6.1 Introduction

The Monte Carlo method is a statistical method for solving deterministic or statistical problems. Statistical estimates are found for quantities of interest. The estimate is obtained by the repetitive playing of a game. The game played is an analog of the physical problem of interest. The game is specified by a set of deterministic rules related to and sets of probabilities governing the occurrences of physical phenomena of interest.

A very simple example will illustrate the nature of the Monte Carlo method. Consider the problem of determining whether or not a conventional die is unbiased, i.e., whether or not it is loaded in favor of one or more faces. A physical determination of any bias could be made by measurements of various types. For instance, measuring the sides to see if the die was a true cube, locating the center of mass, and measuring the principal moments of inertia. The measurements lead to a deterministic answer regarding the bias or lack of bias. An alternative procedure is empirical in nature. Suppose the die is rolled many times and the occurrence of various faces in the upright position recorded. A statistical determination of the probability of obtaining any particular face will permit an analysis of any bias in the die. This second procedure could be termed a Monte Carlo study.

The above example is trivial in theory but serves to illustrate the conceptual simplicity of the Monte Carlo method. There are several points to consider in the example which are universal to all Monte Carlo studies. First, although the problem has a deterministic solution, a statistical procedure was adopted which consisted of the repetitive playing of a game. The game was so constructed that the desired result could be found. In the example, the game to be played is straightforward.
In more complicated problems the analog to be constructed is more complex. In any case, it is characteristic of the Monte Carlo method that one replaces a deterministic problem by an analog which consists of a reasonably straightforward game to be played many times.

The second point about the example is the method of playing the game, i.e., rolling the die. Obviously, if the results are to be meaningful the actual roll of the die must be random, i.e., the process of rolling must not favor any particular face of the die. In more complex problems, it may be necessary to play the game according to some given probability distribution function.

Third, the desired results are found by statistical study. We should expect variations and fluctuations in the answers obtained. If the die was unbiased, we expect the mean occurrence of any particular face to be 1/6. However, the mean value will only be approached asymptotically. The statistical nature of the results is inherent in all Monte Carlo problems.

Our second example concerns the transport of neutrons within a reactor. In this case the reactor's construction may be simulated within a digital computer. The neutrons within the reactor may traverse or attempt to traverse various materials, such as the moderator, fuel elements, cladding, and so forth. When penetrating these materials, the neutron may experience various nuclear events, such as elastic collision, fissions, absorption, and so on. The sequence of events experienced by each neutron is called its history. Interesting pertinent details may be recorded during the history of each neutron, and when enough histories have been followed, a census of these details recorded earlier may be compiled into statistical averages over the population studied. In following a particle we shall use Newton's laws to determine its trajectory. Neutrons, being neutral, move in straight lines with constant velocity. During the course of motion, the neutron may experience a nuclear collision. In such an encounter, only the probabilities with which various events take place are known. To decide which of them occurs, a random number is used (see Section 6.2 for definition, etc.). For example, one random number may be used to decide between a radiative capture and an elastic scattering, and a second random number may be used to determine the direction of the emergent neutron if an elastic scattering occurred. Conservation of momentum and energy may then be used to find the speed and energy of the emergent neutron.

The Monte Carlo method is tremendously flexible in that almost any physical effect and problem can be treated. It is applicable to transport problems, the evaluation of multiple integrals, the composition of music, problems in economics, and war games. However, the Monte Carlo method is not well adapted to the direct study of problems in which
many particles simultaneously interact, e.g., the mutually induced oscillation of electrons and ions in a plasma. The use of the Monte Carlo method is indicated for problems involving complicated geometries, for the study of systems only a few mean free paths in size, for the calculation of the effects of beam holes or control elements, for the computations of resonance escape probabilities, and the like.

In spite of its power, the Monte Carlo method should only be used where there is no other method available. Because of the use of random numbers, the Monte Carlo method is seldom as accurate in practice as other nonstatistical methods. Since the statistical fluctuations decrease only as the square root of the number of particles studied and because a large number of histories must be followed, a large amount of computer time is needed to get reasonable accuracy. Further, the logic of a coded program for a problem of some complexity is more intricate than that for almost any other coded program.

It is usually difficult to estimate the accuracy of a Monte Carlo calculation. The fluctuations in the results found after a large number of histories may be used to this end, but extreme care must be used to be sure the fluctuations are truly random. Each neutron must be followed for many lifetimes. Several generations are required to erase statistical fluctuations in an earlier population, such as an arbitrarily selected initial distribution.

The aim of this chapter is to illustrate the Monte Carlo method, particularly as applied to problems of reactor analysis. In order to understand the method, it is necessary to consider the problem of constructing the analog, selection from distributions, and some elementary statistics. In the next sections we consider the selection from the various distributions. We then review some basic statistics and the central limit theorem upon which most Monte Carlo studies are based. Next, we consider some examples of constructing the analog to certain problems. Finally, we consider some techniques for modifying the basic game in order to improve the method.

### 6.2 Random Numbers

In almost all Monte Carlo studies it is necessary to use numbers obtained from the random distribution, i.e., random numbers. Consider the interval \( a \leq x \leq b \). The random distribution function for the interval is defined as

\[
f(x) \Delta x = \frac{1}{b - a} \Delta x, \quad (6.2.1)
\]
i.e., a flat distribution. Since any value of $x$ in this distribution is as likely as any other $x$, the distribution is called random. A number selected from the distribution (6.2.1) is called a random number. It is usually convenient to consider random numbers in the interval $0 \leq x \leq 1$, in which case

$$f(x) = 1.$$  \hfill (6.2.2)$$

The selection of numbers from the distribution (6.2.2) may be accomplished in several ways in a digital computer. One consists in storing a large table of random numbers, which are obtained otherwise than by machine. Usually so many random numbers are required that insufficient memory space exists to hold a table.

Arithmetic procedures are used almost exclusively at present. The procedures all involve arithmetic operations with numbers and do not generate truly random numbers. The numbers computed by such methods are called pseudorandom since each of the techniques yields predictable chains of numbers and hence cannot be truly random. However, the methods do generate numbers which are approximately random as determined by their distribution function, the occurrence of particular digits, digit pairs, etc. The methods do provide large chains of numbers which can be assumed random. Furthermore, the predictability of a sequence of numbers is not really a disadvantage, since this predictability permits rerunning of problems for testing or debugging purposes.

One of the many methods of generating random numbers will be discussed: the congruential multiplicative method. This method is the most frequently used. Successive random numbers are generated by the algorithm

$$x_{n+1} = \alpha x_n (\mod N),$$  \hfill (6.2.3)$$

where $n$ is the iterate number, $\alpha$ is a scale factor, and $N$ is an integer.

The selection of the parameters $\alpha$, $x_0$, and $N$ is based upon the following observations. First, the integer $N$ is taken to be a little larger than the digit capacity of the computer so that all of the $x_n$ are scaled between $0 \leq x_n \leq 1$, for convenience. The scale factor should be so chosen that the period of the string $x_n$ is very long. The selection of appropriate scale factors may be studied by classical methods of number theory. Such a study is well beyond the scope of this book (see, however, Reference 11). For binary machines $\alpha$ is usually taken to be

$$\alpha = 5^y,$$  \hfill (6.2.4)$$
where \( g \) is the largest odd integer for which \( \alpha \) is less than a full word in the machine. If the machine has \( p \) binary bits, if the appropriate value of \( \alpha \) is chosen, and if \( x_0 = 1 \) (mod 5), then it can be shown that the resultant string of pseudorandom numbers has a period of approximately \( 2^{p-2} \) (Reference 11). For a 36 bit machine the period is of the order of \( 10^{10} \), which seems adequate for most purposes. Strings of different length may be found by modifying various factors in the multiplicative algorithm (6.2.3).

6.3 Distribution Functions

Decisions in Monte Carlo problems must often be made not on the basis that some phenomenon surely occurs, but rather that the given phenomenon occurs in accord with a given distribution function. The distribution of occurrences of an event is usually a more complicated function than the simple flat or random distribution. In this section we discuss methods of selection from distribution functions. We consider first a few elementary definitions and then techniques for selection.

Distribution functions are of two types: integral and differential probability distributions. The probability \( f(x) \Delta x \) that the random variable \( x \) has a value between \( x \) and \( x + \Delta x \) is called the differential distribution function and also the probability distribution function, and is frequently abbreviated as p.d.f. If the variable is defined in the range \( a \leq x \leq b \), then \( f(x) \) must be such that

\[
\int_a^b dx f(x) = 1.
\] (6.3.1)

The probability \( F(x) \) that the random variable \( x' \) is less than \( x \) is called the integral distribution function or the cumulative distribution function, sometimes abbreviated as c.d.f. The c.d.f. is defined as

\[
F(x) = \int_a^x dx' f(x').
\] (6.3.2)

Obviously, since the probability that something happens is unity,

\[
F(b) = \int_a^b dx' f(x') = 1.
\] (6.3.3)

An example of a p.d.f. and the corresponding c.d.f. is shown in Fig. 6.3.1. Since a probability is always positive, i.e., since

\[
F(x) \geq 0, \quad a \leq x \leq b,
\] (6.3.4)
it follows that $F(x)$ is a monotonically increasing function of $x$. Since the probability that $x$ takes on some value less than or equal to $a$ is zero, then $F(x)$ must be zero for $x \leq a$, as Eq. (6.3.2) indicates.

Distribution functions of more than one variable may be defined by analogous means. Thus, if $f(x, y)$ is the p.d.f. for the random variables $a \leq x \leq b, c \leq y \leq d$, then

$$F(x, y) = \int_{a}^{x} dx' \int_{a}^{y} dy' f(x', y').$$

(6.3.5)

The function $f(x, y)$ is called the joint p.d.f., whereas $F(x, y)$ is called the joint c.d.f. Many related distribution functions may be defined from the joint distribution functions.

![Integral and differential distribution functions](image)

**Fig. 6.3.1.** Differential and integral distribution functions of one variable.

The selection of a variable distributed according to a given probability distribution is of central interest in Monte Carlo investigations. One of the several ways is as follows: If $f(x)$ and $F(x)$ represent the p.d.f. and c.d.f. respectively of a random variable $x$, also called a stochastic variable, if $\kappa$ is a random number distributed between 0 and 1, and if $x$ is such that

$$F(x) = \kappa,$$

(6.3.6)

then for each $\kappa$ there is a corresponding $x$, and the variable $x$ is distributed according to the distribution $f(x)$. To prove this statement let $p(\kappa) = 1$ denote the probability distribution function for the random variable $\kappa$. For each $\kappa$ in the range $\kappa$ to $\kappa + \Delta \kappa$ there is a corresponding $x$ in the
range $x$ to $x + \Delta x$. Denote the probability distribution for $x$ as $g(x)$. We now show that for $x$ as given by Eq. (6.3.6), the p.d.f., $g(x)$, is in fact $f(x)$. We have

$$g(x) \Delta x = p(\kappa) \Delta \kappa = \Delta \kappa = F(x + \Delta x) - F(x),$$

and hence

$$g(x) = \frac{dF(x)}{dx} = f(x).$$

Therefore, the stochastic variable

$$x = F^{-1}(\kappa)$$

is distributed according to the p.d.f. $f(x)$. Further, the function $F^{-1}$ always exists.

As an example of the use of the above result, consider the distribution

$$f(x) = \alpha e^{-\alpha x}, \quad 0 \leq x \leq \infty.$$  

The corresponding c.d.f. is

$$F(x) = 1 - e^{-\alpha x}.$$  

To generate values of $x$ distributed according to Eq. (6.3.10), we first generate a random number $\kappa$ and compute $x$ by the prescription

$$x = -(1/\alpha) \ln(1 - \kappa).$$

Note that if $\kappa$ is randomly distributed from 0 to 1, then $1 - \kappa$ is randomly distributed from 1 to 0; hence we might as well use the formula

$$x = -(1/\alpha) \ln \kappa.$$  

In many cases the cumulative distribution function $F(x)$ is so complicated that computation of the stochastic variable $x = F^{-1}(\kappa)$ is impractical. A large table of values of $F(x)$ stored in the computer is particularly useful in such a case. For a given random number $\kappa$, the corresponding value of $x$ may be found by interpolation if necessary. If $\kappa$ is such that $F(x_{j-1}) < \kappa \leq F(x_j)$, then linear interpolation yields

$$x = x_j - \frac{F(x_j) - \kappa}{F(x_j) - F(x_{j-1})} (x_j - x_{j-1}).$$

This linear approximation assumes $x$ is uniformly distributed in the interval $x_{j-1}$ to $x_j$ (see problem 1).
VI. THE MONTE CARLO METHOD

A method of selection from differential distributions is the rejection method. We shall introduce it for one dimensional distributions and then illustrate for three dimensions. Let the p.d.f. be given as shown in Fig. 6.3.1. The maximum value of \( f(x) \) is denoted by \( f_{\text{max}} \), the minimum by \( f_{\text{min}} \). Consider the rectangle bounded by \( a, b, f_{\text{max}}, \) and \( f_{\text{min}} \). The area of the rectangle is denoted by \( A \). For any given random number \( \kappa \), the random numbers

\[
s(\kappa) = (b - a) \kappa + a, \\
g(\kappa) = (f_{\text{max}} - f_{\text{min}}) \kappa + f_{\text{min}}
\]

(6.3.15)

are uniformly distributed over the intervals \( a \) to \( b \) and \( f_{\text{min}} \) to \( f_{\text{max}} \), respectively. For any two random numbers \( \kappa_1, \kappa_2 \), the associated pair \( s(\kappa_1), g(\kappa_2) \) define a point randomly distributed over the rectangle. If \( g > f(s) \), then the point lies above the curve of \( f(x) \) and is rejected. Two new random numbers \( \kappa_3, \kappa_4 \) are found and new values of \( s, g \) are computed. Sooner or later a pair of numbers is found such that \( g < f(s) \) in which case the value of \( s \) is accepted. Geometrically it is evident that the values of \( s \) accepted are distributed according to the function \( f(x) \).

The relative efficiency, \( E \), with which the values of \( s \) are accepted is given by

\[
E = \frac{1}{A}.
\]

(6.3.16)

The average number of trials needed to find an acceptable value is merely \( 1/E \) as may readily be seen (see problem 2). If the area \( A \) is very large compared with one, the rejection method is very inefficient. For distribution functions with large peaks, either other methods must be used or the rejection method must be modified. In general it is desirable to select from a cumulative distribution, since such a method is 100\% efficient, i.e., every \( \kappa \) yields an \( x \) from \( f(x) \). In the usual case where \( F^{-1} \) is very difficult to compute or not explicitly known, then table look-up is used. In particular, for multidimensional distributions, table look-up is the only practical procedure. The rejection method is attractive in those cases where the efficiency is high.

The determination of the direction cosines of an isotropically scattered neutron provides a useful example of the rejection method. A neutron is isotropically scattered if the probability of passing through any one element of area of a sphere circumscribed about the point of scattering equals the probability of the neutron being scattered through any other element of equal area. Let \( \theta \) be the colatitude angle and \( \varphi \) the azimuthal
angle of the scattered neutron. Then elements of area for which $\Delta \cos \theta$ and $\Delta \varphi$ are equal will be of equal area $\Delta A$:

$$\Delta A = \Delta \cos \theta \Delta \varphi .$$ (6.3.17)

If, now, the values of $\cos \theta$ and $\varphi$ are chosen randomly and independently, then the probability of $\cos \theta$ lying in the range $\Delta \cos \theta$ and $\varphi$ lying in the range $\Delta \varphi$ is

$$f(\theta, \varphi) \Delta \cos \theta \Delta \varphi = \frac{\Delta \cos \theta \Delta \varphi}{2},$$ (6.3.18)

since $-1 \leq \cos \theta \leq 1$ and $0 \leq \varphi \leq 2\pi$. For the randomly selected values of $\cos \theta$ and $\varphi$, we have

$$f(\theta, \varphi) \Delta A = \frac{1}{4\pi} \Delta A ,$$ (6.3.19)

which is quite independent of either $\theta$ or $\varphi$, the condition for isotropic scattering. Thus, isotropic scattering is equivalent to $\cos \theta$ and $\varphi$ being randomly distributed variables.

A number of rejection techniques are in use for the determination of the direction cosines of a random scattering. Only one will be described here, two others being left for the problems. Since a random direction is characterized by a random azimuth, such an azimuth may be selected by choosing the coordinates of a point within a unit circle randomly. If $\eta_1$ and $\eta_2$ are random numbers in the interval between $-1$ to $+1$, then this pair is accepted if

$$\eta_1^2 + \eta_2^2 \leq 1 ,$$ (6.3.20)

for then these random numbers may be considered to describe a point within the unit circle. Otherwise, they are rejected, for they will then describe a randomly selected point within the circumscribed unit square outside the circle. Further pairs are generated until one is acceptable. The efficiency of selecting a random azimuth is seen to be $(\pi/4)1^2/1^2 = 78 \%$. The cosine of the colatitude angle is randomly selected by identifying it with a third random number $\eta_3$ lying in the interval between $-1$ and $+1$. The direction cosines are then given by

$$\alpha_d = \eta_1[(1 - \eta_3^2)/(\eta_1^2 + \eta_2^2)]^{1/2} ,$$

$$\beta_d = \eta_2 \alpha_d/\eta_1 ,$$

$$\gamma_d = \eta_3 .$$ (6.3.21)
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A second example of the use of the rejection technique is provided by a frequently used method of calculating the logarithm \( \ln \eta_1 \) of a random number. Basically the procedure consists in selecting a subinterval from the interval between 0 and 1 and of selecting a number within the subinterval chosen, both the subintervals and the number within the subinterval being chosen such that the logarithm of a random number \( \eta_1 \) is computed.

The subintervals are selected as follows: Let \( H \) be some number between 0 and 1. Subdivide the interval from 0 to 1 starting at 1, by marking the points \( 1-H \), \( (1-H)^2 \), \( (1-H)^3 \), and so on, as shown in Fig. 6.3.2. Number the subintervals as illustrated, the first being labeled as 0. The length of the \( n \)th interval is then

\[
(1-H)^n - (1-H)^{n+1} = H(1-H)^n. \tag{6.3.22}
\]

In particular the length of the 0th interval is \( H \).

Now consider the following. The probability that a random number between 0 and 1 will lie within the 0th interval is \( H \) and that it lie outside this interval is \( 1-H \). The probability that a series of \( n \) random numbers all between 0 and 1 not lie within the 0th interval is \( (1-H)^n \) and that the next, the \( (n+1) \)st random number, lies within the 0th interval is \( (1-H)^n H \). On the other hand, the probability that a random number between 0 and 1 lie in the \( n \)th interval equals its length. Equation (6.3.22) then merely states that the probability that a random number lie within the \( n \)th interval is equal to the probability that \( n \) random numbers in sequence lie outside the 0th interval while the \( (n+1) \)st random number lies inside the 0th interval. A subinterval is chosen according to the equality by determining the least number of random numbers required before one of them lies inside the 0th interval.

Attention is now turned toward determining the point of interest within the subinterval selected. If \( \kappa_2 \) is a random number between 0 and 1, then \( (1-H\kappa_2) \) is a random number between \( 1-H \) and 1. For the particular values of \( n \) just found, the number \( (1-H)^n(1-H\kappa_2) \) ranges completely over and only over the \( n \)th interval from \( (1-H)^{n+1} \) to \( (1-H)^n \). Since the \( n \)th interval has been chosen with a probability equal...
to its length by the indirect procedure mentioned above, the ensemble of numbers

$$\kappa_1 = (1 - H)^n(1 - H\kappa_2)$$  \hfill (6.3.23)

is randomly distributed from 0 to 1, i.e., is a random number in the interval from 0 to 1.

The ease with which \(\ln \kappa_1\) can be calculated justifies the labor in getting it.

$$\ln \kappa_1 = n \ln(1 - H) + \ln(1 - H\kappa_2)$$  \hfill (6.3.24)

by Eq. (6.3.23). We may rewrite the argument of the second logarithm to facilitate convergence of a power series expansion:

$$\ln \kappa_1 = n \ln(1 - H) + \ln \left[ \left(1 - \frac{H\kappa_2}{2 - H\kappa_2}\right) \left(1 + \frac{H\kappa_2}{2 - H\kappa_2}\right)^{-1} \right],$$

$$= n \ln(1 - H) - \frac{2\kappa_2 H}{2 - \kappa_2 H} \sum_{k=1}^{\infty} \frac{1}{2k + 1} \left(\frac{H\kappa_2}{2 - H\kappa_2}\right)^{2k},$$  \hfill (6.3.25)

$$= n \ln(1 - H) - \frac{2\kappa_2 H}{2 - \kappa_2 H}.$$

The present rejection method may be summarized as follows:

1. Choose a number \(H\). Compute \(\ln(1 - H)\) once and for all.
2. Generate a number of random numbers and select the first random number such that \(1 - H < \kappa_3 < 1\), counting the number \(n + 1\) of trials required.
3. Generate one more random number, \(\kappa_2\).
4. Compute \(\ln \kappa_1\) from Eq. (6.3.25).

If \(H = 0.2\), then the efficiency of the method of selecting the first acceptable random number is 20\% and the error introduced by truncating the power series at one term is less than 0.5\%.

6.4 Statistical Estimation

Results of Monte Carlo calculations are inevitably expressed as average values of variables determined from many trials of some game. In order to understand whether or not a given analog game will yield the desired results and how accurate the results are, it is necessary to consider the statistical basis of the calculation. Some elementary statistical quantities are defined below, and the important central limit theorem is discussed.
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Let \( f(x) \) be a probability distribution function in the interval \(-\infty\) to \(+\infty\). If \( g(x) \) is an integrable function of \( x \), then the mean value

\[
\langle g \rangle = \int_{-\infty}^{\infty} dx \, g(x) f(x)
\]  

(6.4.1)

exists and is known as the expected value of \( g(x) \). The expected value is merely the first moment of \( g(x) \) about the origin. The second moment about the origin is

\[
\langle g^2 \rangle = \int_{-\infty}^{\infty} dx \, g^2(x) f(x).
\]  

(6.4.2)

The variance is defined to be the second moment of \( g(x) \) about its mean

\[
V = \int_{-\infty}^{\infty} dx (g(x) - \langle g \rangle)^2 f(x) = \langle g^2 \rangle - \langle g \rangle^2.
\]  

(6.4.3)

The square root of the variance is called the standard deviation.

If \( N \) values of the random variable \( x \) are chosen from the p.d.f. \( f(x) \) and denoted as \( x_i \), \( i = 1, 2, ..., N \), then an estimate of \( \langle g \rangle \) is given by

\[
\bar{g} = \frac{1}{N} \sum_i g(x_i).
\]  

(6.4.4)

How good an estimate \( \bar{g} \) is of \( \langle g \rangle \) depends upon the number of trials \( N \) and upon the variance of \( g(x) \). A bound for the estimate is given by the central limit theorem. This theorem states in part that

\[
\lim_{N \to \infty} \text{probability} \left\{ \langle g \rangle + \frac{\alpha \sqrt{V}}{\sqrt{N}} \leq \bar{g} \leq \langle g \rangle + \frac{\beta \sqrt{V}}{\sqrt{N}} \right\} = \frac{1}{\sqrt{2\pi}} \int_\alpha^\beta e^{x^2} dx,
\]  

(6.4.5)

where \( \alpha \) and \( \beta \) are constants. It is assumed that the events leading to the statistical average are independent of each other. Thus, the probability that \( \bar{g} \) lie within an interval \( \pm \sqrt{V} / \sqrt{N} \) of \( \langle g \rangle \) is approximately 60\% , while the probability that \( \bar{g} \) lie within \( \pm 3\sqrt{V} / \sqrt{N} \) is approximately 99\%.

Relation (6.4.5) is an analytic statement of a rather intuitive concept, viz., that the more trials one uses in computing an average the more accurate the average is. The central limit theorem states that if many estimates of \( \langle g \rangle \) are obtained, each estimate of \( \langle g \rangle \) involving \( N \) trials, then
the variable \( \bar{g} \) is normally distributed about \( \langle g \rangle \) to terms of accuracy \( O(1/\sqrt{N}) \).\(^1\) Equation (6.4.5) is the limiting form of the theorem as \( N \to \infty \).

For a given estimate \( \bar{g} \) the mean square error, i.e., the variance \( V \) of \( \bar{g} \) is

\[
V(\bar{g}) = \langle (\bar{g} - \langle g \rangle)^2 \rangle = \langle \bar{g}^2 \rangle - \langle g \rangle^2.
\] (6.4.6)

We are interested in \( V(\bar{g}) \) as a measure of the accuracy of \( \bar{g} \). By Eq. (6.4.4), we have

\[
\langle \bar{g}^2 \rangle = \frac{1}{N^2} \left\langle \sum_i g(x_i) \sum_j g(x_j) \right\rangle = \frac{1}{N^2} \left\langle \sum_i g^2(x_i) + \sum_{i \neq j} g(x_i) g(x_j) \right\rangle.
\] (6.4.7)

Note that

\[
\left\langle \frac{1}{N} \sum_i g^n (x_i) \right\rangle = \left\langle \bar{g}^n \right\rangle = \langle g^n \rangle.
\] (6.4.8)

(See proof below for \( N = 1 \).) By Eqs. (6.4.2) and (6.4.7) we have

\[
\langle \bar{g}^2 \rangle = \frac{1}{N^2} \left[ N \langle g^2 \rangle + N(N - 1) \langle g \rangle^2 \right] = \frac{\langle g^2 \rangle}{N} + \frac{N - 1}{N} \langle g \rangle^2.
\] (6.4.9)

The variance of \( \bar{g} \) is thus

\[
V(\bar{g}) = \frac{1}{N} \left[ \langle \bar{g}^2 \rangle - \langle g \rangle^2 \right] = \frac{V}{N}.
\] (6.4.10)

The fractional square error associated with a given estimate \( \bar{g} \) is

\[
e^2 = \frac{1}{N} \left[ \frac{\langle g^2 \rangle}{\langle g \rangle^2} - 1 \right].
\] (6.4.11)

The magnitude of the error decreases as \( 1/\sqrt{N} \); thus to reduce the error by a factor of 10 requires 100 times as many trials. This is the essence of the difficulty with and the disadvantage of using the Monte Carlo method.

In many cases the first and second moments of \( g(x) \) are unknown. In such cases the statistical data may be used to find approximate expressions for the moments. The expected value of \( \bar{g} \), i.e., \( \langle \bar{g} \rangle \), is given as

\[
\langle \bar{g} \rangle = \frac{1}{N} \left\langle \sum_i g(x_i) \right\rangle = \frac{1}{N} \sum_i \int_{-\infty}^{\infty} dx_i f(x_i) g(x_i) = \frac{1}{N} \sum_{i=1}^{N} \langle g \rangle = \langle g \rangle.
\] (6.4.12)

\(^1\) See remarks concerning the references at the end of the chapter.
The estimate \( \tilde{g} \) is said to be an unbiased estimate of \( \langle g \rangle \) since the expected value of \( \tilde{g} \) is \( \langle g \rangle \). However,

\[
\langle g^2 \rangle \neq \langle g \rangle^2:
\]

for from Eq. (6.4.9) we have

\[
\langle g \rangle^2 = \frac{N}{N-1} \left[ \langle \tilde{g}^2 \rangle - \frac{\langle g^2 \rangle}{N} \right],
\]

(6.4.13)

and hence \( \tilde{g}^2 \) is not an unbiased estimate of \( \langle g \rangle^2 \). Obviously \( \langle \tilde{g}^2 \rangle = \langle g^2 \rangle \), and hence, by Eq. (6.4.10), \( V(\tilde{g}) \) can be approximated by

\[
V(\tilde{g}) \approx \frac{1}{N-1} \left[ \frac{\tilde{g}^2}{\langle \tilde{g}^2 \rangle} - 1 \right],
\]

(6.4.14)

while the fractional error may be approximated by

\[
e^2 \approx \frac{1}{N-1} \left[ \frac{\tilde{g}^2}{\langle \tilde{g}^2 \rangle} - 1 \right].
\]

(6.4.15)

For large \( N \) the bias is unimportant, i.e., \( N - 1 \approx N \). Equations (6.4.14) and (6.4.15) may also be derived by finding the expected value of the sample variance

\[
V_s = \frac{1}{N} \sum_i (g(x_i) - \tilde{g})^2
\]

(6.4.16)

(see problem 5).

As a very elementary example of the application of the above formulas, we consider the die rolling problem. If the die is unbiased, the probability of rolling any face is \( \frac{1}{6} \). Let the true probability of rolling a particular face be \( \rho \), which will not equal \( \frac{1}{6} \) if the die is biased. For \( N \) rolls with \( x \) successes an estimate of \( p \) is

\[
\tilde{p} = x/N.
\]

(6.4.17)

The probability of obtaining \( x \) successes in \( N \) rolls is

\[
f(x) = \rho^x(1 - \rho)^{N-x} \frac{N!}{x!(N - x)!}.
\]

(6.4.18)

Equation (6.4.18) follows by noting that the probability of \( x \) straight successes followed by \( N - x \) failures is merely \( \rho^x(1 - \rho)^{N-x} \). All possible distinct permutations then yield Eq: (6.4.18). The distribution (6.4.18) is the well-known binomial distribution.
The sample mean $\bar{p}$ is given by

$$\bar{p} = \langle x \rangle / N,$$  \hspace{1cm} (6.4.19)

where

$$\langle x \rangle = \sum_{x=0}^{N} x f(x).$$ \hspace{1cm} (6.4.20)

But

$$\langle x \rangle = \sum_{z=1}^{N} p^z (1 - p)^{N-z} \frac{N!}{(x-1)!(N-x)!}$$

$$= Np \sum_{z=1}^{N} p^{z-1} (1 - p)^{N-z} \frac{(N-1)!}{(x-1)!(N-x)!}.$$ \hspace{1cm} (6.4.21)

With the substitution $y = x - 1$, the second form of Eq. (6.4.21) yields

$$\langle x \rangle = Np \sum_{y=0}^{N-1} p^y (1 - p)^{N-1-y} \frac{(N-1)!}{y!(N-1-y)!} = Np,$$ \hspace{1cm} (6.4.22)

since the sum is unity. We then have by Eq. (6.4.19)

$$\bar{p} = p,$$ \hspace{1cm} (6.4.23)

as we expect.

It is easily shown that the variance of the binomial distribution is

$$V = Np(1 - p)$$ \hspace{1cm} (6.4.24)

(see problem 12). According to Eq. (6.4.10), the variance in $\bar{x}$ is then

$$V(\bar{x}) = p(1 - p),$$ \hspace{1cm} (6.4.25)

while the variance in $\bar{p}$ is

$$V(\bar{p}) = p(1 - p) / N.$$ \hspace{1cm} (6.4.26)

The magnitude of the fractional error is thus

$$| \epsilon | = \sqrt{(1 - p) / Np}.$$ \hspace{1cm} (6.4.27)

As expected intuitively we can improve the error in an estimate $\bar{p}$ by taking more trials, i.e., rolling the die more times. Notice that for small $p$ the fractional error may be quite large; thus we need many trials and many successes for a reduced error.
In the case of neutron penetration through a shield, the probability of penetration may be so small that the error indicates the standard Monte Carlo method cannot be profitably used. In this case and certain others, it is necessary to modify the game being played so that \( p \) is increased. The objective is to reduce the variance by altering the game and hence such modifications are collectively known as variance reduction methods. We consider several such procedures in Section 6.6.

6.5 Analogs of Two Simple Problems

In this section we shall illustrate the problem of constructing a statistical game to simulate a deterministic problem by two examples. In all of the examples the utility of variance reduction techniques will become apparent.

Numerical integration by statistical procedures will serve as our first example. The rejection techniques of Section 6.3 will be applied. If the integral

\[
I = \int_{a}^{b} dx \, s(x)
\]  

(6.5.1)

is to be evaluated, then a rectangle which bounds the function \( s(x) \) in the interval \( a \) to \( b \) is constructed. For the moment we shall assume \( s(x) \geq 0 \) in the interval \( a \) to \( b \). If the maximum of \( s(x) \) is known to be \( s_{\text{max}} \), then the bounding rectangle is as shown in Fig. 6.5.1.

The Monte Carlo game to be played consists of generating points randomly distributed over the rectangle and of counting each point.
that lands beneath the curve \( s(x) \). If the total number of successes is \( n \) out of \( N \) trials, then obviously

\[
I = \frac{n}{N}
\]

(6.5.2)
is the statistical estimate of the area. From the results of the previous section we know the fractional error associated with \( I \) is given by

\[
|\varepsilon| = \sqrt{(1 - p) / Np}
\]

(6.5.3)
with \( p \) defined as the ratio of \( I \) to the total area. Clearly, if \( p \) is very small, as might occur if \( s(x) \) had a tall, thin peak, then the number of trials required for reasonable accuracy is prohibitive by the straightforward application of this method.

Frequently an integral of the form

\[
I = \int_a^b dx g(x)f(x)
\]

(6.5.4)
ocurs, where

\[
\int_a^b dx f(x) = 1 .
\]

(6.5.5)
Every definite integral may be factored into the form (6.5.4) and hence the integral may be interpreted to be the expected value of \( g \), i.e.,

\[
I = \langle g \rangle ,
\]

(6.5.6)
and a Monte Carlo game to evaluate \( I \) would consist of picking values of \( x_i \) distributed according to \( f(x) \) and computing

\[
\bar{g} = \frac{1}{N} \sum_i g(x_i) .
\]

(6.5.7)
Equation (6.5.1) is a special case of Eq. (6.5.4) with

\[
f(x) = \frac{1}{(b - a)} ,
\]

(6.5.8a)
\[
g(x) = (b - a) s(x) .
\]

(6.5.8b)
However, the two methods differ with regard to the scoring procedure. In the first game a score of 0 or 1 is tallied depending upon whether or not a random variable is greater than or less than \( s(x_i) \). In the second game a score of \( g(x_i) \) is tallied for every point \( x_i \). The two different games obviously produce the same asymptotic values for the integral.
and standard deviation. The second method is somewhat more general in that it lends itself readily to variations which can be exploited to reduce the variance. We shall consider such ideas later.

Although the discussion has considered functions of only one variable, it is evident that the procedures carry over to multidimensional integrals. Indeed one would hardly consider using the Monte Carlo method for problems in fewer than three dimensions since classical methods of numerical integration are both feasible and accurate in such cases. Classical methods are slow and cumbersome for integrals involving many dimensions because of the large amount of data that must be stored and the large amount of calculation that must be performed.

Boundary value problems can also be solved by statistical sampling methods. We shall now discuss a classical statistical solution to an ordinary differential equation as our second example. First we consider the ordinary differential equation

\[ \frac{d^2y}{dx^2} + 2g(x) \frac{dy}{dx} = 0 \]  

(6.5.9)

with \( g(x) > 0 \) for \( x \) in the interval \( 0 \leq x \leq a \). The boundary conditions are

\[ y(0) = y_0, \]  

(6.5.10a)

\[ y(a) = y_n. \]  

(6.5.10b)

As usual, we divide the interval into \( K + 1 \) segments numbered 0, 1, ..., \( K \). The differential equation is replaced by a simple difference approximation

\[ \frac{\delta^2 y_k}{h^2} + 2g_k \frac{\Delta y_k}{h} = 0, \]  

(6.5.11)

which yields

\[ y_k = \frac{1 + 2g_k h}{2(1 + g_k h)} y_{k+1} + \frac{1}{2(1 + g_k h)} y_{k-1} \]

\[ = a_k y_{k+1} + b_k y_{k-1}, \quad k = 1, 2, ..., K - 1. \]  

(6.5.12)

Notice that \( a_k + b_k = 1 \) for all \( k \).

A statistical game may now be constructed to find the values of \( y_k \), the game being called a random walk. Consider a unit element at point \( k \). We interpret the quantities \( a_k, b_k \) as the probability of the element moving to point \( k + 1 \) or \( k - 1 \), respectively. If a unit element at \( k \) is allowed to move randomly through the mesh, then sooner or later the element will arrive at point 0 or \( K \). Depending upon which boundary
the element reaches first, a score of \( y_0 \) or \( y_a \) is tallied, and the game is
terminated. Let the score tallied, whichever boundary is reached, be
denoted by \( s_1 \). Another element is started from point \( k \) and allowed to
move through the mesh until a boundary is reached and a score \( s_2 \)
tallied. After \( N \) games, the mean value for \( y_k \) is

\[
\bar{y}_k = \frac{1}{N} \sum_i s_i .
\]  

(6.5.13)

The actual playing of the game is very simple. Starting at the point \( k \),
we compute the probability \( a_k \), or look it up in a table. A random num-
ber \( r \) between 0 and 1 is generated. If \( r < a_k \), then \( k + 1 \) replaces \( k \), i.e.,
the element moves to the right one place. Conversely, if \( r > a_k \), then
\( k - 1 \) replaces \( k \), i.e., the element moves to the left one place. After
each move a test must be made to see if a boundary has been reached. In
such a case, an appropriate score is tallied, and the game is terminated.
Otherwise, the process is repeated until a boundary is reached.

It is easy to show that the mean value computed by Eq. (6.5.13) does
approach the analytic solution of the difference equation (6.5.12). The
proof that \( \tilde{y}_k \) approaches \( y_k \) is developed as follows (see Reference 7):
Let \( v_m(k, K) \) be the probability of an element starting at point \( k \) and
reaching point \( K \) before reaching 0 in \( m \) or fewer moves. Similarly let
\( v_m(k, 0) \) be the probability of reaching point 0 before reaching point \( K \)
in \( m \) or fewer moves. Let \( v_m(k) \) be the mean score attained in a game of
\( m \) or fewer moves, the rules of scoring being as follows:

1. Nothing is added to the tally if neither \( k = 0 \) nor \( k = K \) is reached.
2. \( y_0 \) is added to the tally if \( k = 0 \) is reached in \( m \) or fewer moves
   before \( k = K \) is reached.
3. \( y_a \) is added to the tally if \( k = K \) is reached in \( m \) or fewer moves
   before \( k = 0 \) is reached.

Obviously we have

\[
v_m(k) = y_0 v_m(k, 0) + y_a v_m(k, K) .
\]

(6.5.14)

From the definition of \( v_m(k) \) and from Eq. (6.5.13), we have\(^2\)

\[
\tilde{y}_k = \lim_{m \to \infty} v_m(k) .
\]

(6.5.15)

To show that \( \tilde{y}_k \) approaches the analytic solution, we must show

\[
\lim_{m \to \infty} v_m(k) = y_k .
\]

(6.5.16)

\(^2\) The probability of spending an infinite number of moves without reaching
a boundary is zero (see Reference 7).
Thus, we must show that \( \lim_{m \to \infty} v_m(k) \) exists and further that the limit obeys the difference equation (6.5.12). We first show that the limit exists.

Consider the function \( v_m(k, 0) \). Obviously \( v_m(k, 0) \) is bounded by unity for all \( m \). Therefore, if we can show \( v_m(k, 0) \geq v_{m-1}(k, 0) \), then a limit to the sequence certainly exists. The function \( v_m(k, 0) \) is related to \( v_{m-1}(k + 1, 0) \) and \( v_{m-1}(k - 1, 0) \) by the recurrence relation

\[
v_m(k, 0) = a_k v_{m-1}(k + 1, 0) + b_k v_{m-1}(k - 1, 0).
\]

Equation (6.5.17) follows since an element at point \( k \) can only go to \( k \pm 1 \) in one move. The probability of reaching point 0 from point \( k \) in \( m \) moves thus consists of two parts: the probabilities of reaching point 0 from the two points \( k \pm 1 \) in \( m - 1 \) moves. The coefficients \( a_k, b_k \) are the probabilities of travel from \( k \) to \( k + 1, k - 1 \) respectively.

Consider the case \( m = 1 \); we have

\[
v_0(k, 0) = 0, \quad k = 1, 2, ..., K - 1,
\]

but

\[
v_1(1, 0) = b_1, \quad v_1(k, 0) = 0, \quad k = 2, 3, ..., K - 1.
\]

And then

\[
v_2(1, 0) = b_1, \quad v_2(2, 0) = b_2 b_1, \quad v_2(k, 0) = 0, \quad k = 3, 4, ..., K - 1.
\]

Therefore, by an obvious induction,

\[
v_m(k, 0) \geq v_{m-1}(k, 0), \quad \text{all } k.
\]

This result is also evident by stating it in words. Similarly,

\[
v_m(k, K) \geq v_{m-1}(k, K), \quad \text{all } k.
\]

Since the sequences \( v_m(k, 0) \) and \( v_m(k, K) \) are bounded and monotonic, they possess limits, say \( v(k, 0) \) and \( v(k, K) \). Consequently \( \lim_{m \to \infty} v_m(k) \) exists and is denoted by \( v(k) \). To prove that \( v(k) \) obeys the difference equation, we use Eq. (6.5.17) in the definition of \( v_m(k) \), Eq. (6.5.14). We have

\[
v_m(k) = y_0 [a_k v_{m-1}(k + 1, 0) + b_k v_{m-1}(k - 1, 0)]
+ y_n [a_k v_{m-1}(k + 1, K) + b_k v_{m-1}(k - 1, K)],
= a_k v_{m-1}(k + 1) + b_k v_{m-1}(k - 1).
\]
Taking limits, we then have

\[ v(k) = a_k v(k + 1) + b_k v(k - 1), \]  

(6.5.19)

which is the desired result.

As a practical matter one would not solve the differential equation (6.5.9) by the random walk method just considered. Obviously the time required to achieve reasonable accuracy is much greater than a straightforward iterative solution. However, for problems in higher dimensions the random walk process becomes more attractive. This is particularly true since the random walk method holds out the possibility of computing the solution in a particular region of a problem without considering the solution elsewhere. Further, in problems involving many dimensions, the length of each individual game and the number of required games are a slowly varying function of the number of dimensions in contrast to conventional iteration methods.

To illustrate the random walk in two dimensions, we outline the steps for solving Laplace's equation in a square. The relevant difference equation is

\[ \phi_{j,k} = \frac{1}{4} [\phi_{j+1,k} + \phi_{j-1,k} + \phi_{j,k+1} + \phi_{j,k-1}]. \]  

(6.5.20)

The boundary conditions are assumed known for \( k = 0, K \) all \( j \), and \( j = 0, J \) all \( k \).

The random walk is initiated at point \( j, k \). A random number is generated, and the probability of going in any one of the four directions used to locate the next mesh point. The walk continues until a boundary is reached, say point \( m, n \). The score \( \phi_{m,n} \) is tallied and another game is begun. The mean tally

\[ \bar{\phi}_{j,k} = \sum_{m,n} \phi_{m,n} \]  

(6.5.21)

is the desired result. Proofs of the scoring procedure and generalizations are found in the references (for particulars, see References 6 and 7).

Random walk problems also show the need of modifying the game or the scoring procedure in some way so as to reduce the variance. For instance, a given walk may take many many steps only to reach a boundary point which contributes little or nothing to the total score. Conversely, an element may oscillate back and forth for a long time before finally reaching a boundary. There is an evident need for improvement of the random walk method outlined above.
In this section we discuss a straightforward application of the Monte Carlo method to a typical reactor problem. Many nuclear calculations require studies of neutrons or photons as they pass through matter. The example considered here is sufficiently general to illustrate many of the aspects of particle processing and is representative of a simple application of the Monte Carlo method. Before outlining the computational steps, we first discuss some general procedures for handling transport problems.

In running time-independent Monte Carlo problems, it is often very convenient to introduce a periodic interval, called a census time, at which the population may be surveyed, statistics compiled and published, or certain changes made in the parameters characterizing a problem. In time-dependent problems, a census period is essential. Censuses are also very useful in reducing the variance in a problem: the use of census periods insures the processing of a representative selection of particles present at the beginning of the census period. If no census were used, then the whole calculation might consist of a study of only one initial particle and its progeny. Thus, the initial distribution would be very poorly represented. Other uses of census periods will be mentioned in the next section. In general the census period should be 1/2 to 2 lifetimes of the particle: shorter times waste machine time because many operations are performed only once per census period, longer times may result in a great change in the number of neutrons in the population. This is bad for reasons that will become clear in the next section. At a census statistics may be compiled and published on the results achieved.

In addition to the optional but advised use of census times, Monte Carlo studies in particle motion involve the following essential steps:

1. The selection of a neutron from a population of neutrons. “Selection” means that the six coordinates, $r, v$, characterizing a neutron are assigned to one to be studied. In a multiplicative problem the initial population may be roughly estimated and selected somewhat arbitrarily from whatever may be known about the problem. It has been the authors’ experience with a number of diverse problems of this class that accurate initial populations hasten the convergence to the final answer only a little for reasons that will become clear later. In a problem involving the detailed study of only a small part of a system, the macroscopic features of the population must be accurately found so that the microscopic features can be accurately determined by the Monte Carlo method.

2. In the digital computer the neutron is followed until it dies, more or less as it would diffuse, interact, moderate its energy, alter its direction,
and so on in the actual system. The neutron is said to die whenever it gets captured, escapes from the system, reaches the end of a census period, or in some problems gets below a certain energy. In any event the coordinates characterizing the interesting properties of the neutron surrounding its death will be recorded; at the end of a census period the coordinates $r, v$ characterizing a neutron will certainly be recorded.

3. If any neutrons have been born in a fission or $(n, 2n)$ event, these will be followed to their death. It is advisable in order to save memory space to follow the one most recently born to its death first.

4. After the original neutron and all its progeny of all generations have been followed to their death, a new neutron will be selected from the population present at the beginning of the census period. It and its progeny are followed to their deaths. This process is repeated until as many of the initial population have been studied as desired.

5. If the problem is nonmultiplicative, it is terminated at this point. If the problem is multiplicative, a new census period may be begun until as many as desired have been examined. The data recorded at the end of the previous census period are used as the population for the beginning of the new census period.

With these general remarks about particle transport, we now consider the problem of the calculation of the fast fission factor for an infinite single fuel rod in a unit cell, as shown in Fig. 6.6.1. The fuel rod consists

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FIG. 6.6.1. Idealized unit cell with associated fuel and moderator regions for the calculation of the fast fission effect.
VI. THE MONTE CARLO METHOD

of $^{235}\text{U}$ and $^{238}\text{U}$ with $N_{^{235}\text{U}}$ and $N_{^{238}\text{U}}$ atoms per unit volume, respectively. The moderator will be taken as a single material with atomic density $N_{\text{mod}}$. Various macroscopic cross sections will be denoted by $\sigma_{se}$, $\sigma_{s1}$, $\sigma_{c}$, and $\sigma_{f}$ for elastic scattering, inelastic scattering, capture, and fission. Where necessary a superscript will be used to identify nuclear species. The thermal neutron flux is denoted by $\phi_{\text{th}}(r)$ in the fuel. The approach taken in this section for the present problem will be somewhat naive. Refinements to reduce variance will be discussed in the next section. If the total number of neutrons produced by thermal fission is denoted by $N_{0}$ and if $\Delta N$ neutrons are produced by fast fission, then the final computation of the fast fission factor $\epsilon_{f}$ is

$$\epsilon_{f} = 1 + \frac{\Delta N}{N_{0}}. \quad (6.6.1)$$

We now consider the details of the computation. In this problem it is assumed that the macroscopic behavior of $\phi_{\text{th}}(r)$ is known. This distribution may be sampled by any of the methods discussed in Section 6.3 to determine the location at which the fission neutron is born. On the average two and a fraction neutrons are born in fission. Therefore, in the Monte Carlo method, two neutrons are certainly created in every fission, and a third is created a fraction of the time equal to the fraction above two neutrons born in fission on the average. If 2.4 neutrons are born in fission, then 40% of the time a third neutron is made: if a random number $\kappa < 0.40$, an additional neutron is made, otherwise not.

The selection of the energy of the fission neutrons is next considered. In the problem at hand, since only neutrons of energy greater than about 1 Mev can cause a fission in $^{238}\text{U}$, only a fraction of the fission spectrum is of interest. Let

$$\alpha = \int_{0}^{1 \text{ Mev}} dE \chi(E), \quad (6.6.2)$$

where $\chi(E)$ is the fission spectrum so normalized that

$$\int_{0}^{\infty} dE \chi(E) = 1. \quad (6.6.3)$$

Fairly accurate analytic expressions exist for the fission spectrum; these expressions could be used to select an energy $E$. However, table look-up is more frequently employed because of the cost in computer time to compute the transcendental functions involved and because the table can be of modest size. The neutron energy is selected then in accord with any of the methods outlined in Section 6.3. In this problem, if the
random number $\kappa$ used to select the neutron energy is less than $\alpha$, the neutron is not processed at all, because it can induce no fast fissions. The direction of the fission neutron may be selected again according to the procedure outlined in Section 6.3, since the angular distribution of fission neutrons is isotropic.

The details of particle motion through the medium can be very complicated when irregular boundaries exist. In general the parameters characterizing the direction in which a particle moves change as the particle moves. Cartesian coordinates have the great advantage that the direction cosines do not change for particles moving in straight lines as the particle moves. For this reason Cartesian coordinates are used even in problems having other than rectangular symmetries, even spherical.

After the neutron has been selected by choice of the parameters characterizing it, one must decide whether it gets to a boundary, experiences a nuclear collision, or reaches the end of the census period. The event that is predicted to occur first is, of course, the one that is actually taken to happen in the Monte Carlo calculation. To effect this decision a random number must be generated to determine the total number of mean free paths $l$ the neutron goes before a collision is experienced. If the total macroscopic cross section is denoted by $\sigma$, then the probability of a collision in an element $\Delta l$ located $l$ mean free paths from the present position of the neutron with no collision in between is

$$p(l) \Delta l = \exp (-l\sigma) \sigma\Delta l.$$  \hfill (6.6.4)\textsuperscript{5}

The c.d.f. may be calculated by integrating Eq. (6.6.4). The number of mean free paths the neutron goes is then decided by identifying the resulting c.d.f. with a random number, as mentioned in Section 6.3. Thus,

$$l = -\frac{1}{\sigma} \ln \kappa,$$  \hfill (6.6.5)

where $\kappa$ is a random number between 0 and 1.\textsuperscript{5}

\textsuperscript{5}The logarithm of $\kappa$ may be computed either by the rejection technique mentioned in Section 6.3 or by the following method. Multiply the random number by such a power $p$ of 2 that the product $\kappa \chi$ lies between $\frac{1}{2}$ and 1.

$$\kappa \chi = 2^p \kappa,$$  \hfill (6.6.6)

and

$$\ln \kappa = a(\kappa - \frac{1}{2}) + b(\kappa - \frac{1}{2})^2 + c(\kappa - \frac{1}{2})^3 + d(\kappa - \frac{1}{2})^4 - (p + 1) \ln 2,$$

where $a = 1.994884$, $b = -1.8851356$, $c = 1.8053480$, $d = -0.9400432$ have been so chosen to make the truncated power series expansion a best fit over the interval $0 \leq 2(\kappa - \frac{1}{2}) \leq 1$ to $\ln [1 + 2(\kappa - \frac{1}{2})]$.
The distance to the nearest boundary must be computed. Unfortunately, to determine this quantity the distance to all boundaries must usually be computed. For example, in Fig. 6.6.1 although we can see that the neutron is within the fuel rod, this fact is not usually "known" to the computer, so it must calculate the distance not only to the cylinder and the north wall, but also to the projection of the east wall. (In this problem it would be practical to keep track of which region the neutron is in, but in more complicated geometries this is usually not the case. It is also usually very time consuming to determine by testing which region of several the neutron may be in if the region is unknown. However, a method that is especially suited to complex geometries will be given later.)

A simple method for calculating the distance to a boundary is now considered. The essential idea is to characterize the geometrical surface by some simple vector equation. For example, if \( \mathbf{n} \) is a unit vector along the axis of our cylinder, then the cylinder is characterized by the statement that

\[
(\mathbf{n} \times \mathbf{r'})^2 = r_0^2,
\]

(6.6.7)

where \( \mathbf{r'} \) is a vector from the origin on the axis of the cylinder to the point of the cylinder at which the neutron will hit the cylinder.

\[
\mathbf{r'} = \mathbf{r} + L\mathbf{\Omega},
\]

(6.6.8)

where \( \mathbf{r} \) is the vector from the origin to the present position of the neutron which goes in the direction specified by the unit vector \( \mathbf{\Omega} \). \( L \) is the distance from the neutron to the point of impact with the bounding cylinder. Now from Eqs. (6.6.7) and (6.6.8), we learn that

\[
(\mathbf{n} \times \mathbf{r'})^2 = (\mathbf{r} + L\mathbf{\Omega})^2 - (\mathbf{n} \cdot \mathbf{r} + L\mathbf{n} \cdot \mathbf{\Omega})^2.
\]

(6.6.9)

Upon equating this expression to \( r_0^2 \) according to Eq. (6.6.7) and solving for \( L \), we find

\[
L = \left( (\mathbf{n} \cdot \mathbf{r})(\mathbf{n} \cdot \mathbf{\Omega}) - (\mathbf{r} \cdot \mathbf{\Omega}) \pm \sqrt{[((\mathbf{n} \cdot \mathbf{r})(\mathbf{n} \cdot \mathbf{\Omega}) - (\mathbf{r} \cdot \mathbf{\Omega})]^2 + [1 - (\mathbf{n} \cdot \mathbf{\Omega})^2][r_0^2 + (\mathbf{n} \cdot \mathbf{r})^2 - r^2]]^{1/2}} \right) [1 - (\mathbf{n} \cdot \mathbf{\Omega})^2]^{-1},
\]

(6.6.10)

the desired relation. The plus sign is used if the neutron is inside the cylinder and the minus sign is used if it is outside. Figure 6.6.2 illuminates some of the vector relations. In the case of a sphere the distance to the boundary is given by

\[
L = -\mathbf{\Omega} \cdot \mathbf{r} \pm \sqrt{(\mathbf{\Omega} \cdot \mathbf{r})^2 + r'^2 - r^2},
\]

(6.6.11)
where the origin is taken at the center of the sphere, the association of the + and − signs being as for the cylinder. The distance to a plane boundary is given by

\[ L = (r' - r) \cdot n/(\Omega \cdot n), \]  

(6.6.12)

where \( n \) is a unit vector perpendicular to the plane through the point of reference. The distance to the closest boundary is selected, and the transit time computed from the known speed with which the neutron travels. In the present example, a neutron upon reaching a plane surface would be reflected there in the calculation, since then the next cell into which the neutron would penetrate in the actual system would be correctly simulated by the one at hand in the calculation.

The neutron will eventually experience a collision. At a collision several decisions must be made. The material with which the neutron collides is found as follows: Define

\[ \Xi_i = \sigma_i / \sum_{j=1}^{N} \sigma_j, \]  

(6.6.13)

where \( \sigma_i \) is the total macroscopic cross section for element \( i \). The quantity \( \Xi_i \) may be regarded as the fraction of the unit interval occupied by the element \( i \). The element may be selected by generating a random number \( \kappa \) and finding the largest \( i \) for which

\[ \sum_{j=1}^{i-1} \Xi_j \leq \kappa. \]  

(6.6.14)
Once the element has been selected, the nature of the collision is determined. The variation of cross sections with energy is usually so complicated that table look-up is the only practical procedure for specifying cross sections as functions of energy. A random number is then used to determine the type of collision. The various types of collisions that one might consider are as follows:

1. **Capture.** In this case the particle history is terminated and another neutron is picked up.

2. **Fission.** In this case the particle history is terminated and appropriate data concerning the vital statistics of the neutron causing fission are recorded. The energy and location of the neutron inducing fission are likely to be of interest in this connection, or one particle can be added to the appropriate energy group tally and to the appropriate spatial zone tally.

3. **Inelastic scattering.** In this event the energy and direction of the scattered particle must be found. In this connection tables of the cross sections for inelastic scattering between various groups \( g \) and \( g' \) are required. One random number may be used to select the energy of the scattered neutron and consequently the group in which this neutron falls. In this problem, if the scattered neutron has an energy below the fission threshold, the particle history is terminated, and if desired, appropriate statistics recorded. Since inelastic scattering is important chiefly only for heavy elements, the neutrons may be assumed isotropically scattered in the laboratory system. The direction cosines may then be chosen as described in Section 6.3.

4. **Elastic scattering.** This case is the one that most frequently occurs. The energy of the scattered neutron can be found from Eq. (B.8) once the cosine of the scattering angle in the center-of-mass system is known. As always, if the energy of the scattered neutron is less than the fission threshold of \(^{238}\text{U}\), the particle history is terminated. If the scattering is isotropic, then, the direction cosines in the center-of-mass frame with its axes parallel to the corresponding axes of the laboratory system may be found by the method indicated in Section 6.3. The direction cosines referred to the laboratory system may then be found by Eqs. (B.21). One the other hand, if the scattering is anisotropic, then the cosine of the angle of scattering must be found from the scattering law and the azimuth chosen randomly about the direction of the incident neutron by the method mentioned in Section 6.3. The scattering law is usually made available to the computer in the form of a table. The direction cosines thus found are transformed from the center-of-mass frame with
its $z$ axis along the direction of the incident neutron to those of the center-of-mass frame with its axes parallel to the corresponding ones of the laboratory frame by Eqs. (B.30). These in turn are transformed to those referred to the laboratory frame by Eqs. (B.21).

Once the particle directional and energy parameters are found after the collision, the computer proceeds to find the times to the next boundary crossing, census, and collision.

It is evident from this problem that, since $\Delta N/N_0$ is on the order of a few percent and since the fuel rods are at most on the order of a mean free path in thickness, many neutrons must be processed per fast fission, and hence very few histories contribute to the result. Large variance is the consequence. Variance reduction methods will be considered in Section 6.7.

It is further evident from the discussion above that in a problem involving a complicated geometry, many boundaries must be checked for each possible boundary crossing and that in checking the distances to curved boundaries, a great amount of calculation is required. Since many histories must be followed to get reasonable accuracy and since the Monte Carlo method is inherently capable of handling complicated geometries, it behooves us to find some more efficient way to treat such geometries (see Reference 10). Two facts may be exploited to this end:

1. The probability of crossing boundaries more removed than three mean free paths is quite low.

2. Tests for the crossing of planes perpendicular to the Cartesian coordinate axes are very simple since they involve only a comparison of the coordinates of the particle with the corresponding ones describing the orthogonal planes. Accordingly, a substantial amount of computer time can be saved if the system is subdivided by a set of planes orthogonal to the coordinate axes. Orthogonal planes are circumscribed around every curved surface with a diameter of curvature one mean free path or more, thus dividing the system into a number of geometrical parts each of which will be called a zone. Some of the boundaries of a zone may be purely mathematical, some may be physical. Parts of the system physically small compared with a mean free path can often be treated sufficiently well by homogenization. To further facilitate the determination of boundary crossings, certain orthogonal planes may be chosen as block boundaries. These should include at least six zones along any edge. The block within which the neutron is located is first determined, a matter that can be executed with great speed in view of the easy comparisons involved. The zone within which the neutron is found is determined by
examining the boundaries of all those and only those zones within this block. Orthogonal planes located too closely together defeat the very purpose for which they are installed in the system; orthogonal planes located too far apart will not be very effective in simplifying the search for the zone within which the neutron is located. About three mean free paths apart is approximately optimum for many problems.

Approximate expressions for the distance to a curved boundary that are less than this actual distance can often be used to expedite the calculations. If a boundary crossing based upon the use of the approximate expression is predicted, the prediction can be checked by a calculation with the exact expression.

### 6.7 Variance Reduction Methods

In the preceding example we have observed the need for modifying a game or scoring procedure in order to reduce the variance or error. A number of variance reducing methods have been examined in the literature partly because of the obvious need for them and partly for their mathematical appeal. We shall display a few of these methods. However, the reader is strongly cautioned against their indiscriminate use. Normally, the lowest possible variance is desired with a given amount of machine time. Complicated variance reduction schemes can cost so much time that a lower variance results by avoiding their use and by using the time saved to follow more histories. It has been the authors' experience in many problems that the reduction of variance by elaborate weighting, for example by assigning different weights to different regions of space and/or to different speed groups, should only be used when mandatory. These cases will make themselves obvious, and the way in which the weighting should be carried out in such cases is usually very obvious from rough calculations or physical intuition. For example, a problem involving huge attenuation through shields is one that can be handled only by suitable weighting. Again, weighting should not be used, for example, in criticality studies of light water systems.

The importance sampling method is the first variance reduction method to be discussed. The basic idea here is to play a game so modified that the variance is reduced by selecting from a distribution other than that suggested by the problem. The technique is perhaps best illustrated by the problem of calculating by the Monte Carlo method an integral

\[
\langle g \rangle = \int_{a}^{b} dx \ g(x) \ f(x) \tag{6.7.1}
\]
with $f(x)$ a p.d.f. A statistical estimate of $\langle g \rangle$ is

$$
\bar{g}_1 = (1/N) \sum_i g(x_i), \tag{6.7.2}
$$

where the $x_i$ are chosen from $f(x)$. Let us now consider modifying the integrand in the form

$$
\langle g \rangle = \int_a^b dx \frac{g(x)}{f^*(x)} f^*(x), \tag{6.7.3}
$$

with $f^*(x)$ a p.d.f. such that $g(x)f(x)/f^*(x)$ exists everywhere in the interval $a \leq x \leq b$.

Obviously, either form gives the same expected value. The statistical estimate

$$
\bar{g}_2 = (1/N) \sum_i g(x_i)f(x_i)/f^*(x_i) \tag{6.7.4}
$$

has the expected value $\langle g \rangle$ when the $x_i$ are chosen from $f^*(x)$. We now compare the variance associated with $\bar{g}_1$ and $\bar{g}_2$. By Eq. (6.4.10), the variance for the first method is given by

$$
V_1(\bar{g}_1) = (1/N) \int_a^b dx (g(x) - \langle g \rangle)^2 f(x) \tag{6.7.5}
$$

$$
= (1/N) \left[ \int_a^b dx g^2(x)f(x) - \langle g \rangle^2 \right],
$$

whereas the variance for the second method is given by

$$
V_2(\bar{g}_2) = (1/N) \int_a^b dx \left( \frac{g(x)f(x)}{f^*(x)} - \langle g \rangle \right)^2 f^*(x) \tag{6.7.6}
$$

$$
= (1/N) \left[ \int_a^b dx \frac{g^2(x)f^2(x)}{f^*(x)} - \langle g \rangle^2 \right].
$$

In general, the two variances $V_1$ and $V_2$ differ. The objective is to choose an $f^*(x)$ which makes $V_2$ smaller than $V_1$. If $g(x) \geq 0$ in $a \leq x \leq b$, then

$$
f^*(x) = g(x)f(x)/\langle g \rangle \tag{6.7.7}
$$

would yield an answer of zero variance. This result is hardly surprising since knowledge of the optimum $f^*(x)$ requires knowledge of the answer. The example does show, however, the possibility of making a very good choice of $f^*(x)$. 

6.7 VARIANCE REDUCTION METHODS
In general the choice of $f^*(x)$ is a difficult matter. Clearly the wrong choice can increase the variance. Intuitively a distribution $f^*(x)$ is desired that concentrates on the portion of the interval which contributes most to the integral, i.e., is the most important to the integral, whence the name of the method.

A special case of importance sampling is the so-called splitting method or Russian roulette. In this method it is recognized that some regions of velocity-configuration space may be more important and contribute more heavily to the final answer than others. Accordingly, these regions should be studied more intensively than those of lesser importance. Consequently the concept of particles carrying weight is introduced, and important regions are studied by many particles having little weight, whereas unimportant regions are studied by few particles having high weight. For example, in a problem in which the attenuation through a shield is being investigated, the particles near the exit face would have a much lower weight than those near the entrance face, since the neutrons near the exit face contribute much more heavily to the final answer than neutrons near the entrance face.

Each particle followed may in general represent many neutrons, since restrictions on the use of machine time usually limit the number of histories followed to less than 10,000, 1000 being frequently followed. The number of neutrons $n$ is related to the weight $W$ of $N$ particles by

$$n = CWN,$$  \hspace{1cm} (6.7.8)

where $C$ is some proportionality constant. This constant needs to be evaluated only in problems involving the accretion and depletion of nuclear matter. This equation governs the reweighting process, for in this process neutrons must be conserved. Thus if for some reason the weight of a particle is to be changed from $W$ to $W'$, then $W/W'$ particles must be followed after the reweighting for each one followed prior to the reweighting in order that the number of neutrons be unchanged. If $W/W'$ is larger than one, then $W/W'$ particles are created with the same relevant coordinates $v, r$ as the particle previously being followed. Should $W/W'$ be an integer plus a fraction, then $\lfloor W/W' \rfloor$ particles are always created, where $\lfloor W/W' \rfloor$ is the greatest integer less than $W/W'$, and an extra particle is followed $W/W' - \lfloor W/W' \rfloor$ of the time. To this end, an extra particle is followed if a random number $\kappa$, scaled between 0 and 1, is less than $W/W' - \lfloor W/W' \rfloor$. The case of $W/W'$ less than 1 is merely a special case of that already discussed. The resulting game is called splitting if $W/W' > 1$ and Russian roulette if $W/W' < 1$.

Variance can be reduced by avoidance of gaming where possible. The
use of weights gives a way of reducing the gaming. For example, if a particle experiences a nuclear event, scattering, fission, and capture may occur with the probabilities $\sigma_s/\sigma$, $\sigma_f/\sigma$, and $\sigma_c/\sigma$, respectively. After the event a particle with weight $\nu_{\sigma_f} W/\sigma$ is recorded in memory with the coordinates $\mathbf{r}, \mathbf{v}$ of the parent; this particle's history would be followed later. The death weight $W(\sigma_c + \sigma_f)/\sigma$ would be tallied, if desired, and a particle of weight $W_{\sigma_s}/\sigma$ and coordinates $\mathbf{r}, \mathbf{v}$ would be followed. Death then can now come to a particle in such a game only by Russian roulette and by being lost from the system. Further, it will be noted that if a number of nuclides are present, the particle experiences an event with an average nuclide if the macroscopic cross sections, $\sigma$, are used with no loss of information and with a reduction of variance. Of course, with this method of gaming, the angular distributions for anisotropic scattering of the different nuclides must be compiled into a composite $f(\theta)$ by means of the macroscopic cross section:

$$f(\theta) = \frac{\sum_i \sigma_i f(\theta)_i}{\sum_i \sigma_i},$$  

(6.7.9)

where $f(\theta)_i$ is the angular distribution for the $i$th nuclide. Likewise, for all other distributions, such as the fission spectra, the spectra resulting from elastic or inelastic scattering, and so forth.

If such a weighting procedure is used, then it is advisable to introduce weight standards for each of the various regions of velocity-configuration space to broadly limit the range over which the weights of the particles may vary for several reasons (see Reference 10).

1. It is inadvisable to reweight the particles at each game because of the increased variance introduced by the gaming. If certain facts are definitely known, such as the relative probability with which various nuclear events may occur, the use of these facts will avoid the playing of a game and the introduction of variance.

2. Since importances are only approximately known in any case, it makes no sense to control the weights of the particles very closely by reweighting at each game.

3. The control of the weights within broad limits will reduce variance by preventing the computer from wasting time in following particles whose weight has been reduced to a very low value.

It seems reasonable then to control the weight of a particle within a factor of two; whenever the weight of the particle exceeds the weight standard by a factor of two, it is split until the weight is reduced to within this factor; whenever the weight is less than the weight standard,
a game of Russian roulette is played with its life at stake with the odds in favor of life given by the ratio of its weight to the weight standard.

Two rather definite rules emerge from experience in the use of weight standards.

1. All weight standards should be equal unless it is mandatory that they be different in order to get an answer with reasonably low variance. Attenuation and perturbation problems require the use of weight standards; criticality studies do not.

2. The use of weight standards in different regions of velocity-configuration space differing by a factor of less than 8 or so in criticality calculations wastes machine time and violates the very reason for which weighting was introduced.

Calculation of the attenuation in shields provides an illuminating example of the use of importance sampling by the use of weights. If no weights were used, then even a study of a million histories might result in no particles penetrating the shield if its attenuation were in excess of a million. The variance would be enormous. In a shield problem, splitting planes are often inserted in such a way that the population of particles studied is maintained approximately constant (see Fig. 6.7.1).

The weight standard of a zone is one-half that of the zone to the left and double that of the zone to the right. Accordingly, particles crossing from left to right across a splitting plane will be doubled in number on the average, and in crossing from right to left will be halved in number. In a problem involving low attenuation, the placement of the splitting planes, i.e., the choice of the weight standards can be found by the relation

\[ z = k \sigma \ln 2 \]

where \( k \) is an integer, and \( \sigma \) is the macroscopic cross section for neutrons.
of the most penetrating energy within the range of energies that neutrons may have. In problems involving great attenuation, if the splitting planes are too far apart, the particle population may approach zero at the exit plane and thus lead to high variance; if the splitting planes are too close, the particle population may drastically increase with consequent increase in variance resulting from an inadequate study of the initial population of injected particles because of limitations of computer time. Accordingly, for problems involving great attenuation the Monte Carlo method must be used to locate the splitting planes. To this end, particles are injected from the left and a plane is located such that half the original number of particles die to the right of the location where the splitting plane will be placed. After insertion of the plane, another set of neutrons is injected, and the second plane is located at that place where half the original number of neutrons injected die to the right. The procedure is repeated until all planes have been placed, after which a large number of particles can be injected to find the attenuation more accurately. The scheme suggested is stable against statistical fluctuations: if a plane is placed too close to the one previously placed, the next will be placed a little farther away to keep the neutron population about constant.

The use of census periods was mentioned in Section 6.6 for the purpose of running time-dependent problems, making parameter changes, auditing the population of both time-independent and time-dependent problems, and so on. Census periods can also be used to reduce variance. At the end of each census period the total population may be audited and new weights established so that the population will be returned to the original number during the next census period. Thus, if the population has decreased because of the attenuation of particles within a shield, it may be restored by reducing the weights. Alternatively, splitting planes a little too close together may be used and the population restored to normal size at the start of each census period. Censuses have proved very useful in practice.

If the statistics of less penetrating particles are desired at the exit face of the shield, then splitting planes can be placed somewhat closer together near this face so that these particles will be forced through.

A complementary procedure to the splitting and weighting just discussed is the use of expected values. Frequently it is simple to compute the probability that a particle penetrates to a given distance, for instance through a shield. For such cases one assumes a fraction $a$ of the particle does penetrate, whereas a fraction $(1 - a)$ is left to diffuse. If the initial weight is $W$, then $Wa$ is tallied for the transmission, and $W(1 - a)$ is the remaining weight. After each collision the expected penetration is tallied, and the remaining weight processed, etc.
VI. THE MONTE CARLO METHOD

Another special case arises in the study of the effect of strong perturbations over small volumes of an assembly. Small perturbations over large volumes are better handled by standard perturbation theory. The following techniques are used in the case of a localized strong perturbation (see Reference 10):

1. The population of particles used to study the perturbed problem is initially identical to that for the unperturbed problem. Further, these populations and the statistical fluctuations remain the same until the particles diffuse into the small region of the large perturbation.

2. Weight standards are chosen so as to enhance greatly the diffusion of particles into the perturbing region. This means that near the perturbation, zones having a low weight standard will be used compared to the weight standards of more distant regions. The values of the weight standards should be selected so that a significant part of the population is within five mean free paths of the perturbed region.

3. The population in the unperturbed problem is allowed to come to equilibrium before starting the calculation of the perturbed problem.

There are many other ways to reduce variance. One of them is called forcing. In this method it is assumed that the expected number of events of each type is known, a tally is kept of the number of each that has actually occurred, and a biased game is played to encourage more of those events which are below the expected number. For example, let \( K \) be a forcing constant and suppose a decision between a reaction [capture, fission, \((n, 2n)\) event] or a scattering (isotropic or anisotropic) is to be made. Assume that \( N_r \) reactions have occurred in \( N \) games. Then if a random number \( \kappa \), scaled between 0 and 1, is such that

\[
\kappa < \frac{\sigma_r}{\sigma} + K \left( \frac{\sigma_r}{\sigma} - \frac{N_r}{N} \right) \tag{6.7.10}
\]

a reaction is decided upon. If too few reactions have taken place, there is a bias in favor of more reactions by an amount proportional to the disparity between the actual and expected values and to the forcing constant. By making the forcing constant large enough, the game can be made deterministic. Determinism in one game within the whole Monte Carlo calculation is all right, but at two or more points there is a danger of correlation. In general, morality is a virtue in gaming as elsewhere: play the game straight and stay out of trouble. Really there is no reason to use forcing at all, since if expected values are known, the method in which weights are changed is better.
Finally we mention a procedure called systematic sampling (sometimes called quota sampling). The method is very similar to forcing. The basic idea is to reduce or eliminate the variance associated with random selection in the first or early stages of the computation. The process is used only for one distribution, and hence no correlation problems arise. As an example, consider the integral in Eq. (6.5.4). Let the interval \( a \) to \( b \) be divided into \( f \) subintervals with the points \( a = x_0 < x_1 < \ldots < x_f = b \). The factors \( p_j \) are defined by

\[
p_j = \int_{x_{j-1}}^{x_j} dx f(x).
\] (6.7.11)

If the integration is to be approximated with \( N \) points, then the expected number of points within the interval \( x_{j-1} \) to \( x_j \) is merely

\[
\bar{n}_j = p_j N.
\] (6.7.12)

The systematic sampling is done by assigning \( \bar{n}_j \) points to the \( p_j \)th subinterval. Within the subinterval the \( \bar{n}_j \) points may be distributed uniformly.

What has been accomplished by this process is the elimination of any variance associated with the initial selection of points for evaluating the integral. Usually the variance reduction is small; however, the method is simple to apply and is frequently used.

6.8 Concluding Remarks

We conclude this chapter with a few remarks concerning the Monte Carlo method:

1. Do not use the Monte Carlo method if any other method is available. It is a method of last resort.

2. Use variance reduction if and only if it is really necessary. Statistical estimates of the variance using computed results should be considered only as suggestive of the true variance. Great caution should be exercised in attributing precision to a result merely from low variance of past histories, since the variance estimate is an asymptotic function of the number of histories. Use known expected values wherever possible.

3. Particles must be followed for many nuclear lifetimes to remove any hereditary influences of the initial population. The fluctuations within one lifetime will be much smaller than those over many lifetimes, and these small fluctuations can give a very false impression of reliability and accuracy.
4. Check the coded program by all possible methods, and check it again.

The checking of Monte Carlo coded programs is especially difficult (1) because of the intensely complex logic, (2) because this logic is not deterministic, (3) because events wrongly calculated may be sufficiently rare to hide the error and yet large enough to influence the results, and (4) because the statistical nature of the calculations masks such errors. Several suggestions are offered to make any errors obvious and to isolate them.

1. Check each individual subroutine before assembling it into the larger routine. Check as many aggregates of subroutines as possible.

2. Run a series of simple, extreme problems so designed as to bound the class of all possible problems for which the Monte Carlo will be used. Artificial substances in which neutrons experience only one type of nuclear event are particularly useful to check the routines with respect to that event. Everything should be checked, such as tallies, the velocities and locations of particles, the conservation of neutrons. Sometimes the injection of particles at one point with one velocity will facilitate precise checks; at other times statistical checks on velocity distributions, for example, on a reasonable sample of particles must be run. Input data should be as troublesome to the computer as possible. Run problems involving simple and complex geometries in which the matter consists of a vacuum to check the crossing of boundaries. If possible, observe the trajectories of the particles on an on-line oscilloscope to check these routines. Boundary crossings are particularly troublesome because of round-off error within the machine. When a particle hits a boundary, design the boundary crossing routine such that a small amount is added to its coordinates to force it across regardless of this round-off.

References

The literature on the Monte Carlo method is surprisingly sparse. There are many articles and chapters devoted to the topic, but no comprehensive review exists to the authors' knowledge. For reasonably broad coverage of the method, References 1–5 are recommended. Certain special topics such as random walk, random number generation, etc. are discussed in References 6–11. References 12 and 13 are two very readable texts on statistics, including the central limit theorem.


Problems

1. A linear interpolation between tabular points \( F(x_i) \) and \( F(x_{i-1}) \) assumes the random variable \( x \) is uniformly distributed over the interval \( x_{i-1} \) to \( x_i \). If \( F(x) \) is known to be concave upward or downward more accurate parabolic interpolation may be used. Show that for \( F(x) \) concave upward we have

\[
x = \sqrt{x_i^2 - \frac{(F(x_i) - \kappa)}{F(x_i) - F(x_{i-1})}(x_i^2 - x_{i-1}^2)},
\]

and for \( F(x) \) concave downward

\[
x = \sqrt{x_i^2 - \frac{(\kappa - F(x_{i-1}))}{F(x_i) - F(x_{i-1})}(x_i^2 - x_{i-1}^2)},
\]

where \( \kappa \) is a random number. What are the advantages and disadvantages of the parabolic interpolation methods?

2. Prove Eq. (6.3.16).

3. Show that the direction cosines of a random direction may be selected by choosing a point randomly within a semicircle and are given by

\[
\alpha_d = \left( \frac{\eta_x^2 - \eta_1^2}{\eta_x^2 + \eta_1^2} \right) (1 - \eta_3^{1/2}),
\]

\[
\beta_d = \left( \frac{2\eta_x\eta_3}{\eta_x^2 + \eta_1^2} \right) (1 - \eta_3^{1/2}),
\]

\[
\gamma_d = \eta_3,
\]
where \( \eta_1 \) and \( \eta_2 \) are acceptable random numbers, scaled between 0 and 1 and between \(-1\) and \(1\), respectively, if and only if

\[
\eta_1^2 + \eta_2^2 < 1
\]

and where \( \eta_3 \) is any random number scaled between \(-1\) and \(+1\). Hint: Consider the trigonometric relations \( \sin 2\varphi \) and \( \cos 2\varphi \), and \( \sin \varphi \) and \( \cos \varphi \).

Show that the efficiency of selection of the random numbers is \(78.5\%\).

4. By selecting a point at random that lies within a unit sphere, show that the cosines of a random direction are given by

\[
\begin{align*}
\alpha_d &= \eta_1[\eta_1^2 + \eta_2^2 + \eta_3^2]^{-1/2} \\
\beta_d &= \eta_3[\eta_1^2 + \eta_2^2 + \eta_3^2]^{-1/2} \\
\gamma_d &= \eta_3[\eta_1^2 + \eta_2^2 + \eta_3^2]^{-1/2}
\end{align*}
\]

where \( \eta_1 \), \( \eta_2 \), and \( \eta_3 \) are acceptable random numbers, scaled between \(-1\) and \(+1\), if and only if

\[
\eta_1^2 + \eta_2^2 + \eta_3^2 < 1.
\]

Show that the efficiency of selecting the cosines of this random direction is \(52.4\%\).

5. Prove Eq. (6.4.16).

6. Suppose \( y = x_1^2 + x_2^2 \), where \( x_1 \) and \( x_2 \) are independent variables distributed according to

\[
f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.
\]

Show that

\[
\begin{align*}
f(y) &= 1/2 e^{-y^{1/2}} \quad \text{if } y > 0 \\
&= 0 \quad \text{if } y < 0
\end{align*}
\]

7. Suppose \( y = \eta_1 - \eta_2 \), where \( \eta_1 \) and \( \eta_2 \) are random numbers scaled between 0 and 1. Show that if \( 0 \leq y \leq 1 \),

\[
f(y) = 2(1 - y).
\]

8. Suppose the probability that \( y \) has a value in the range \( dy \) centered at \( y \) is \( f(y)dy \), where \( f(y) = 3y^2 \) and suppose that \( 0 \leq y \leq 1 \). Show that \( y = \eta/3 \), where \( 0 \leq \eta \leq 1 \).

9. The differential probability distribution of \( y \) is \( f(y) = 4/\pi(1 + y^2) \), where \( 0 \leq y \leq 1 \). Show that \( y = \tan \eta\pi/4 \), where \( 0 \leq \eta \leq 1 \).

10. The differential probability distribution of \( y \) is \( f(y) = 2/\pi \sqrt{y}(1 + y) \). Devise a rejection technique for choosing \( y \) from this distribution. Find the efficiency.

11. Suppose \( y = \eta', \) where \( 0 \leq \eta \leq 1 \). Show that the probability that \( y \) has a value in the interval \( dy \) centered at \( y \) is

\[
\frac{1}{\eta} y^{-(\eta-1)} dy.
\]

13. Prove Eqs. (6.6.11) and (6.6.12).

14. Flow chart a Monte Carlo routine in which isotropic elastic scattering, anisotropic elastic scattering, capture, inelastic scattering, \((n, 2n)\) events, and fissions are each considered individually.

15. Devise a boundary crossing routine for zones consisting of concentric spheres only, taking round-off error into account.

16. Devise a boundary crossing routine for zones consisting of only coaxial cylinders infinitely long, taking round-off error into account.

17. We have coded a program that has no provision for recording the coordinates of the particles that leak out of a reactor but that has a provision for recording the coordinates of each neutron in each zone within the reactor. Devise a simple method for finding the spectrum and angular distribution of neutrons that leak out of the reactor.

18. Program a subroutine to calculate the logarithm of a random number according to the rejection technique discussed.

19. Program a Monte Carlo routine in which isotropic elastic scattering and anisotropic elastic scattering are considered as one nuclear event and capture, fission, \((n, 2n)\) events, inelastic scattering are considered as another event.

20. Devise a generalized boundary crossing routine for zones consisting of spheres, cylinders, planes, cylindrical cones, elliptical cones, elliptical cylinders, and ellipsoids. Hint: Consider that such boundaries can be described by a formula of the type

\[
ax^2 + by^2 + c(z - z_0)^2 - K = 0. 
\]

Show that the distance to any boundary is given by

\[
\frac{-e + j \sqrt{e^2 - hr}}{h}
\]

where

\[
e = a\alpha x + b\beta y + c\gamma (z - z_0),
\]

\[
h = a\alpha^2 + b\beta^2 + c\gamma^2,
\]

\[
r = ax^2 + by^2 + c(z - z_0)^2 - K,
\]

and \(j = 1\) if the expression (1) changes from negative to positive as the neutron crosses the boundary and \(j = -1\) if the expression (1) changes from positive to negative. A neutron is inside the \(a\) zone if \(jr > 0\) for any of the boundaries.

21. Program a Monte Carlo routine that takes delayed neutron emitters into account. Hint: Devise a routine to consider representative times, then extrapolate past results. Calculate what the sources will be and use them to inject neutrons.

22. Suppose we have an infinite plane slab used as a shield. The attenuation of neutrons through the slab is very great.
(a) Program a routine that will automatically locate particle splitting planes stably.

(b) Program a routine that will calculate accurately the number of neutrons that leave the slab through a small spot on the surface.

23. Discuss the merits and faults of the following criteria for locating splitting planes:

(a) The planes are so located that the number of deaths in the zone on the left of the prospective position, i.e., the space between itself and the most recently placed boundary, is one-half the original number.

(b) The prospective boundary is to be so placed that the number of deaths to its right will be half the number of particles that emerge from the preceding boundary.

(c) The prospective boundary is so placed that as many more deaths above the initial number of particles injected occur in the region to its right as occurred short of the required number to the right of the preceding boundary.

All of these schemes for locating splitting planes are inferior to the one mentioned in the text.