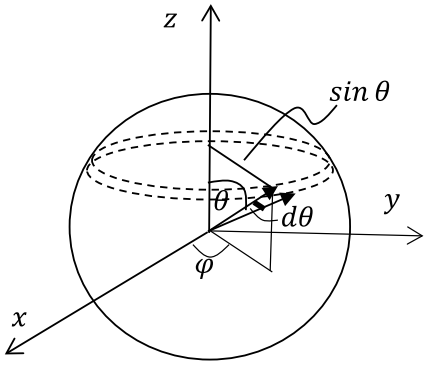


Fig. 7.8 Sampling of a source particle direction (θ, φ) in the spherical volume



unit sphere (4π). The strip is a ring of radius $\sin\theta$ and thickness $d\theta$. Therefore, the strip area is $2\pi \sin\theta d\theta$. The PDF is $f(\theta) = \frac{2\pi \sin\theta}{4\pi} = \frac{\sin\theta}{2}$ And the CDF is

$$\zeta = F(\theta) = \frac{\frac{1}{2}\int_0^\theta \sin\theta d\theta}{\frac{1}{2}\int_0^\pi \sin\theta d\theta} = \frac{1}{2}(1 - \cos\theta)$$

from which $\theta = \cos^{-1}(1 - 2\zeta)$ The angle φ is selected as in the case of the angle φ of the position coordinates $\varphi = (2\zeta - 1)\pi$. Finally, the random direction coordinates are defined as $\left[\cos^{-1}(1 - 2\zeta), (2\zeta - 1)\pi\right]$. Of course, the selection of direction parameters are independent of the shape of the spatial selection in the source volume. In the case of an isotropic surface source, the direction should be selected randomly from a 2π half-space

$$\zeta = F(\theta) = \frac{\frac{1}{2}\int_0^\theta \sin\theta d\theta}{\frac{1}{2}\int_0^{\pi/2} \sin\theta d\theta} = 1 - \cos\theta \text{ and } \theta = \cos^{-1}\zeta$$

Non-isotropic distributions can be considered as well.

7.3.2 Path Length

The path length along the parameters of initial direction defines the point at which an interaction occurs.

1. *Path length in a single region*:

Assume initially a single infinite region through which particles are being tracked. If the total macroscopic cross section of the region is $\Sigma_t(E)$, then the number of particles of energy E (making no collisions scattering or absorption) penetrating to depth L (Fig. 7.9) out of N_0 trials is $N_0 e^{-\Sigma_t(E)L}$, hence the probability of penetration to depth L without making a collision is just

$$P(L) = \frac{\text{number penetrating to depth } L}{\text{number of trials}} = e^{-\Sigma_t(E)L}$$

The probability of particle interaction at some path length less than or equal to L is thus given by

$$F(L) = 1 - P(L) = \left[1 - N_0 e^{-\Sigma_t(E)L}\right]$$

If the path length L to first collision is to be sampled at random, the random number, ζ is set equal to $F(L)$, or

$$\zeta = F(L) = \left[1 - e^{-\Sigma_t(E)L}\right] \text{ or}$$

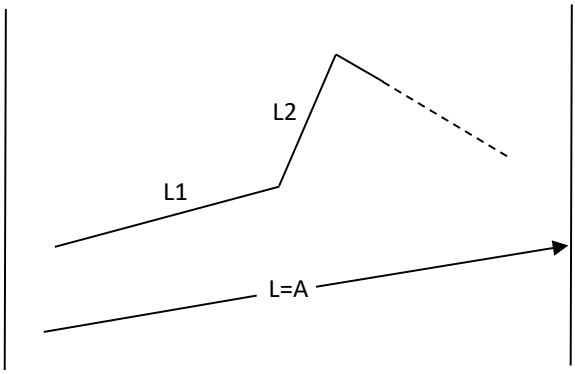


Fig. 7.9 Path length in a single region

$$1 - \zeta = e^{-\Sigma_t(E)L}$$

giving

$$L = -\frac{1}{\Sigma_t(E)} \ln(1 - \zeta)$$

Since $(1 - \zeta)$ is distributed in the same manner as ζ, we can rewrite:

$$L = -\frac{1}{\Sigma_t(E)} \ln \zeta$$

Suppose now that a single region is bounded such that the boundary is encountered at path length $= A$, then, if the randomly selected path length exceeds the value of A then the particle will be assumed to have escaped the system and history will be terminated, otherwise, collision will be assumed to have occurred at the selected point and collision parameters will be calculated. As a matter of fact, the value of A will be a function of the initial direction of the particle and the geometry of the region boundary and it is not the *region thickness* per say. It should be calculated after the source direction has been selected so that it will be available for test against L.

2. *Path length in a multi-region*:

Consider Fig. 7.10 where a point source is outside several homogenous layers with different properties. A ray extending in the direction of the particle motion encounters region boundaries in the various regions given by $A_1, A_2, \ldots A_N$ with associated total x-sections given by

$$\Sigma_{t1}(E), \Sigma_{t2}(E), \cdots\cdots \Sigma_{tN}(E)$$

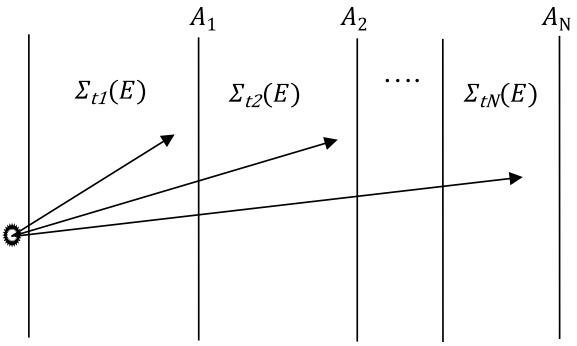


Fig. 7.10 Interaction probabilities for several homogenous layers

The effect of successive probabilities is such that the escape probabilities from the entire system is equal to the product of the individual zone penetration probabilities. The total escape probability will be given by

$$p = e^{-(\Sigma_{t1}A_1+\Sigma_{t2}A_2+\cdots\cdots\Sigma_{tN}A_N)}$$

The fate of the particle along the track could be determined in the following ways:

First method:

1. Select a path length at random assuming an infinite medium with cross section $\Sigma_{t1}(E)$ using the equation $L = -\frac{1}{\Sigma_{t1}(E)}\ln\zeta$ above.
2. If $L1$ exceeds $A1$, move the particle to the point where its track intersects the boundary between region 1 and region 2.
3. Select a path length at random in the original direction, assuming an infinite medium with a x-section $\Sigma_{t2}(E)$.
4. If $L2$ exceeds $A2$, move the particle to the point where its track intersects the boundary between region 2 and region 3.

This procedure is repeated until one of the $L_i \leq A_i$ or until the particle escapes.

Second method:
Instead of selecting path length in each of the materials successively as described in the first method, it would be perhaps simpler to decide the fate of the particle by selecting only one random number. For this purpose, we will define $b = \sum_i A_i\Sigma_{ti}(E)$ where A_i are defined as before lying along the particle path between the source point and the first collision. Then the total escape probability will be given by

$$p = e^{-(\Sigma_{t1}A_1+\Sigma_{t2}A_2+\cdots\cdots\Sigma_{tN}A_N)} = e^{-b}$$

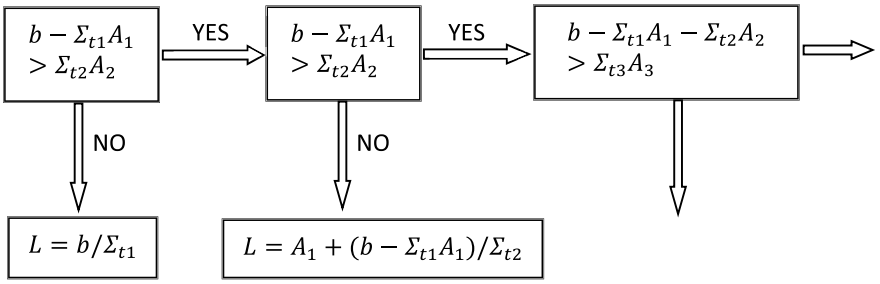


Fig. 7.11 Path length selection method for several homogenous layers

The probability of interaction at some path length ($\leq L$) is given by

$$\zeta = F(L) = \left[1 - e^{-b}\right]$$

hence, $b = \ln\zeta$. The process of finding the path length corresponding to the selected value of b is symbolized in the flow chart of Fig. 7.11.

7.3.3 Collision Parameters

When it has been determined on the basis of total material cross section that a collision has occurred, it is then necessary to determine which of the possible nuclear species is involved and which of the possible interactions of that species has taken place.

7.3.3.1 Type of Material

In a material containing several elements of atomic density N_i and total x-section σ_{ti} such that the total cross section is defined as $\Sigma_t = \sum_{i=1}^{N} N_i\sigma_{ti}$, the probability of a particle species being involved is given by the fraction of the total cross section represented by that species $\frac{N_i\sigma_{ti}}{\Sigma_t}$. The nucleus involved in a collision can be obtained by selecting a random number ζ and comparing it to the cumulative distribution function

$$F(k) = \frac{\sum_{i=1}^{k} N_i\sigma_{ti}}{\Sigma_t} = \zeta$$

Solving for k (the kth species) where k is an integer between 1 and N. Figure 7.12 shows the scale by total cross sections of the material mixture.

7.3.3.2 Type of Interaction

The type of interaction can be determined by comparing the random number ζ to the CDF $F(l) = \frac{\sum_{j=1}^{l}\sigma_{ij}}{\sigma_{ti}} = \zeta$ where σ_{ij} is the jth type of interaction belonging

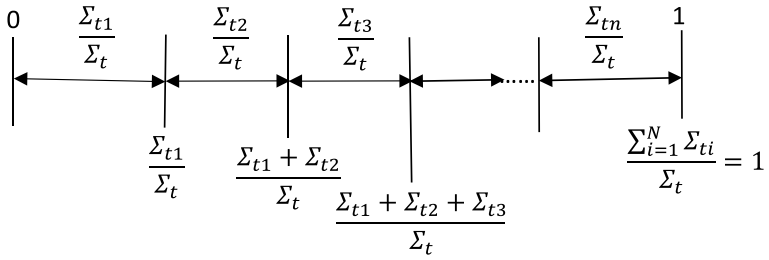


Fig. 7.12 Random selection of material type from material mixture

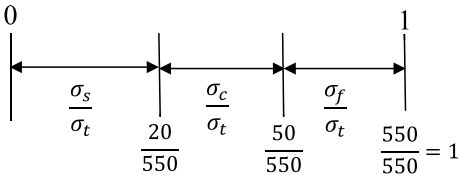


Fig. 7.13 Random selection the type of interaction

to the ith type nucleus determined previously and l is an integer between 1 and M and M is the total number of interaction types. For neutrons, σ_{ij} can be the microscopic cross section for elastic scattering, absorption, $(n.n')$, $(n.2n)$, $(n.\alpha)$, etc. Secondary neutrons or gamma rays resulting from the interaction are stored (banked) and later processed. Therefore, tracking is delayed until the histories of the incident particles are terminated in a separate program. For gamma rays,σ_{ij} can be the cross section for Compton scattering (Cs), photoelectric absorption (pe), or pair production (pp) (electron–positron pair). In the case of pp and pe history will be terminated although two photons are eventually emitted by positron annihilation.

Example
Consider the x-sections $\sigma_s = 20b, \sigma_c = 30b, \sigma_f = 500b$, and $\sigma_t = 550b$ (Fig. 7.13).

To select which type of interaction has occurred check the following: if $\zeta < \frac{20}{550}$ then the interaction is scattering; if $\frac{50}{550} > \zeta \geq \frac{20}{550}$ then the interaction is capture; and if $1 > \zeta \geq \frac{50}{550}$ then it is fission. The choice of collision parameters is not an easy task. First, a large amount of x-section data has to be formatted and coded properly in libraries with the associated interpolation subroutines.

7.3.3.3 Parameters After Collision

After determining the path length, we automatically assume a collision has taken place so the type of nucleus is determined followed by the type of collision. If the type of collision leads to the termination of particle history, then tracking is

stopped. Secondary particles if created are banked for later tracking. Otherwise, a scattering collision is assumed and the parameters after collision must be determined. Neutron transport in the reactor and hence criticality calculations are our main concern, therefore only MC applications to the interactions of neutrons are discussed in this chapter and MC simulation of gamma and electron interactions are excluded.

1. *Elastic scattering*: (σ_e)

In elastic scattering, the incident neutron gives off some of its energy to the recoiling nucleus. It is isotropic in the COM for light elements. For heavy elements, it becomes more complicated and forward. Anisotropic scattering becomes important as the energy of the incident neutrons increases. The elastically scattered neutron energy is given by

$$\frac{E'}{E} = \frac{A^2 + 2A\cos\theta_c + 1}{(A+1)^2}$$

The angles in both systems are related by

$$\cos\theta_L = \frac{A\cos\theta_c + 1}{\left(A^2 + 2A\cos\theta_c + 1\right)^{1/2}}$$

A schematic diagram for elastic scattering in the LAB and COM before and after collision is shown in Fig. 7.14. The final energy is minimum (maximum energy loss) when the neutron is backscattered ($\theta_C = \pi$), and hence $\frac{E_{\min}}{E} = \left[\frac{A-1}{A+1}\right]^2$. In the case of isotropic scattering in the COM the average cosine of the scattering angle in the LAB is given by $\overline{\cos\theta_L} = \frac{2}{3A}$. The angle in the COM is selected randomly from $\mu = \cos\theta_c = 2\zeta - 1$. For other distributions, the differential angular scattering cross section $\sigma(\theta_c, E)$ is used for random selection of the angle. The CDF is calculated from

$$F(\theta_c, E) = \frac{\int_0^{\theta_c} \sigma(\theta_c, E)d\theta_c}{\int_0^{\pi} \sigma(\theta_c, E)d\theta_c} = \zeta$$

Once the scattering angle in the COM is obtained, the energy loss is calculated from relations which were presented previously. Once the angle and energy are obtained, the azimuthal angle φ ($0 \le \varphi \le 2\pi$) should be randomly selected from an isotropic distribution, hence $\varphi = 2\pi\zeta$. Figure 7.15 shows the steps of random calculations for elastic scattering angles and emerging energies.

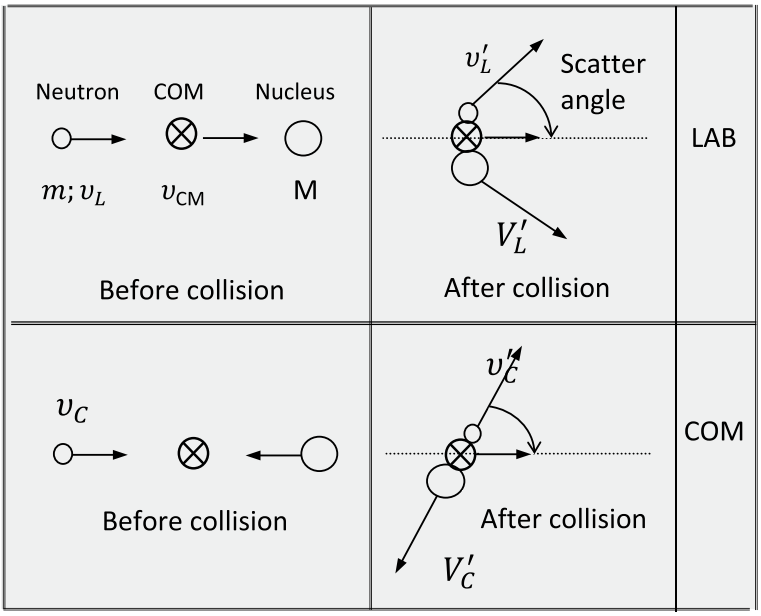


Fig. 7.14 Elastic scattering in the LAB and COM before and after collisions

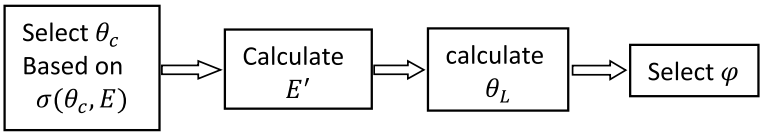


Fig. 7.15 Random selection of elastic scattering angles from the differential cross section

2. *Inelastic scattering*: (σ_{in})

In inelastic scattering, the neutron is absorbed by the target nucleus forming the compound nucleus which gives off a neutron and remains in the excited state which subsequently decays by photon emission. Neutron energies must be high enough to cause an inelastic reaction. It requires higher energies for light nuclei and lower energies for heavier nuclei. It is worth mentioning that the energy loss mechanism is via elastic scattering in the case of collisions with light nuclei and via inelastic scattering in the case of heavy nuclei.

The total inelastic cross section is divided into two components firstly, $\sigma_{nn'}(L)$ which is the probability that the nucleus is excited to any level L from which

gamma rays are emitted and secondly, $\sigma_{nn'}(C)$ which is the probability that the nucleus is excited to the region where levels are closely spaced and the emission is continuous.

The kinematic equation for inelastic scattering is given by

$$\frac{E'}{E} = \frac{1}{(A_i+1)^2}\left[1 + A_i^2\left(1 - \frac{\varepsilon}{E}\right) + 2A_i\cos\theta_c\left(1 - \frac{\varepsilon}{E}\right)^{1/2}\right]$$

$$\cos\theta_L = \frac{1 + A_i\cos\theta_c\left(1 - \frac{\varepsilon}{E}\right)^{1/2}}{\left[1 + A_i^2\left(1 - \frac{\varepsilon}{E}\right) + 2A_i\cos\theta_c\left(1 - \frac{\varepsilon}{E}\right)^{1/2}\right]^{1/2}}$$

The neutron energy required for an excitation of particular level is

$$E > [(A+1)/A]\varepsilon$$

where angles are defined as before and ε is the excitation energy of the target nucleus. Sampling from inelastic scattering cumulative distribution function is treated in the same manner as in elastic scattering.

3. *Calculation of the emergent direction cosines*:

If the direction cosines of the incident particle before the reaction are (α, β, γ) and the direction cosines after scattering are $(\alpha', \beta', \gamma')$, and the scattering angle in the LAB is θ_L and the azimuthal angle is φ the relations between the two cosines are given by

$$\alpha' = \alpha\cos\theta_L + \gamma\alpha\frac{\sin\theta_L\cos\varphi}{(1-\gamma^2)^{1/2}} - \beta\frac{\sin\theta_L\sin\varphi}{(1-\gamma^2)^{1/2}}$$

$$\beta' = \beta\cos\theta_L + \gamma\beta\frac{\sin\theta_L\cos\varphi}{(1-\gamma^2)^{1/2}} - \alpha\frac{\sin\theta_L\sin\varphi}{(1-\gamma^2)^{1/2}}$$

$$\gamma' = \gamma\cos\theta_L + (1-\gamma^2)^{1/2}\sin\theta_L\cos\varphi$$

if $\left(1-\gamma^2\right) \to 0$

$$\alpha' = \sin\theta_L\cos\varphi$$
$$\beta' = \sin\theta_L\sin\varphi$$
$$\gamma' = \gamma\cos\varphi$$

7.4 Variance Reduction Methods

7.4.1 Particle Weight

If the simulation is exactly a physical transport, then each simulated particle would represent one physical particle and would have a unit weight. However, for computational efficiency, the simulation allows many techniques that do not exactly simulate physical transport. For instance, each simulated particle might represent a number w of particles emitted from a source. This number w is the initial weight of particle simulation. The w physical particles all would have different random walks, but the *one* simulated particle representing these w physical particles will only have one random walk. Clearly this is not an exact simulation; however, the true number of physical particles is preserved in the simulation in the sense of statistical averages and therefore in the limit of a large number of simulated source particles (of course including particle production or loss if they occur). Each simulated particle result is multiplied by the weight so that the full results of the w physical particles represented by each simulated particle are exhibited in the final results (tallies). This procedure allows users to normalize their calculations to whatever source strength they desire. A second normalization to the number of Monte Carlo histories is made in the results so that the expected means will be independent of the number of source particles actually initiated in the calculation. Therefore, the result is given *per one source particle* and the more histories simulated the better the statistics. The real number of particles at any point is just [3, 7, 8, 9]:

$$[\text{the actual } source\ strength \times \text{MC } result]$$

Noting that:

Sometimes the number of sampled source particles are artificially increased in some direction or energy bins or position by a specified factor hence increasing the number of histories in order to improve statistics. At the end of the random walk, bias is neutralized by dividing the MC results by the same factor.

7.4.2 Source Biasing Parameters

In certain calculations it may be desirable to prejudice the selection of one or more source parameters to favor those most likely to contribute to the quantity of interest such as shield leakage or detector response. This can be done by selecting a larger number of source particles in the favored direction and assigning to each particle a number called its weight to adjust for a bias that was introduced. The benefit is to reduce drastically the tracking time.

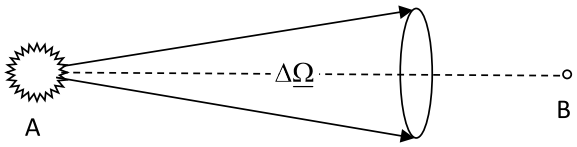


Fig. 7.16 Biased tracking toward point B

Table 7.1 Weight balance in a biased case

	Unbiased case		Biased case	
	No. of histories	Weight (w)	No. of histories	Weight (w)
Histories in $\Delta\underline{\Omega}$	2000	1	8000	1/4
Histories outside $\Delta\underline{\Omega}$	9000	1	3000	3
Total	11,000		11,000	

Example
Suppose there is a total of 10,000 source particle histories to be tracked from which 2000 in $\Delta\underline{\Omega}$ (Fig. 7.16). However, the detector recording at B is the main objective of the calculation. Therefore, we will bias the flux in $\Delta\underline{\Omega}$ and make it 6000 and leave the 4000 outside $\Delta\underline{\Omega}$. This will require weight of (1/3) in $\Delta\underline{\Omega}$ and weight of (2) in the outside in order to neutralize the bias. In order to obtain a near true measurement at the detector, $\Delta\underline{\Omega}$ should be carefully chosen. Table 7.1 explains the weight balance in this biasing case.

Situations where biasing might be used include:

(1) selecting more source points near the periphery of the reactor
(2) selecting more particles with an initial direction toward the shield or detector
(3) selecting more particles with a high energy or with an energy corresponding to a low total cross section.

It is important to remember that an adjustment of one category (e.g. angle bin or energy group) effects not only the bin or group but the entire distribution.

7.4.3 Variance Reduction Techniques

When most of the computation time is spent on more probable particle histories that do not contribute to the desired result, extra effort is required to increase the sample size seeking accuracy in the less probable more important rare events. The wasteful effort may lead to exceeding the Random Number Generator (RNG) capability giving rise to correlated samples. Therefore, not just computer time and

economics are of concern, rather the RNG finite period may be exceeded. Therefore, is it possible to reduce the relevant numerical and statistical uncertainty errors associated with the MC calculation without increasing sample size? The answer is through the variance reduction technique, the computer time can be reduced and still obtain results of sufficient precession. Common variance reduction techniques in Monte Carlo calculations are listed below:

1. *Energy cutoff*

Particles are terminated when their energy falls below a predetermined energy cut off. It should be noted that: It is a user supplied low limit on energy.

- If particle energy falls below the specified limit it is killed with zero probability.
- It should be used only when it is known that the low energy particle is not important.

Remembering that:

1. Low energy neutrons may produce high energy ones e.g. fission.
2. Low energy neutrons may be in some regions have more importance e.g. reactor core.
3. Neglecting weight of low energy particles by zero kill probability may make the answer biased low. Russian roulette (RR) is played to preserve weight.
4. If particle is not killed with RR, it is continued but weight is increased by the reciprocal of the survival probability to conserve weight.

2. *Time cutoff*

Particles are terminated when their time exceeds the time cutoff. It is for time dependent problems.

3. *Importance*

We define the importance of a cell as the expected score when a unit weight particle will generate after entering a cell.

$$\text{Importance(expected score)} = \frac{\begin{array}{c}\text{total score generated by particles}\\ \text{(and thier progony) entering the cell}\end{array}}{\text{total weigt entering the cell}}$$

After the importances have been generated the weights are assigned inversely proportional to the importances. Zero importance regions imply killing particles e.g. a surrounding infinite void where tracking is no longer desired.

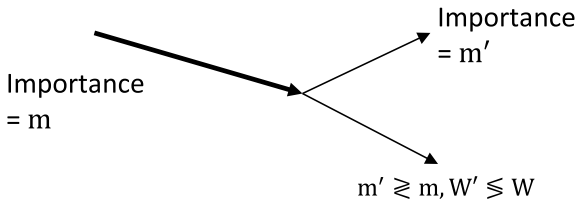


Fig. 7.17 Particle splitting

4. *Geometry splitting/Russian roulette*

Particles are increased in number when move to important directions (Fig. 7.17).

1. When $m' > m$, the particle is split into $\frac{m'}{m} \sim 2$ or $4\ldots$ splits, however weight is reduced by $\frac{m}{m'}$ to become $W' = \frac{m}{m'}W$.
2. When $m\prime < m$ Russian roulette is played and the particle is killed with a probability of $\left(1 - \frac{m\prime}{m}\right)$.
3. Or followed further with a probability m'/m and weight $W' = \frac{m}{m'}W$.

Russian roulette procedure (play) is used to *randomly* terminate particle history moving toward less important phase space regions. The importance number assigned to a region is dictated by how important it is and the number assigned will determine the action taken weather it is 1 or (2 or 3).

5. *Energy splitting/Russian roulette*

In space energy problems, particles are more important in some energy ranges than in others. For example, in a reactor core where fission occurs by thermal neutrons with a high probability so in the case of small number of fissions are taking place. Once a neutron falls below a certain energy level it can be split into several neutrons with appropriate weight adjustment.

6. *Weight cutoff*

It is a lower bound on weight e.g. if the weight of a particle reaches a preset lower bound Russian roulette is played and its weight is transferred to other particles.

7.4.4 Neutron/Photon Problem

When photons are produced in a neutron problem where photons are also tracked, such as in shielding problems, the weight of photons is

$$W_P = \frac{W_n \sigma_\gamma}{\sigma_t}$$

where,

W_n neutron weight
σ_γ photon production x-section
σ_t total neutron x-section

σ_γ, σ_t are calculated at the energy of the incident neutron.

1. *Capture*

(1) In analog capture, the particle is killed with a probability $\frac{\sigma_a}{\sigma_t}$ and $\sigma_a = \sigma_{n,\gamma}, \sigma_{n,\alpha}, \sigma_{n,d}, \cdots$. Neutron energy and weight are deposited in the collision cell when particle is killed.
(2) In Implicit capture, weight is reduced to $W_n^{'}$ as follows:

$$W_n' = \left[1 - \frac{\sigma_a}{\sigma_t}\right] W_n \text{ or } W_n' = \left[\frac{\sigma_s}{\sigma_t}\right] W_n$$

It represents the probability of survival (no capture) and $W_n - W_n^{'} = \left[\frac{\sigma_a}{\sigma_t}\right] W_n$ is deposited in addition to energy. If $W_n^{'}$ is equal to a problem weight cut off (on a cut card), Russian Roulette is played and of course its weight is transferred to other particles resulting in fewer particles with larger weight.
(3) Implicit capture along a flight distance to scatter $l = -\frac{1}{\Sigma_s} \ln(1 - \zeta)$. The particle weight is reduced at the scattering point by the capture loss $W' = We^{-\Sigma_a l}$ since capture did not take place.

A final remark on the variance reduction methods is that all the schemes employed aim at varying the importance sampling. One should be cautious in implementing schemes because they may increase variance. Fortunately, in criticality problem calculations we only need some simple schemes of cell importance.

7.5 Criticality Calculations

Nuclear criticality is the ability to sustain a chain reaction by fission neutrons, and characterized by k_{eff} is thought of as the ratio between the number of neutrons in successive generations, with the fission process regarded as the birth event that separates generations of neutrons. In criticality applications, the effective multiplication factor of an assembly is of primary interest [3, 10, 11].

7.5.1 k_{eff} Cycle

A group of neutron histories is often referred to as a k_{eff} cycle or neutron generation with the multiplication factor of the assembly given by the ratio of the

number of neutrons generated at the end of the k_{eff} cycle (i.e., those created in fission events in this cycle) to the number of neutrons whose histories are evaluated in this cycle (i.e., the number at the start of a generation). In short,

$$k_{\text{eff}} = \frac{\text{number of neutrons in a generation}}{\text{number of neutrons in a previous generation}}$$

A *generation* is defined as the period between birth of a neutron to its death by escape, parasitic capture, or absorption leading to fission. It is the computational equivalent by MC to a fission generation. $(n, 2n), (n, 3n)$ are not considered as termination and are internal to the cycle. It is optional to include delayed neutrons.

The expected value of the multiplication factor is then estimated by averaging over the events in the k_{eff} cycle. In the same way, the expected value of the leakage probability or the fraction of events leading to capture can also be obtained. The relative error in the estimate of the effective multiplication factor will usually decreases as the number of k_{eff} cycles increase. Thus, numerous cycles are necessary to arrive at a good estimate of k_{eff}. In addition, the first few cycles are inaccurate because the spatial neutron source has not converged. Because the distribution of source (fission) neutrons in a system is dependent on the eigenvalue of the system and on its geometry, it takes a number of inactive cycles for the Monte Carlo spatial neutron distribution to approach the converged distribution. For this reason, the first few cycles are ignored in the final estimate of k_{eff}. The estimates of k_{eff} from the remaining cycles are averaged to obtain a mean value for the effective multiplication factor. Criticality calculation in a Monte Carlo code such as MCNP (A General Monte Carlo N-Particle Transport Code) is performed through a special card known as KCODE card which describes the initial source distribution, skipped cycles, total cycles, etc. For example, let's say we evaluated G generations and discarded the first D of them. (It is recommended that $G - D > 100$ to observe any trends in the calculations.) Then the estimated effective multiplication factor of the system is given by

$$\overline{k_{\text{eff}}} = \frac{1}{(G - D)} \sum_{i=D+1}^{G} k_{\text{eff}}^{i}$$

where $\overline{k_{\text{eff}}}$ is the estimated system multiplication factor and k_{eff}^{i} is the multiplication factor determined from the ith cycle. The repeatability of the estimate (i.e., if the same calculation is performed with different random numbers, how much different will the estimate of k_{eff} be?) is determined from the estimated standard deviation of the mean. The standard deviation of the mean is calculated using the standard deviation, σ_S, of the distribution of k_{eff}-values.

$$\sigma_S = \sqrt{\frac{1}{(G - D - 1)} \sum_{i=D+1}^{G} \left(k_{\text{eff}}^{i} - \overline{k_{\text{eff}}}\right)^2}$$

For a valid Monte Carlo calculation, the range $\overline{k_{\text{eff}}} - \sigma$ to $\overline{k_{\text{eff}}} + \sigma$ should include the precise k_{eff} result about 68% of the time. The final result of the Monte Carlo calculation would be reported as $\overline{k_{\text{eff}}} \pm \sigma$ for a nominal 68% confidence interval,$\overline{k_{\text{eff}}} \pm 2\sigma$ for 95% and $\overline{k_{\text{eff}}} \pm 2.6\sigma$ for a 99% confidence interval for large N. These percentages refer to the fraction of the time the precise value of $\overline{k_{\text{eff}}}$ included in a confidence interval. MCNP has three different estimators for k_{eff}: collision, absorption, and track length between collisions. A statistically combined average is used as the final k_{eff}.

7.5.2 k_{eff} Estimators

There are several estimators for the multiplication factors, such as collision, absorption, track length, and prompt removal lifetime. The difference between implicit absorption k_{eff}^{A} and collision k_{eff}^{C} estimators is that in the absorption estimator only the nuclides involved in collision are used for the estimation of the k_{eff} rather than an average of all nuclides in the material for the collision estimator. The track length estimator $k_{\text{eff}}^{\text{TL}}$ is accumulated every time the neutron traverses a distance in a fissionable material cell. Monte Carlo codes Sampling the probability distributions during particle history simulation are taken from the detailed physics of the problem. They are deducted from the deterministic formulae of the relevant physics of interaction. This direct approach is called the *physical analogue approach* which is quite lengthy and time-consuming. The modern MC codes rather develop sampling procedure from the *integral* form of the transport equation. The reader may consult specialized references for the mathematical details. There are many codes based on the Monte Carlo method. They have developed so rapidly as the capabilities of computers evolved. Some of these codes are MORSE, MCN, NCNG (LASL), Tripoli, TART (LLL), and more recently the well-known MCNP (LASL) series. Figure 7.18 shows the general organization of an MC code.

7.6 Particle Scoring

The discussion so far has been concerned with the generation of source particles, tracking to the first collision and the determination of the new particle direction and energy following a collision. This is continued until particle history is terminated. Large number of histories and variance reduction methods must be employed in order to obtain acceptable statistics for the physical quantities desired in the energy, angle bins and spatial cells defined. Such physical quantities are [3]:

(1) Flux density as a function of space, energy, and direction
(2) The penetration dose or flux
(3) Time dependence of arriving particles
(4) The energy and angular distributions of the penetrating particles

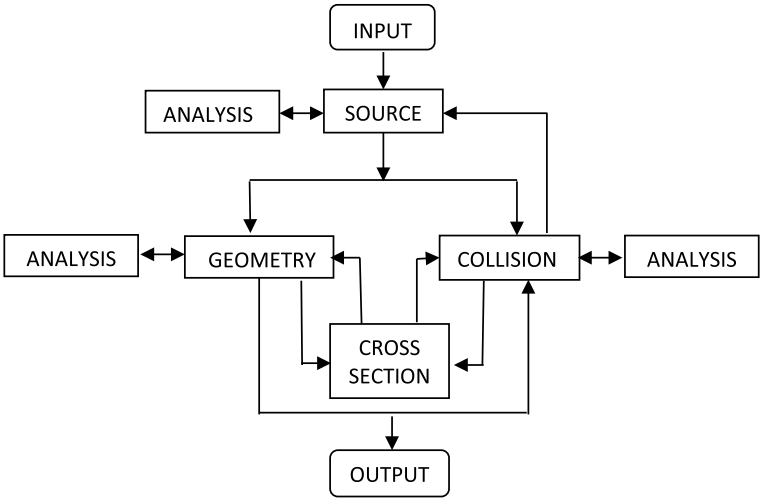


Fig. 7.18 The general organization of an MC code

7.6.1 Neutron Tallies

A Monte Carlo code like MCNP provides:

1. A standard summary information that includes:
   - Creation and loss of tracks and their energies
   - Tracks entering and reentering a cell and track population in the cell
   - Number of collisions in the cell
   - Average weight, mean free path, energy tracks in the cell
   - Activity of each nuclide in cell (interactions of with each nuclide in the cell, not radioactivity)
   - A complete weight balance for each cell
2. Seventeen standard tally types: 7 (neutron tallies); 6 (photon tallies); 4 (electron tallies). They can be modified by the user in many ways. They are normalized per starting particle except in KCODE criticality problem, which are normalized to be per fission neutron generation. There is also a plotter for displaying results.

Table 7.2 lists the basic standard tally types. N, E, P refer to neutrons, electrons, and photons respectively. Table 7.3 shows the mathematical definitions of the physical quantities defined by the tally. The starred tallies are the same physical quantities in units of energy.

Note that cell flux becomes a surface flux when the cell becomes so thin. Also, the units of the flux follow the units of the source, e.g. S (n/s) give a flux in units of (n/cm^2-s). In criticality calculations since the sources are fission sources the

Table 7.2 MCNP standard tallies

Fn	Unit	Name	*Fn	Unit
F1:N,E,P		Surface current	E	MeV
F2:N,E,P	$1/cm^2$	Surface flux	E	MeV/cm^2
F4:N,E,P	=	Track length estimate of cell flux	E	=
F5a:N,P	=	Flux at a point or ring detector	E	=
F6:N,E,(N,P)	MeV/g	Track length estimate of energy deposition	1.6022E-22	Jerks/g
F7:N	=	Track length estimate of fission energy deposition	1.6022E-22	=
F8:N,E,P,(P,E)	Pulses	Pulse height tally	E	MeV

Table 7.3 MCNP mathematical definitions of the tally physical quantities

Fn	Physical quantity
F1	$\boldsymbol{J} = \int_A \boldsymbol{dA} \int_\mu \boldsymbol{d\mu} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE}\lvert\boldsymbol{\mu}\rvert\boldsymbol{A\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\mu}, \boldsymbol{t})$
F2	$\overline{\boldsymbol{8}}_s = \int_A \frac{\boldsymbol{dA}}{\boldsymbol{A}} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$
F4	$\overline{\boldsymbol{8}}_V = \int_V \frac{\boldsymbol{dV}}{\boldsymbol{V}} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$
F5	$\overline{\boldsymbol{8}}_{PD} = \int_t \boldsymbol{dt} \int_E \boldsymbol{dE\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$
*Fn	Physical quantity $\times$ MeV
*F1	$\int_A \boldsymbol{dA} \int_\mu \boldsymbol{d\mu} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE}\boldsymbol{E}\lvert\boldsymbol{\mu}\rvert\boldsymbol{A\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{\mu}, \boldsymbol{t})$
*F2	$\int_A \frac{\boldsymbol{dA}}{\boldsymbol{A}} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE}\boldsymbol{E\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$
*F4	$\int_V \frac{\boldsymbol{dV}}{\boldsymbol{V}} \int_t \boldsymbol{dt} \int_E \boldsymbol{dE}\boldsymbol{E\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$
*F5	$\int_t \boldsymbol{dt} \int_E \boldsymbol{dE}\boldsymbol{E\Phi}(\boldsymbol{r}, \boldsymbol{E}, \boldsymbol{t})$

units are deduced from the reactor power. The following conversion is used:

$$\left(\frac{\mathrm{J/s}}{\mathrm{w-s}}\right)\left(\frac{1\ \mathrm{MeV}}{1.602\times10^{-13}\mathrm{J}}\right)\left(\frac{\mathrm{fissions}}{180\ \mathrm{MeV}}\right) = 3.467\times10^{10}\mathrm{fissions/w-s}$$

Therefore, in order to produce a power of P watts we need (3.467×10^{10}P) fissions/s. this power level produces $\left(3.467\times10^{10}\mathrm{P}\,\overline{\nu}\right)$neutrons/s which is the neutron source strength per second for a power level P in watts.

7.7 Accuracy, Precision, Relative Error, and Figure of Merit

A systematic error (true value of $x - \overline{x}$) is a measure of how close is the expected value of ($\overline{x}$) to the true value of x, which is seldom known [12].

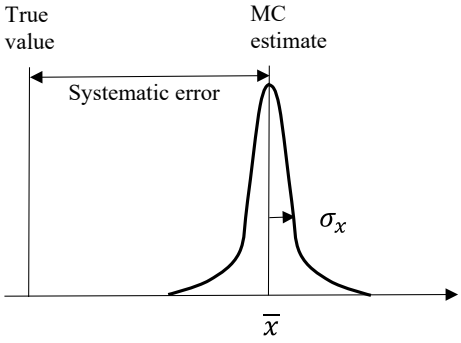


Fig. 7.19 The meaning of precision and accuracy

Table 7.4 Interpretation of the relative error

Range of $R = S_{\overline{x}}/\overline{x}$	Quality of tally
0.5–1	Completely unacceptable
0.2–0.5	Still unacceptable
0.1–0.2	Questionable (undependable)
<0.1	Generally reliable (not for point detector)
<0.05	Generally reliable (for point detector)

7.7.1 Precision

The standard deviation $\sigma_x = \sqrt{\overline{x^2} - \overline{x}^2}$ is a measure of precision of the Monte Carlo estimate. However, it is possible to get a highly precise result that is far from the true value if the model is not faithful. Figure 7.19 shows the meaning of precision and accuracy.

7.7.2 Relative Error

The relative error is a measure of calculation precision. Based on the long experience of MC practitioners, Table 7.4 presents the recommended interpretation for various values of the relative error R associated with an MCNP tally.

7.7.3 Figure of Merit

The estimated relative error squared, R^2, should be proportional to $\frac{1}{N}$ that is $R^2 \propto \frac{1}{N}$ where N is the number of histories. The computer time T should be proportional to N ($T \propto N$). Therefore, $R^2 T = \text{const}$. The figure Of Merit (FOM) is defined as $\text{FOM} = \frac{1}{R^2 T}$. The FOMs should always be examined against the number of histories for each tally that are approximately constant. It is a good measure of the efficiency of the Monte Carlo method (the higher the FOM the better the statistics).

Exercises

1. Get acquainted with any MC code input and output files and the selection of x-section tables. Use the code for modeling of a heterogeneous core *fuel cell* and *fuel assembly* of a thermal reactor of your choice. In particular,
   (a) Find the multiplication factor for the fuel cell
   (b) Vary the enrichment until it becomes near critical within two decimal points
   (c) Repeat the same calculation for the fuel assembly (ignore BP and CR)
2. Table below gives the geometrical and material composition of Godiva assembly, a bare sphere

Composition	Enrichment	Radius (exp.)	Radius (calc)	Critical mass of fuel	U-235 density
U235-U238	93.9%	8.71 cm	8.67 cm	48.7 kg	17.59 g/cm^3

   (a) Show that the density of Godiva constituents (U-235 and U-238) is 18.74 g/cm^3.
   (b) Run a Monte Carlo code such as MCNP for Godiva and study results:
      (i) Use the multiplication Fm cards to find the various reaction rates
      (ii) Use the energy card and the Hansen-Roch energy group structure to obtain the neutron spectrum. Draw the spectrum of the 16-group structure
      (iii) Does the composition of Godiva reveal a fast neutron spectrum?
      (iv) What is the main mechanism of neutron moderation?

References

1. N.M. Schaeffer, *Reactor Shielding for Nuclear Engineers* (Organization for Economic Cooperation and Development, Nuclear Energy Agency, France, 2008)
2. J. Duderstadt, W. Martin, *Transport Theory* (Wiley, New York, 1979)
3. X-5 Monte Carlo Team, *MCNP - A General Monte Carlo N-Particle Transport Code Manual*, vols. I–III (2005)
4. L. Carter, E. Cashwell, *Particle Transport Simulation with the Monte Carlo Method* (Loss Alamos Scientific Laboratory, 1975)
5. D.A. Usikov, Estimate of perturbations in solving nonuniform neutron transport problems by the Monte Carlo method. At. Energy **42**(1) (1977)
6. S. Maire, D. Talay, On a Monte Carlo method for neutron transport criticality computations. IMA J. Numer. Anal. (2006)
7. V.A. Velizhanin, I.G. Dyad'kin, Simulation of neutron transport in a low-capture medium by the Monte Carlo method. At. Energy **60**(1) (1986)
8. L.L. Carter, N.J. McCormick, Coupled sampling with the Monte Carlo method in neutron transport calculations. Nucl. Sci. Eng. **39**(3) (1970)
9. T. Mori, M. Nakagawa, M. Sasaki, Vectorization of continuous energy Monte Carlo method for neutron transport calculation. Nucl. Sci. Eng. (1992)
10. T. Goorley, *Criticality Calculations with MCNP5: A Primer*, 2nd edn. (Los Alamos National Laboratory, X-5)

11. G. Zhu et al., Monte Carlo burnup code development based on multi-group cross section method. Prog. Nucl. Energy **110** (2019)
12. I.M. Sobol, *A Primer for the Monte Carlo Method* (eBook, Published 30 Sept 2017)