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Monte Carlo Particle Transport Methods

Neutron and Photon Calculations

Iván Lux, László Koblinger

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Monte Carlo Particle Transport Methods: Neutron and Photon Calculations

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PREFACE

With this book we try to reach several more-or-less unattainable goals, namely:

- To comprise in a single book all the most important achievements of Monte Carlo calculations for solving neutron and photon transport problems;
- To present a book which discusses the same topics in the three levels known from the literature;
- To write a book which gives useful information for both beginners and experienced readers;
- To list both the well-established old techniques and the newest findings;
- To fulfill the functions of both a textbook and a handbook; and last but not least,
- To formulate everything in a manner that is understandable (and, perhaps, sometimes even enjoyable) for the interested readers.

These are the goals . . . The judgement whether we were at least partly successful in reaching them is for the readers.

Iván Lux
László Koblinger

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Chapter 1

SCOPE AND STRUCTURE OF THE BOOK

Monte Carlo methods are being efficiently used for solving widely varying types of physical problems. Although Monte Carlo is trivially a straightforward tool to stimulate random processes, it can also be used for solving problems that have no immediate probabilistic interpretation.

The first inventions of the method go back very far in history,[4] however, extensive applications came along with the construction and use of modern digital computers, i.e., from the late 1940s.

Historically, the Monte Carlo method has first been successfully used to solve particle transport problems and this is still one of the areas of most extensive use.[1]

The general method was originally developed by Fermi, Ulam, and von Neumann,[2] the first comprehensive review was published by Kahn,[6] and the high quality of this early contribution cannot be better evaluated than by stating that people interested in the use of Monte Carlo are well advised even nowadays to start with Kahn's report.

The first book written exclusively for photon and neutron random walk simulations was published by Cashwell and Everett,[2] a newer review[1] — also from the Los Alamos group — appeared in 1975.

Neutron transport is discussed with higher mathematical apparatus by Spanier and Gelbard.[9]

There are many books describing the particle transport in general — in these books, Monte Carlo is studied as one of the tools, generally in a separate chapter.[10,11] On the other hand, many reviews dealing with diverse aspects of Monte Carlo contain chapters devoted to particle transport.[5,7,8]

The novelty of this book — and therefore the justification of its edition — can be briefly summarized in two points.

First, the latest textbook[9] deals only with specific problems and since it was published more than 20 years ago, it obviously does not cover the developments of the last decade. The newest methods, the rigorous and unified theory of which is the product of the last 6 or 7 years, can only be found in journal articles. In our judgment, these new methods (variance reducing techniques, efficiency analyses, combined scoring schemes, etc.) have now reached the point where they can be discussed in a precise and comprehensive way, in such a manner that is necessary for a textbook.

Secondly, the present situation in the relevant literature is the following: There exist several introductory books or chapters[2,11] which describe the simplest direct simulation procedures. Other reviews[10,3,1] already discuss several more advanced methods, however, such complicated though generally the most efficient techniques are only briefly mentioned, and not all of them at all. For the present users of Monte Carlo there might seem to be a gap between the level of the existing books and the much more refined description of the newest methods in the journal papers.

This book aims to constitute a bridge over the gaps of the different levels. We do hope that this treatise in a single book at successively deeper levels, will satisfy an existing demand.

The structure of the book is planned to coincide with the above-mentioned purpose.

After an Introduction (Chapter 2) describing the basic sampling processes and precisely defining the later used quantities, Chapter 3 deals with the heuristically obvious methods: the one-to-one numerical simulation of the original physical processes and those modifications which are easily understood without rigorous and tiring mathematical derivations.

In Chapter 4 the integral form of the Boltzmann Equation is the starting point. Here,

by a little bit more mathematics, the introduction of several more advanced techniques (such as the adjoint treatment) becomes possible.

In Chapter 5 the whole treatment is based on the moment equations. The investigation of the equations that govern various moments of the Monte Carlo estimates are extremely helpful for increasing the efficiency of the methods.

Special games (correlated, perturbation and differential Monte Carlo; criticality and flux at a point calculations) are discussed in Chapter 6 — based on the mathematical treatment introduced in the previous part.

The last Chapter is devoted to optimization of the techniques (splitting, path stretching, Russian roulette, etc.) widely used in deep-penetration Monte Carlo calculations.

Our intention was to compile the book in such a way that readers whose interest extends just to the depth of the first or to the second level, are provided with a concise and easily intelligible treatise of all the necessary tools for preparing Monte Carlo programs and solving problems. Though the real novelties are necessarily subjects of the later Chapters, we do hope that the reader can find new approaches, or descriptions of well-known techniques from a new, and hopefully interesting, point of view even in the first Chapters.

We also hope that the understanding of the first level treatment will trigger out the curiosity of many readers to start to study the second and even further, the third level.

Readers of the last three Chapters become familiar with the complete set of the most sophisticated weapons of the Monte Carlo arsenal.

An essential feature of the book is that the same nomenclature and a unified notation is used throughout the different Chapters, wherever possible.

Cross references between the various levels (particularly from higher levels to lower ones) make it obvious for the reader that the different approaches represent different projections of the very same physical phenomena.

References are given at the end of each Chapter, therefore, several basic sources are listed more than once in the book. From our point of view, such repetitions are not unnecessary, but rather make the reader's orientation easier.

It is clear for us that the inclusion of all the knowledge accumulated during 4 decades by a lot of scientists is impossible. Apart from the limitation mentioned already in the title of the book, i.e., that we deal only with transport of neutrons and photons, the most serious stipulation is that with very few exceptions, the whole treatment is restricted to time-independent, or steady-state problems. There are also many minor points not treated, for example we do not discuss the construction and tests of the basic random number generators. In these cases the reader is directed to the literature.

REFERENCES

1. **Carter, L. L. and Cashwell, E. D.,** Particle-Transport Simulation with the Monte Carlo Method. ERDA *Crit. Rev. Ser.*, National Technical Information Service, Springfield, MA, 1975.
2. **Cashwell, E. D. and Everett, C. J.,** *A Practical Manual on the Monte Carlo Method for Random Walk Problems*, Pergamon Press, London, 1959.
3. **Ermakov, S. M. and Mikhailov, G. A.,** *Course of Statistical Modelling* (in Russian), Nauka, Moscow, 1976.
4. **Halton, J. H.,** A Retrospective and Prospective Survey of the Monte Carlo Method, *SIAM Rev.*, 12, 1, 1970.
5. **Hammersley, J. M. and Handscomb, D. C.,** *Monte Carlo Methods*, John Wiley & Sons, New York, 1964.
6. **Kahn, H.,** Applications of Monte Carlo. AECU-3259 Report, Rand Corporation, Santa Monica, CA, 1954.

7. **Shreider, Y. A., Ed.,** Method statisticheskih ispytani (Monte Carlo) (in Russian) Fizmatgiz, Moscow (1961) — German translation: Die Monte Carlo Methode und ihre Verwirklichung mit elektronischen Digitalrechnern. B.b. Teubner Verlags gesellschaft, Leipzig, 1964. — English translation: The Monte Carlo Method, Pergamon Press, New York, 1966.
8. **Sobol, I. M.,** *The Monte Carlo Calculational Method,* (in Russian), Nauka, Moscow, 1973.
9. **Spanier, J. and Gelbard, E. M.,** *Monte Carlo Principles and Neutron Transport Problems,* Addison-Wesley, Reading, MA, 1969.
10. **Stevens, P. M. and Trubey, D. K.,** Methods for Calculating Neutron and Gamma-ray Attenuation. *Weapons Radiation Shielding Handbook,* Report DNA-1892-3, Nuclear Defense Agency, Washington, D.C., 1972, Chap. 3.
11. **Wood, J.,** *Computational Methods in Reactor Shielding,* Pergamon Press, Oxford, 1982.

Chapter 2

INTRODUCTION

When we started to think about writing a book on Monte Carlo techniques for neutron and photon transport calculations it was clear that in the very first sentence a nice definition of the Monte Carlo method itself should be given. This task seemed to be very easy: just have a look on the earlier textbooks and copy the well-established definition! However, after reading more and more introductions it became more and more hopeless to find this sentence. Instead of exact definitions we have rather found illustrations and examples.

In the book, which is the most sophisticated earlier description of the Monte Carlo applications on neutron transport,[33] the authors, J. Spanier and E. M. Gelbard frankly confess that they found "it difficult to construct a definition which characterizes the Monte Carlo method accurately, completely and concisely". Their next sentence, however, already catches a basic feature of Monte Carlo, namely that "this method, in all its forms, involves some sort of random sampling process". And, really, *random* is the only word obligatorily contained in all definitions.

Anyhow, after listing our excuses, we cannot avoid giving *our definition,* which may not be accurate, complete, and concise, but can help the reader begin to have a rough image about the method.

In all applications of the Monte Carlo method a stochastic model is constructed in which the expected value of a certain random variable (or of a combination of several variables) is equivalent to the value of a physical quantity to be determined. This expected value is then estimated by the average of several independent samples representing the random variable introduced above. For the construction of the series of independent samples, random numbers following the distributions of the variable to be estimated are used.

There are two requirements imbedded in this definition, viz.:

First, a stochastic model adequate to the problem has to be constructed. Secondly, in the actual Monte Carlo calculations, the user has to be able to select random numbers with various distributions.

There are basically two different ways to construct a stochastic model. In certain cases — as in particle transport, the topics of this book — the physical process is per se stochastic and thus the most straightforward Monte Carlo calculation is simply a numerical (or computer) simulation of the real physical events. Such direct simulations are called *analog* Monte Carlo games. When the computational process deviates more or less from the one-to-one simulation of the actual physical process, the game is called *nonanalog*. The distinction is not always clear. Several authors tolerate small deviations and still call simulations slightly differing from the straightforward one analog. (In our book at the beginning the strictness of this distinction has no importance, however, from Chapter 5 on, the term "analog" is used exclusively for the really analog simulations.)

The other extreme case is when the stochastic model is constructed artificially, just for solving deterministic equations by Monte Carlo.

In the simulation of a physically stochastic process, two expected values: that of the physical quantity and that of the average of random samples, must equal one another. Both expected values have their own variances, which may have no direct relationship. In the correct solution of a deterministic problem, the expected value of the random sample average equals the *real value* of the quantity in question which is not accompanied by any statistical uncertainty.

Though the distinction between the two cases described above is clear, in transport calculations one can seldom — or rather never — find algorithms or computer codes based purely on one-to-one simulation of the physical processes, and — on the other hand — in

the procedures derived for solving the deterministic equations of the expected values (generally collision densities), one can still find many resemblances to a particle's random walk. Here we have again attained one of the aims of this book: we should like to illustrate with as many examples as possible that heuristically introduced plausible modifications of the simple simulations lead to techniques, the validity of which can be mathematically correctly proved by analysis of the deterministic transport equations. The opposite statement is not always true, there are special procedures which are hardly understandable heuristically.

An immediate question arises: why are refined nonanalog methods worked out, if we know that an accurate, analog simulation of the real physical process does not necessarily serve us with correct results? The answer is very simple: to save computer time. In the physical experiments millions of particles are usually emitted from the source and only a small fraction of them is observed by a receptor (the word receptor is used hereafter in a most general sense, it may be, e.g., a physical detector, a cell in a reactor core, an organ in a human body). In the computation — even on the fastest machine — the simulations of all the interreactions of so many particles is impossible within reasonable running times. The use of less source particles may result in a very small number (none, in the extreme) of them reaching the receptor, thus causing very poor statistics, i.e., nonconfident results. This answer directly involves a precondition against the nonanalog techniques: they are worth application only if they decrease the computer time as compared to that of the analog simulation, assuming that the statistical uncertainties are the same in the two cases. Needless to say the first precondition is that the result, the expected value of the physical quantity to be determined in any accepted nonanalog technique, must be the same as in the physical reality or in the direct simulation of the process.

The second requirement for building Monte Carlo games is the ability to select the proper random numbers.

This is the topic of the next sections.

I. SAMPLING PROBABILITY DISTRIBUTIONS

In most practical cases, sampling of any probability distribution is based on sampling one or more random number(s) uniformly distributed (or equidistributed) over the interval (0,1) (hereafter: random number) and on a transformation of it (them).

The probability density function (PDF) of the random numbers is:

$$p(\xi) = \begin{cases} 1, & \text{if } 0 \leq \xi < 1 \\ 0, & \text{otherwise} \end{cases}$$

the expected value is:

$$M(\xi) = \int_0^1 \xi p(\xi) d\xi = \frac{1}{2}$$

and the variance is:

$$D(\xi) = \{M(\xi^2) - [M(\xi)]^2\}^{1/2}$$

Since

$$M(\xi^2) = \int_0^1 \xi^2 p(\xi) d\xi = \frac{1}{3}$$

thus,

$$D(\xi) = \sqrt{\frac{1}{12}}$$

As it is proved[6] — and is so plausible that we do not think it necessary to repeat this derivation — an n digit binary random number is constructed by just lining up n 0 or 1 digits after the binary point. Since in any realization n is finite, these random numbers do not fill in continuously the (0,1) interval, the mathematically correct term for their distribution is "quasi-uniformly" distributed.

There are two essentially different ways how one can obtain a random series of 0's and 1's.

The first way is the use of physical random number generators where the inherently random nature of a physical phenomenon is utilized. The generally used random processes are the radioactive decay and the electronic noise. Though there are several physical generators[31] constructed for use in Monte Carlo calculations, their application is disadvantageous for two reasons. Partly because they need continuous hardware maintenance, partly because due to the really random and therefore never repeated series they generate, the user cannot repeat a former run and thus the debugging of a program is cumbersome.

Instead, the use of computational algorithms is practically unanimously preferred. These algorithms supply series of numbers which are determined by the generation formula, however, if a sequence of the so generated numbers passes the same randomness tests as the real, physical random numbers, one can use them in the same way; (in some works these artificially constructed random numbers are called pseudorandom numbers.)

Many papers in the literature deal with the description of random number generators[19,29,34,31,26,10,35] and with tests suggested to check the randomness.[16,11,4,31,2,5,12]

Here, we do not go into detail, partly because the selection of the generator is strongly influenced by the type of computer, but assume that there is a carefully designed and tested generator at the user's disposal.

Sampling from an arbitrary distribution can be realized by transformation of one or more random numbers uniformly distributed on (0,1). In the next subsections the most frequently used transformation methods are overviewed.

Many special techniques are listed in the very early report of Kahn,[15] in the Monte Carlo samplers of Everett and Cashwell,[7,8,9] or in the report of McGrath et al.[27]

Procedures used exclusively in photon and neutron transport (e.g., for selecting energies of particles after collisions) are described in the appendices of Chapter 3.

Before turning to the summary of the most common continuous selection procedures, let us start with the special case of sampling from a discrete distribution. The procedure is also heuristically obvious and is often met in conjunction with more sophisticated selection methods.

Theorem 2.1 — Let $p_1, p_2, \ldots, p_n$ be probabilities of the $e_1, e_2, \ldots, e_n$ mutually exclusive events and assume that:

$$\sum_{i=1}^{n} p_i = 1$$

For the selection of one of the discrete events let us first select a random number ρ equidistributed on (0,1). Then the event e_i is selected if the inequality

$$p_1 + \ldots + p_{i-1} \leq \rho < p_1 + \ldots + p_i \tag{2.1}$$

is fulfilled.

Proof. The proof of the selection rule is quite straightforward since the probability that the value of ρ is between

$$\sum_{j=1}^{i-1} p_j \quad \text{and} \quad \sum_{j=1}^{i} p_j$$

is just p_i.

□

For selecting a value of a continuous random variable, a number of techniques are described in the following section. We assume that the random variable has a probability density function so that

$$p(\xi) \geq 0 \quad \text{and} \quad \int_{-\infty}^{\infty} p(\xi)d\xi = 1$$

A. THE INVERSE DISTRIBUTION METHOD

Theorem 2.2 — If $p(x)$ is the PDF of a variable x, $a \leq x < b$, then an x value determined by the relations

$$\begin{aligned} \rho &= P(x) = \int_a^x p(x)\,dx \\ x &= P^{-1}(\rho) \end{aligned} \tag{2.2}$$

falls with a frequency $p(x)dx$ between x and $x + dx$, i.e. if ρ_i $(i = 1, 2, \ldots, n)$ are independent random numbers then the $x_i = P^{-1}(\rho_i)$ values are independent realizations of the x random variable. Shortly, we can say that x_i's are selected from $p(x)$.*

Proof. Let us denote the probability that a selected x is less than x_o by $P'(x < x_o)$. Then from Equation (2.2)

$$P'(x < x_o) = P'(\rho < P(x_o))$$

Now since ρ is equidistributed over (0,1):

$$P'(x < x_o) = P'(\rho < P(x_o)) = P(x_o)$$

i.e., $P(x)$ is really a cumulative distribution function (CDF) of x.

□

If the exact solution of Equation (2.2) is complicated or even impossible (due to the complexity of the PDF) approximation of the PDF or iterative solution of Equation (2.2) can be used or, rather, another selection method is suggested.

There are cases, when there is no difficulty in selecting x by Equation (2.2), but other techniques are faster. Examples will be given in Sections I.D. and I.E.

* In a rigorous mathematical treatment, different symbols for the argument in the PDF and CDF and the actual values selected from them should be used, however, we hope, that the use of the same symbol hereafter does not lead to confusion, but rather simplifies the notation.

B. THE PROBABILITY MIXING METHOD

Theorem 2.3 — If the PDF p(x) can be broken up to the sum of n non-negative functions:

$$p(x) = \sum_{i=1}^{n} \tilde{p}_i(x), \qquad \tilde{p}_i(x) \geq 0, \qquad a \leq x \leq b$$

then sampling can be realized by a two-step procedure. First, the i-th term is selected with a probability

$$p_i = \int_a^b \tilde{p}_i(x)\,dx \tag{2.3}$$

according to Equation (2.1):

$$\sum_{j=1}^{i-1} p_j \leq \rho_1 < \sum_{j=1}^{i} p_j$$

then — by the use of a second random number — x, the actual realization is selected from the PDF of $\tilde{p}_i$:

$$\rho_2 = P_i(x) = \frac{1}{p_i} \int_a^x \tilde{p}_i(\xi)\,d\xi$$

Proof. The probability that a selected x lies between x and x + dx is a sum of conditional probabilities:

$$\sum_{i=1}^{n} P\left(\sum_{j=1}^{i-1} p_j < \rho_1 < \sum_{j=1}^{i} p_j\right) \cdot P(x < \rho_2 < x + dx) =$$

$$\sum_{i=1}^{n} p_i \cdot \frac{1}{p_i} \tilde{p}_i(x)\,dx = \sum_{i=1}^{n} \tilde{p}_i(x)\,dx = p(x)\,dx$$

□

This technique is easily extendable for cases where the p(x) PDF is expanded into an infinite series of terms.

C. THE REJECTION TECHNIQUES

Rejection techniques, proposed by Neumann[29] are widely used for producing independent samples when the solution of Equation (2.2) is extremely complicated.

Theorem 2.4 — In the simplest form of the rejection technique we assume that p(x) is again a PDF of the variable x, $a \leq x \leq b$, and there is a positive finite number M, for which $p(x) \leq M$ (see Figure 2.1).

Let a point be chosen randomly from the rectangle with a base of b-a and height of M. If the point selected falls below the graph of p (ξ) accept the abscissa as a sample, if not, reject it and try again. Thus, if ρ_1 and ρ_2 are two independent random numbers, then

$$x = a + \rho_1(b - a)$$

is accepted if and only if

$$\rho_2 M \leq p(x) \tag{2.4}$$

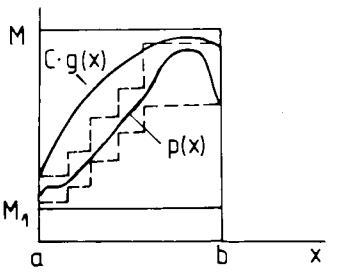

FIGURE 2.1. Illustration of the rejection technique.

Proof. (Before we present the proof, it is worth noting that the correctness of the procedure is plausible from the graphical explanation in Figure 2.1.)

The probability density function of x is the conditional density of x given that

$$\rho_2 < \frac{p(x)}{M}$$

The joint density of x and ρ_1 is

$$p'(x,\rho_1) = \begin{cases} \dfrac{1}{b-a}, & \text{if } a < x < b \\ 0, & \text{elsewhere} \end{cases}$$

Thus,

$$P\left(x < x_o < x + dx \middle| \rho_2 < \frac{p(x)}{M}\right) = \frac{P'(x < x_o < x + dx)}{P\left(\rho_2 < \frac{p(x)}{M}\right)}$$

$$= \frac{\dfrac{1}{b-a}\displaystyle\int_0^{p(x)/M} d\rho_1}{\dfrac{1}{b-a}\displaystyle\int_a^b dx \int_0^{p(x)/M} d\rho_2} = \frac{p(x)/M}{1/M} = p(x)$$

□

Two consequences are obvious:

- the generation of at least two independent random numbers is necessary for obtaining one sample value,
- the ratio of the successful first trials to all selections, i.e., the efficiency (E) of the procedure, is just the ratio of the area below the graph to that of the rectangle:

$$E = \frac{\displaystyle\int_a^b p(\xi)\,d\xi}{(b-a)M} = \frac{1}{(b-a)M}$$

It is easy to prove[15] by summing up the probabilities of accepting the sample after $n = 1, 2 \ldots$ trials that the average number of trials, $\bar{n}$ is

$$\bar{n} = \frac{1}{E}$$

There are many different ways to improve the efficiency of the rejection procedure.

Theorem 2.5 — More generally,[3] if one can write p(x) in the form

$$p(x) = Cg(x)f(x) \tag{2.5}$$

where f(x) is also a PDF and C is chosen such that the

$$0 \leqslant g(x) \leqslant 1$$

inequality holds for $a \leqslant x \leqslant b$ (i.e. Cg(x) is a majorant of p(x), see Figure 2.1), then the following procedure can be applied:

- select an x value from f(x)
- select a random number ρ
- accept x if and only if

$$\rho \leqslant g(x)$$

Proof. The conditional density (q) of x, given that $\rho < g(x)$, is

$$q[x|\rho < g(x)] = \frac{f(x)\int_0^{g(x)} d\rho}{\int_a^b dx\, f(x)\int_0^{g(x)} d\rho} = \frac{f(x)g(x)}{\int_a^b dx f(x)g(x)} = Cf(x)g(x)$$

□

In most practical cases the formulation (2.5) is reasonable if f(x) is a quite simple function, and for the selection of x from f(x) the inverse distribution method can be applied (using only one random number).

The efficiency of the method is trivially[3]

$$E = \frac{1}{C}$$

For widely varying functions very often a step function is used for Cq(x) (the broken line in Figure 2.1), leading to the application of the different subintervals of the abscissa.

Another efficiency-improving method is the combination of the rejection with other techniques. If the PDF is broken into terms as in Section I.B., rejection can be applied in sampling from any term. In the simplest case if

$$p(x) \geqslant M_1 \qquad a \leqslant x \leqslant b$$

$$p(x) = \tilde{p}_1(x) + \tilde{p}_2(x)$$

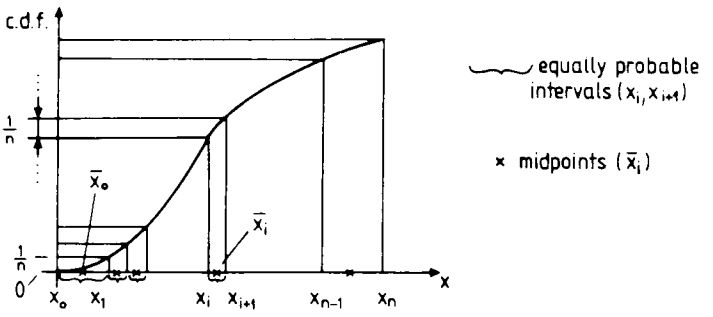

FIGURE 2.2. A sketch of the table lookup method.

where

$$\tilde{p}_1(x) \equiv M_1$$

$$\tilde{p}_2(x) = p(x) - M_1$$

sampling from M_1 is straightforward and the efficiency of the rejection is increased to

$$E = \frac{1}{(b - a)(M - M_1)}$$

Furthermore, the lower limit M_1 can also be set differently to different subintervals, thus further improving the efficiency.

The actual measure, how far we can proceed in taking out simple parts of a complicated PDF depends partly on the computer time balance (how much time we gain by improving the rejection efficiency and how much we lose by setting more and more criteria). Moreover, there may be some programs where even the shape of the actual distribution changes during the computation and thus only very loose criteria can be set in advance.

A generalization for the rejection technique for PDFs that can be expanded into McLaurin series is given by Lux,[20] where an "iterative rejection" method is proposed in which — roughly speaking — the g(x) and f(x) functions of Equation (2.5) are changed after each unsuccessful trial.

D. THE TABLE LOOKUP METHOD

One of the fastest, though trivially approximate, selection methods applicable for arbitrary distribution is the table lookup method, where midpoints of equally probable intervals of the variable to be selected are picked up randomly from a table (Figure 2.2).

The table here contains the x coordinates of the finite number midpoints from which an actual value is selected with equal probabilities.

The accuracy of this method is improved by increasing the number of intervals (n), which in turn increases both the core requirement and the selection time. Another easy way for improvement is applied if the midpoints are not just the middle of the intervals:

$$\bar{x}_i = \frac{1}{2}(x_{i+1} - x_i)$$

but the most probable values:

$$\bar{x}_i = \frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} p(x)\,dx$$

In case of complicated density functions the determination of the limits of the equal probability intervals themselves may be complicated and time consuming, however, one has to bear in mind that this task is to be solved only once for a given PDF.

Another restriction is that the method cannot be applied directly to the distribution functions defined over an infinite domain since the tail of the distribution has to be truncated if a table of finite dimensions is used. There are several cases when this disadvantage can be overcome by tricky methods. A nice example was proposed by Frank-Kamenietzky (described in Reference 22) for the exponential distribution.

Here, the PDF is

$$p(x) = e^{-x}$$

and samples can very easily be obtained by solution of the inverse distribution Equation (2.2),*

$$x = P^{-1}(\rho) = -\ln\rho \tag{2.6}$$

however, the execution of logarithm is very time consuming.

Instead, let us write the realization of x in the form

$$x = k \cdot \ln 2 - z \tag{2.7}$$

where $k > 0$ and $0 < z \leq \ln 2$. Let us select a random number ρ and determine a value k such that

$$2^{-k} \leq \rho \leq 2^{-(k+1)}$$

It can be seen[30] that choosing k in this way the cumulative distribution function of z in Equation (2.7) reads

$$P(z) = e^z - 1 \qquad 0 < z \leq \ln 2$$

Since the random variable z is defined over a finite interval it can be selected by table lookup and the z value so selected along with the integer k value above determines the exponentially distributed random variable x according to Equation (2.7).

An actual realization of the above procedure is detailed in Reference 22.

E. SELECTION FROM POWER FUNCTIONS

$$\text{Let} \quad p(x) = (n + 1)x^n \qquad 0 \leq x \leq 1 \tag{2.8}$$

* Here, the term (1-ρ) derived from Equation 2.2 is replaced by ρ since both are equidistributed on (0,1).

thus the CDF is

$$P(x) = \int_0^x p(x)\,dx = x^{n+1}$$

i.e., the direct inverse distribution method can be applied, a random sample x is obtainable by Equation (2.2):

$$\rho = x^{n+1} \qquad x = \rho^{1/(n+1)} \tag{2.9}$$

This method is not fast enough in most computers since the execution of the a^b operation is quite slow if b is not an integer. Therefore, if n is an integer, the following method can replace the execution of Equation (2.9).

Theorem 2.6 — Let x (the sample) be the maximum of n+1 random numbers, then the x is a representative sample from Equation (2.8).

Proof: The probability, that a random number ρ_i is equal or less than x_o ($0 \leq x_o \leq 1$) is just x_o. The probability that all random numbers from a set of n+1 independent element is less than x_o is

$$P(\rho_1 \leq x_o, \quad \rho_2 \leq x_o, \ldots, \rho_{n+1} \leq x_o) = \prod_{i=1}^{n+1} (\rho_i \leq x_o)$$
$$= \prod_{i=1}^{n+1} x_o = x_o^{n+1}$$

□

In the method proposed here, a set of n+1 random numbers has to be generated. In most computers the generation of the elementary random numbers is much faster than the execution of Equation (2.7), however, especially for large values of n, it might be advised to check the actual computer times before the selection of one of the two procedures.

If x is equidistributed on (a,b) then the transformation $z = (x-a)/(b-a)$ should first be applied.

F. SAMPLING FROM THE NORMAL DISTRIBUTION

From the positive half of the Gaussian distribution,

$$p(x) = \sqrt{\frac{2}{\pi}} \exp(-x^2/2) \tag{2.9}$$

a simple rejection method is given in Reference 15:

$$\text{let:} \quad x' = -\log\rho_1$$
$$y = -\log\rho_2$$

accept x′ if, and only if

$$\frac{1}{2}(x' - 1)^2 \leq y$$

and give a random sign (by the use of a third random number) to x′:

$$x = s \cdot x'$$

$$s = \begin{cases} +1, & \text{if } \rho_3 \geq 0.5 \\ -1, & \text{if } \rho_3 < 0.5 \end{cases}$$

The efficiency of this procedure is fairly high:

$$E = \sqrt{\frac{\pi}{2}} \exp(-1/2) \approx 0.76$$

Approximate Gaussian PDF sampling can be realized by the use of the central limit theorem: according to which the sum of a large number of independent and identically distributed random variables (with finite variance) is asymptotically normally distributed. If the x_i variables are uniformly distributed on (0,1), then their expected value is

$$a = \frac{1}{2}$$

with a variance of

$$s = \frac{1}{\sqrt{12}}$$

then $x = \Sigma_{i=1}^{n} x_i$ is asymptotically ($n \rightarrow \infty$) normally distributed with a residual expected value of

$$a_n = an = \frac{n}{2}$$

and a variance of

$$s_n = \sqrt{n} \cdot s = \sqrt{\frac{n}{12}}$$

Therefore, if samples from a normal distribution with $a = 0$, $s = 1$ (Equation 2.9) have to be generated then the

$$x = \sqrt{\frac{12}{n}} \left[\sum_{i=1}^{n} \rho_i - \frac{n}{2} \right] \tag{2.10}$$

rule is to be applied, with $n \rightarrow \infty$. In practice $n = 4 \ldots 8$ is enough.

Sobol[32] proposes a fast method where five random numbers in Equation (2.10) are used and a squared term is added for decreasing the truncation error: the sample x is generated by

$$x = 0.01\, n(97 + n^2)$$

where

$$n = \sqrt{\frac{12}{5}}\left[\sum_{i=1}^{5} \rho_i - \frac{5}{2}\right]$$

The fastest procedure[27] which is completely accurate and does not need considerable storage was recommended by Marsaglia et al.[24] It works basically with the probability mixing method (see Section I.B., of this Chapter). The normal distribution is composed of three terms where the first two have the major contributions and are very simple and easy to sample. Actually, in about 86% of the selections three, in a further 11% two random numbers have to be summed as in Equation (2.10) and only in less than 3% is a rather complicated algorithm used.

The flow chart of this procedure is given in Figure 2.3.

Many procedures for generating normally distributed random numbers are collected and compared in the paper of Ahrens and Dieter[1] and Kinderman and Ramage.[18]

G. EFFICIENT SELECTIONS FROM THE EXPONENTIAL DISTRIBUTION

The simplest method for selecting random variables from the exponential distribution is to use the inverse solution, as given by Equation (2.6). A faster method was already described in Section I.D. Other rapid but generally large storage-requiring methods based also on the use of tables prepared in advance are elaborated by Marsaglia[23,25] and Ahrens and Dieter.[1]

Von Neumann[29] suggested a simple rejection technique, the scheme of which is given in Figure 2.4.

The efficiencies of the different selection methods are compared in Reference 1.

H. THE USE OF THE FIRST DERIVATIVE OF THE PDF

Lux[20] presented a special method that uses the first derivative of the density function to be sampled. The procedures suggested in his paper originate from two theorems, viz.:

Theorem 2.7 — Let p(x) be a continuous PDF on (0,A) and let

(i) $p(x) = 0 \quad \text{if} \quad x \leq 0 \quad \text{or} \quad x > A$

(ii) $\frac{dp(x)}{dx} = p'(x)$ be continuous on (0,A)

(iii) $$g(y) = \frac{1}{d}[\alpha p(y) + p'(y)]\{1 - \exp[\alpha(y - A)] \geq 0, \quad \text{if} \quad 0 \leq y < a \qquad (2.11)$$

where α is an arbitrary real number. Thus, g(y) is again a PDF and if η is a sample from g(y) then

$$\zeta = -\frac{1}{\alpha}\ln[e^{-\alpha\eta} - (e^{-\alpha\eta} - e^{-\alpha A})\rho] \qquad (2.12)$$

is a sample from p(x).

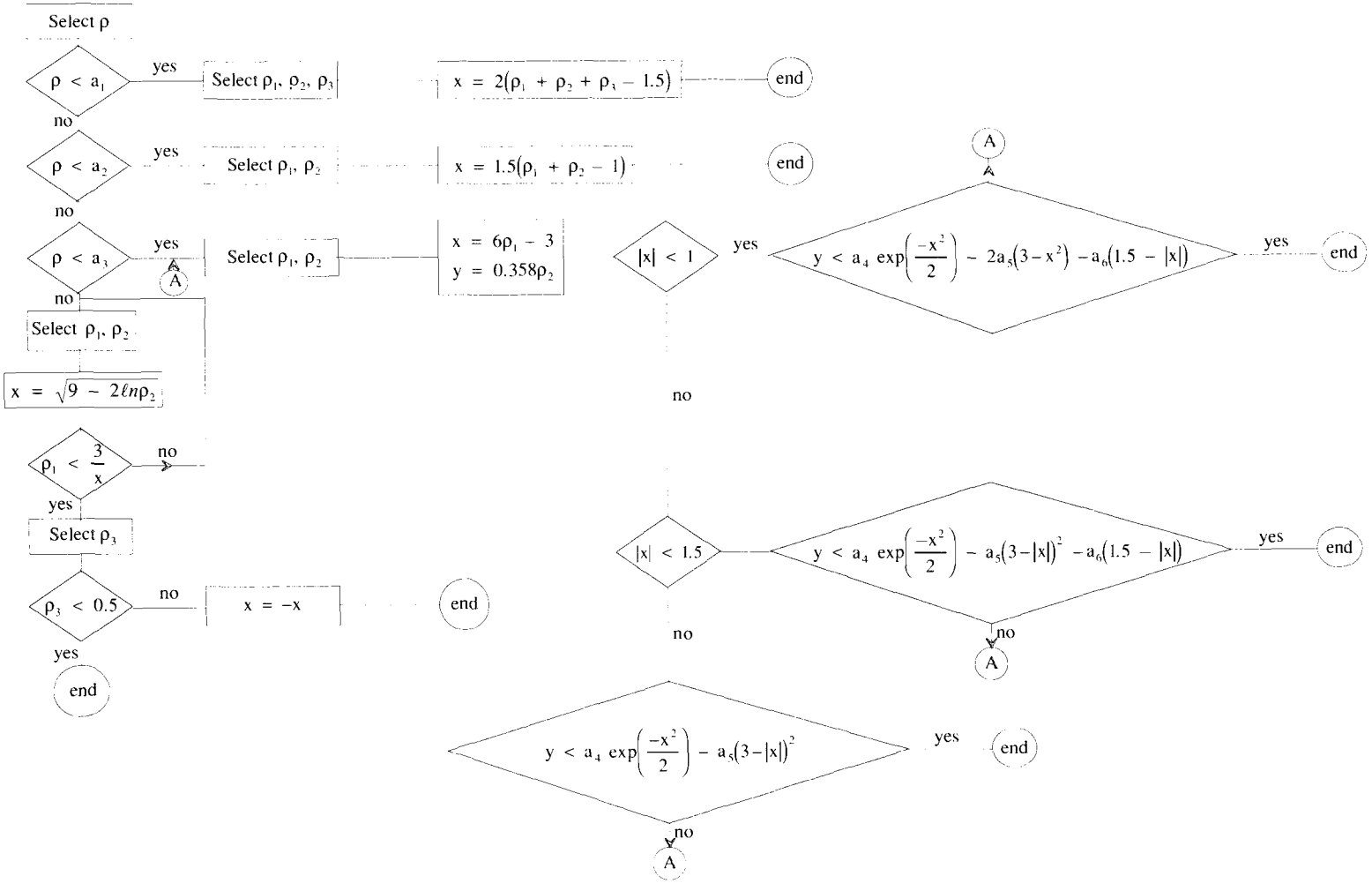

FIGURE 2.3. Flow chart for selecting x from the normal distribution.[27] $a_1 = 0.8638$; $a_2 = 0.9745$; $a_3 = 0.997302039$; $a_4 = 17.49731196$; $a_5 = 2.36785163$; $a_6 = 2.15787544$.

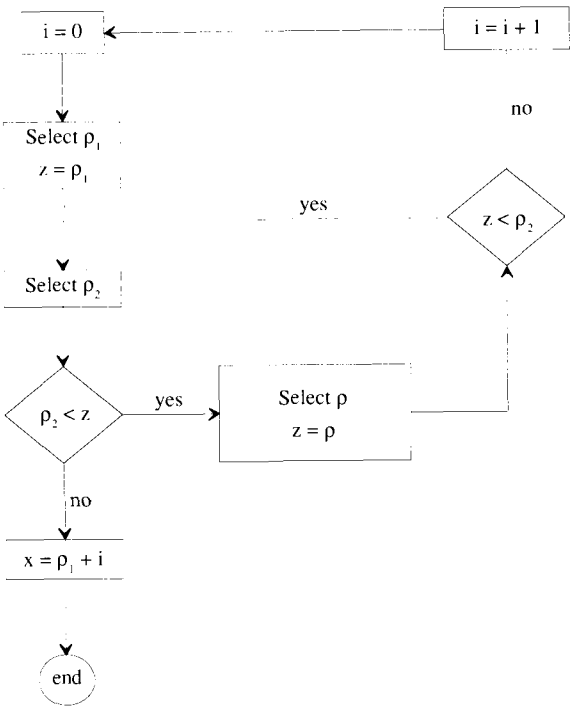

FIGURE 2.4. Flow chart for selecting x from the exponential distribution.[27]

Proof.

$$\int_0^A g(y)\,dy = \int_0^A \frac{1}{\alpha}\,[\alpha p(y) + p'(y)]\{1 - \exp[\alpha - (y - A)]\}\,dy$$

$$= 1 + \frac{1}{\alpha}\,p(A) - \frac{1}{\alpha}\int_0^A [p(y)e^y]'e^{-\alpha A}dy = 1$$

i.e., g(y) is really a PDF. To get the density function $p_\xi(x)$ of ξ one has to use that

$$p_\xi(x) = \int_0^A p_\xi(x|y)p_\xi(y)\,dy$$

where

$$p_\xi(x) = \begin{cases} e^{-\alpha x}/(e^{-\alpha y} - e^{-\alpha A}), & \text{if } y \leqslant x \leqslant A \\ 0, & \text{elsewhere} \end{cases}$$

and

$$p_y(y) = g(y)$$

After substitution and integration one gets

$$p_\xi(x) = p(x)$$

□

Theorem 2.8 — Let p(x) again be a PDF continuous for $x > 0$ and continuous from the right at $x = 0$ and let:

(i) $p(x) = 0$, if $x < 0$

(ii) $p'(x)$ continuous, if $x > 0$

(iii) $g(y) = \frac{1}{\alpha}[\alpha p(y) + p'(y)](1 - e^{\alpha y}) \geq 0$, if $y \geq 0$

(iv) $\lim_{n\to\infty} p(y)e^{\alpha y} = 0$

where α is again an arbitrary real number. The g(y) defined in this way is again a PDF and if η is a sample from g(y) then

$$\xi = -\frac{1}{\alpha}\ln[1 - (1 - e^{-\alpha\eta})\rho]$$

is a sample from p(x).

The proof is analogous to that of Theorem 2.7. and is thus not detailed here.

Several illustrative applications of the above theorems are given in the original paper of Lux,[20] here we call the attention of the reader to one only which fits to our special field:

If in Theorem 2.7 α is set to unity and A tends to infinity, then from Equation (2.11)

$$g(y) = p(y) + p'(y)$$

and if g(y) is non-negative then according to Equation (2.12)

$$\xi = -\ln\rho + \eta$$

This selection procedure was first recommended by Mikhailov[28] for sampling of the fission neutron spectrum and the Maxwell energy distribution.

I. SELECTING RANDOM VECTORS

Very often, a random vector of an n dimensional phase space (that is n coordinates of a random point) has to be selected. In the simplest cases the multidimensional probability distribution can be factorized into a product of one dimensional PDFs of mutually independent random variables.

A simple example of it for $n = 2$ is the selection of points in a square:

Here both ξ and η are equidistributed on (0,1) and their representative values x and y can be set by the use of two successive random numbers:

$$x = \rho_1$$

$$y = \rho_2$$

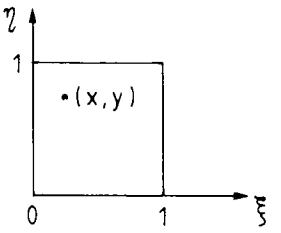

FIGURE 2.5. A random point in a square.

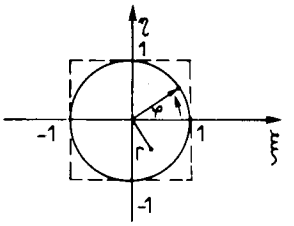

FIGURE 2.6. Selection of a random unit vector in two dimensions.

If the PDFs cannot be separated for the variables (i.e., the borders of the domain are complicated) generally only the rejection technique works.

Let the n-dimensional domain — from which the samples are to be taken — be defined by the relation

$$F(\xi_1,\xi_2,\ldots \xi_n) \leq 0$$

and $a_i \leq \xi_i \leq b_i$ for $i = 1, 2 \ldots ,n$ then select x_i's with

$$x_i = a_i + (b_i - a_i)\rho_i$$

and accept the point $(a_1, a_2, \ldots a_n)$ if and only if

$$F(x_1,x_2,\ldots,x_n) \leq 0$$

J. SELECTING TWO- AND THREE-DIMENSIONAL RANDOM ORIENTATIONS

There are practically no transport codes where there is no need for the generation of randomly oriented two- and/or three-dimensional unit vectors.

In two dimensions, according to the notation in Figure 2.6, the connection between the Cartesian coordinates and the angle φ is

$$\xi = \cos\varphi$$

and

$$\eta = \sin\varphi$$

and φ is equidistributed in $(0,2\pi)$.

Thus, for the random selection of the two coordinates a quite straightforward method is given by:

$$\varphi = 2\pi\rho$$

and

$$\begin{aligned} y &= \cos\varphi \\ x &= \sin\varphi \end{aligned} \tag{2.13}$$

An alternate method was first suggested by von Neumann[29] where the circle is covered by a square. The procedure is as follows:

$$\tilde{\rho}_1 = 2\rho_1 - 1$$

$$\tilde{\rho}_2 = 2\rho_2 - 1$$

except if

$$\tilde{\rho}_1^2 + \tilde{\rho}_2^2 \leq 1 \tag{2.14}$$

i.e., the $(\tilde{\rho}_1,\tilde{\rho}_2)$ point lies within the circle. A simple normalization will give:

$$x(=\cos\varphi) = \frac{\tilde{\rho}_1}{\sqrt{\tilde{\rho}_1^2 + \tilde{\rho}_2^2}}$$

$$y(=\sin\varphi) = \frac{\tilde{\rho}_2}{\sqrt{\tilde{\rho}_1^2 + \tilde{\rho}_2^2}}$$

The square roots in the denominators can be eliminated by the use of the double-angle formulae of trigonometry and the final procedure is:

$$\tilde{\rho}_1 = 2\rho_1 - 1$$

$$\tilde{\rho}_2 = 2\rho_2 - 1$$

except if:

$$\tilde{\rho}^2 = \tilde{\rho}_1^2 + \tilde{\rho}_2^2 \leq 1$$

then

$$x = \frac{\tilde{\rho}_1^2 - \tilde{\rho}_2^2}{\tilde{\rho}^2}$$

and

$$y = \frac{2\tilde{\rho}_1\tilde{\rho}_2}{\tilde{\rho}^2} \tag{2.15}$$

The efficiency is trivially the ratio of the circle to the square areas, i.e.,

$$E = \frac{\pi}{4} \simeq 0.785$$

Though the straightforward procedure (2.13) seems to be much simpler than (2.15), in most computers both the generation of random numbers and the execution of the other elementary operations of (2.12) are less time consuming than the evaluation of the sine and cosine of an angle.

If not a unit vector, but rather a point from the circle area has to be selected then Equation (2.13) should be supplemented by

$$r = \max(\rho_1,\rho_2)$$

(since: $p(r) = 2r\,dr$) and x and y should be multiplied by r.

In the rejection method Equation (2.14) gives directly the necessary coordinates (there is no need for normalization), thus its preference to the direct method in Equation (2.12) is even more obvious.

In three dimension the coordinates of a random unit vector are[31]

$$z = \omega$$
$$x = \sqrt{1 - \omega^2}\cos\varphi$$
$$y = \sqrt{1 - \omega^2}\sin\varphi$$

where ω is equidistributed on $(-1,1)$ and $\cos\varphi$ and $\sin\varphi$ can be generated by one of the methods listed above.

A point from inside of a sphere can again be selected by the rejection method, where the sphere is boxed in a cube. The efficiency here is the ratio of the sphere to the cube *volumes:*

$$E = \frac{\pi}{6} \simeq 0.523$$

II. BASIC PHYSICAL QUANTITIES

The reader is assumed to be familiar with the basic physical quantities that are characteristic to particle transport that will be used in the following Chapters of this book. There are, however, several quantities which are named differently in different papers (e.g., fluence, flux, flux density . . .), or which have equivalent physical interpretations but different names in different contexts (macroscopic cross-section and linear attenuation coefficient). Even a larger variety is found in the use of symbols for a number of terms.

Considering all the above arguments it seems appropriate to give a systematic review of the basic quantities, their notations, definitions, and symbols as well as the derivation of the basic relations between several quantities.

The main source of the definitions given in the following sections is the most recent booklet of the International Commission on Radiation Units and Measurements (ICRU),[13]

though many quantities not listed there are taken from other sources and several notations are specifically introduced for later use in this book.

The survey of the definitions is arranged in sections collecting quantities describing similar phases of the radiation transport.

A. THE PHASE SPACE

A migrating particle (neutron or photon) is represented by a set of coordinates that uniquely determine the state of the particle. The notations of the relevant coordinates are given below.

The three spatial *Cartesian coordinates* x, y and z of the particle are often denoted by the single vectorial symbol **r**.

The three-dimensional unit *direction vector* is denoted by $\boldsymbol{\omega}$ and, if necessary, its components parallel to the x, y, and z coordinates are denoted by ω_x, ω_y and ω_z, respectively.

The symbol E represents the energy of a particle.

Since in many cases the *energy and the direction* of a particle change simultaneously, sometimes the coordinates ($\boldsymbol{\omega}$, E) are simply denoted by a single vector **E**. (If somebody does not like to see the "energy" described by a "vector", we would like to remind them that — at least for neutrons — the direction vector + the energy coordinates might have been replaced by the velocity of the particle, i.e., by a real vector quantity.)

Further simplifying the notation, a set of the *spatial, direction, and energy coordinates* are united and described by a point in the six-dimensional phase-space: P.

In the *integrations* $\iiint \ldots dx\,dy\,dz$ may be replaced by $\int \ldots d\mathbf{r}$, similarly $\iint \ldots d\boldsymbol{\omega}$ dE is often reduced to $\int \ldots d\mathbf{E}$ and the shortest way to denote an integration over the whole phase-space is $\int \ldots dP$.

B. THE PARTICLE SOURCES

The *intensity* of a neutron or photon source is denoted by Q and Q(P) means the number of particles emitted with coordinates in dP about P.

Generally, for the Monte Carlo calculations the equations are established for one starting particle, i.e.,

$$\int Q(P)\,dP = 1$$

and hence Q is called the *source density*.

For radioactive sources the term *activity* is used which is the "quotient of dN by dt, where dN is the number of spontaneous nuclear transformations which occur . . . in the time interval dt". This quantity of the ICRU differs from our *intensity* in two respects:

1. Since we deal with stationary processes in most of this book, the differentiation with respect to time is not necessary for us, we shall consider all quantities (e.g., collision densities, reaction rates) as integrated over an arbitrary time interval (e.g., unity);

2. there are many isotopes where e.g., beta decay is the elementary "nuclear transformation" and gammas are emitted only in a fraction of decays thus the number of transformations (activity) is higher than the number of photons emitted (intensity).

Neutron sources are often characterized by the *yield* which is the number of neutrons leaving the source. Thus in case of extended sources, the yield is decreased by self-absorption.

In many cases, the sources are isotropic, monoenergetic, or point-like. In such cases the argument is simplified from (P) $\equiv$ ($\mathbf{r},\boldsymbol{\omega}$,E) to ($\mathbf{r}$) or ($\mathbf{r}$,E) or in any other way but the symbol Q is preserved even in these cases. Therefore, equations like

$$Q(\mathbf{r}) = \int Q(\mathbf{r},E)\,dE \qquad (2.15a)$$

are written, and here the difference in the argument indicates the difference in the quantities and necessarily in their units.

C. FLUX-TYPE QUANTITIES

This is the point where perhaps the most loose use of words can be found in the literature. By the ICRU definition "the *fluence*, Φ, of particles is the quotient of dN by da, where dN is the number of particles which enter a sphere of cross-sectional area da". The argument **r** is naturally joinable to the symbol Φ since it specifies the point around which the sphere is placed.

The time derivative of the fluence ($\varphi = \dot{\Phi}$) is called by the ICRU as *flux density or fluence rate,* however, in most of the books and papers both fluence and flux density are simply called *flux,* and this word is used throughout our book too.

Flux also can be considered as differential by energy and/or direction of flight, then it is denoted as

$$\varphi(\mathbf{r},E) \quad \text{or} \quad \varphi(\mathbf{r},\boldsymbol{\omega}) \quad \text{or} \quad \varphi(P)$$

In reactor physics, many times an alternative definition of flux is preferred. In such cases the particle density (n) is first introduced: n(P) is the number of particles per unit phase-space volume. Then the flux density is defined as

$$\varphi(P) = vn(P)$$

where v is the particle's speed ($\sqrt{2E/m}$ for neutrons and it equals to c, the speed of light, for photons).

The speed of an individual particle is its *track-length* per unit time. Hence, the total flux can be conceived as the sum of track-lengths traced out by the particles per unit volume.

A similar final result can be derived from the ICRU definition, if we take into account that for a convex body the mean length of randomly oriented chords ($\bar{d}$) is[17]:

$$\bar{d} = 4V/A \tag{2.16}$$

where V is the volume and A is the surface area.

In the ICRU fluence definition

$$\Phi = \frac{dN}{da} = \frac{dN \cdot \bar{d}}{dV} \tag{2.17}$$

since for spheres $A = 4a$, $dA = 4da$.

The numerator in the R.H.S of Equation (2.17) is just the total chord length of the dN particles crossing the infinitesimal sphere.

Flux is characteristic to the number of particles crossing an infinitesimal sphere — regardless of their orientation. If one is interested in the *direction* of the flow the *current vector* (**J**) can be introduced as

$$\mathbf{J}(P) = \boldsymbol{\omega}\Phi(P)$$

Obviously, if a unit area normal to the unit direction vector ***n*** is placed into the phase space at about **r**, then the number of particles crossing it (J_n) is:

$$J_n = \mathbf{J}(\mathbf{r})\mathbf{n}$$

D. ELEMENTARY INTERACTIONS OF PARTICLES WITH MATTER

Neutrons and photons interact with matters in many ways. *Interactions or collisions* can lead to:

- *Absorption,* when the original particle entering the collision is absorbed and no particle of the same type is emitted, or
- *Scattering,* if the incoming particle continues its flight after the collision but possibly with altered direction and energy, or
- *Multiplicative effects,* where after certain nuclear transformations more than one of the same type particles leave the collision than that entered.

There are interactions when the type of the outcoming particle(s) is different from that of the colliding particle, e.g., reactions (n,γ) or (n,nγ). The outputs of these events give *additional source terms* in the joint neutron-photon transport calculations.

The probabilities of these interactions both for neutrons and photons, depend on the colliding particle's energy and on the knocked element.

The interaction probabilities are described by the *cross-sections.*

The total *microscopic cross-section* is defined as the probability of an interaction in a mass element divided by the product of the number of nuclei and the fluence. Its unit is therefore cm^2, and the generally used symbol is σ, however, we shall denote it by σ*.

In the formulae of the transport processes another quantity is much more frequently used:

$$\sigma = \rho N_A \frac{\sigma^*}{M} \tag{2.18}$$

where ρ is the density of the material, N_A is the Avogadro constant, and M is the molar mass of the target element. The quantity defined by Equation (2.18) has the unit of 1/cm and in neutron physics it is called the *macroscopic cross-section* and denoted by Σ, whereas in photon interactions the term *linear attenuation coefficient* and the symbol μ are preferred.

Since in this book we deal with the transport of both particles the symbol σ and the simple name *cross-section* is used for the quantity of Equation (2.18) and if the microscopic cross-section is referred, we distinguish it with the obligate attribute "*microscopic*" and the *superscript asterisk.*

If the matter investigated is a compound of n elements then the resultant cross-section is the weighted sum of the elementary microscopic cross sections

$$\sigma = \rho N_A \sum_{i=1}^{n} w_i \frac{\sigma_i^*}{M_i} \tag{2.19}$$

where w_i is the weight fraction, σ_i^* is the microscopic cross-section, and M_i is the molar mass of the i-th component.

In most cases different types of interactions may occur at a certain collision and thus the total cross section can be expressed as the sum of *partial* cross-sections. If σ_{ij}^* denotes the partial microscopic cross-section of the j-th type of interaction on the i-th element, then the total cross-section is:

$$\sigma = \rho N_A \sum_{i=1}^{n} \frac{w_i}{M_i} \sum_{j=1}^{m} \sigma_{ij}^* \tag{2.20}$$

where we assumed that altogether m types of interactions can occur in the case investigated.

By introducing the partial macroscopic cross-sections as

$$\sigma_{ij} = \rho N_A \frac{w_i}{M_i} \sigma^*_{ij}$$

Equation (2.20) reduces to

$$\sigma = \sum_{i=1}^{n} \sum_{j=1}^{m} \sigma_{ij} \tag{2.21}$$

The cross-section is a function of the incident particle's energy and in inhomogeneous media it also varies from site to site, thus generally has two arguments:

$$\sigma(\mathbf{r},E)$$

In non-absorption events, differential cross-sections can be introduced where

$$\sigma_j(\mathbf{r},\boldsymbol{\omega},E\rightarrow\boldsymbol{\omega}',E')d\boldsymbol{\omega}'\,dE'$$

is proportional to the probability that the particle entering a collision of type j with direction $\boldsymbol{\omega}$ and energy E leaves it with new direction and energy coordinates in $d\boldsymbol{\omega}'$ about $\boldsymbol{\omega}'$ and between E′ and E′ + dE′, respectively.

Again only the argument will indicate whether differential or integrated quantities are mentioned, i.e., similarly to Equation (2.15a), formulae like

$$\sigma_j(\mathbf{r},\mathbf{E}) = \int \sigma_j(\mathbf{r},\mathbf{E}\rightarrow\mathbf{E}')\,d\mathbf{E}'$$

can occur.

Another quantity important for the study of scattering events is the *expected number* of the outcoming particles. One can assign such an expected number (ν) to every type of interactions. This number will be trivially 0, for an absorption, 1, for simple scattering events, 2, for (n,2n) reactions, etc.

For fission interactions of neutrons ν is usually not an integer which indicates that different numbers of neutrons can be emitted even if the same type of nuclei are split by neutrons of the same incident energy.

If a complete set of ν_{ij}-s are assigned to possible interactions with σ_{ij} cross-sections, then the expected number of the outcoming particles $<n>$ is

$$<n> = \frac{\sum_i \sum_j \nu_{ij}\,\sigma_{ij}}{\sigma}$$

which may be either less or larger than one.

The probability of the occurrence of a certain reaction (type j) with a partial cross-section σ_j is

$$\frac{\sigma_j}{\sigma}$$

and this quantity, from its definition could easily be called reaction rate (or more definitely

absorption, scattering, etc. rate if the type of reaction is definitely denominated). However, the term reaction rate shall be used in a much more general sense, as defined in Section G. of this Chapter.

E. FREE-PATHS, DISTANCES

In a homogeneous medium the mean free path between two collisions is

$$\lambda = \frac{1}{\sigma}$$

since the PDF of the path length (R) is

$$p(R) = \sigma e^{-\sigma R} \tag{2.22}$$

and thus

$$\lambda = \langle R \rangle = \int_0^\infty R e^{-\sigma R} dR = \frac{1}{\sigma}$$

Actual selected paths will also be denoted by R.

In inhomogeneous media, where the cross-section changes during the flight between two collisions the PDF of Equation (2.19) is changed to:

$$p(R) = \sigma(R) \exp\left(- \int_0^x \sigma(R') dR' \right)$$

The quantity

$$\tau(R) = \exp\left(- \int_0^R \sigma(R') dR' \right) \tag{2.23}$$

is called the optical distance from the starting point to the next collision site at a geometrical distance of R.

In most of the practical cases, the material does not change continuously, but there are different, clearly separated regions filled with different media and thus the integral in Equation (2.23) is replaced by a sum (see Figure 2.7):

$$\tau(R) = \sum_{i=1}^{n} \sigma_i R_i$$

F. COLLISION DENSITIES

In Section D. the elementary probabilities of interactions were described. The expected number of collisions occurring in a phase-space element dP about P are characterized by two functions, two collision densities.

$$\chi(P) dP$$

is the number of particles *leaving* a collision with coordinates lying in dP about P and is sometimes briefly called the *outgoing density,* whereas

$$\psi(P) dP$$

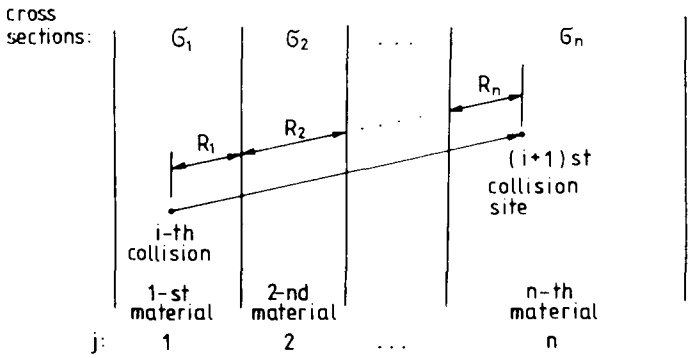

FIGURE 2.7. A particle flight crossing boundaries of zones of different materials.

denotes the number of particles *entering* a collision with coordinates dP about P and its name is *incoming density,* or simply *collision density.*

From the above definitions it is clear that none of these functions is a "density function" since generally the normalization conditions

$$\int \chi(P)\,dP = 1$$

and

$$\int \psi(P)\,dP = 1$$

are not satisfied.

The incoming density is closely related to the flux. Let us recall the definition of the flux (fluence, by the rigorous ICRU terminology):

$$\phi(\mathbf{r},\mathbf{E})\,da\,d\mathbf{E}$$

is the number of particles entering an infinitesimal sphere of radius dr, cross-sectional area of $da = \pi\,(dr)^2$ with direction and energy $d\mathbf{E}$ about $\mathbf{E}$. The expected path length $<d\ell>$ of these particles is (see Equation 2.14)

$$<d\ell> = \frac{4}{3}\,d\rho$$

Thus the expected number of particles entering collisions in the infinitesimal sphere (i.e. the collision density) is

$$\begin{aligned}\psi(\mathbf{r},\mathbf{E})\,d\mathbf{r}\,d\mathbf{E} &= \sigma(\mathbf{r},E) < d\ell > \phi(\mathbf{r},\mathbf{E})\,da\,d\mathbf{E} \\ &= \sigma(\mathbf{r},E)\,\phi(\mathbf{r},\mathbf{E})\,d\mathbf{r}\,d\mathbf{E}\end{aligned}$$

therefore:

$$\psi(P) = \sigma(\mathbf{r}_1,E)\,\phi(P) \tag{2.24}$$

The inverse relation

$$\phi(P) = \frac{1}{\sigma(\mathbf{r}_1,E)}\,\psi(P) \tag{2.25}$$

is valid only if $\sigma \neq 0$, which condition clearly reflects the very simple physical fact that *in vacuum* the flux is still a reasonable quantity whereas no collisions can happen if no material is present.

G. QUANTITIES TO BE DETERMINED: REACTION RATES, RESPONSES, SCORES

Generally, the aim of a Monte Carlo calculation is the estimation of the value of a *physical quantity* or values of several quantities. For the sake of simplicity we restrict our discussion to the determination of a single quantity. Extension of the considerations to parallel examination of several quantities is straightforward.

These quantities can represent a great number of physically interpretable data varying from the number of collisions in a space element to leakage probabilities, detector responses or doses absorbed in certain regions of the core of a reactor or even in organs of an anthropomorphic phantom. Just to preserve generality of the discussion all these quantities will be called either as *receptor responses* or *reaction rates*.

A common feature of these responses is that they can be formulated as weighted integrals (or functionals) of one of the collision densities.

Thus a response (or reaction rate) is most generally formulated as:

$$R = \int f_\chi(P)\chi(P)\,dP \tag{2.26}$$

or

$$R = \int f_\psi(P)\psi(P)\,dP$$

The f_χ and f_ψ weight function are derived from the *physical* connection between the collision density and the quantity to be determined. The integrations are extended to the region of interest, or, by other words the f weight functions have to vanish outside the range of interest. Since the subscript of f is trivial from the type of collision density used in the integrals of (2.26) it is generally omitted.

Naturally if R is calculated not for a finite range but only for a point, e.g., for $\mathbf{r}_o$, then the weight function contains a Dirac-delta component:

$$f(P) = f_1(\mathbf{E})\delta(\mathbf{r} - \mathbf{r}_o)$$

Simply, if the number of collisions are to be computed for a phase space domain P_o, then

$$f(P) = \begin{cases} 1, & \text{if } P \in P_o \\ 0, & \text{otherwise} \end{cases}$$

Another simple example can be derived from Equation (2.25), the formula for the flux integral in a phase-space domain P_o is

$$\phi = \int \sigma^{-1}(\mathbf{r},E)\psi(P)\, dP$$

i.e.,

$$f_\psi(P) = \sigma^{-1}(\mathbf{r},E) \qquad \text{here.}$$

A Monte Carlo estimate of the reaction rate is called the (actual) *score*, and every simulated event has a — many times zero — *contribution to the score*. A reaction rate is usually estimated by several independent Monte Carlo histories and the final estimate will be the average of the individual scores.

H. OTHER QUANTITIES

There are many other quantities — which may or may not have direct physical meaning — introduced in the next chapters. They are, however, used only in connection with certain special examples or techniques and will be defined at the appropriate places.

A general rule of our notation is that if a quantity is denoted by x in the analog simulation (in the numerical "copy" of the real physical process) then its counterpart used in the nonanalog simulations (e.g., simulations deviating from the physical process) will be denoted by $\hat{x}$.

The statistical weights necessarily introduced for nonanalog simulations are denoted by W and the factors modifying it at a single step by w.

REFERENCES

1. **Ahrens, J. H. and Dieter, U.,** Computer Methods for Sampling from the Exponential and Normal Distributions, *Comm. ACM,* **15,** 873 (1972).
2. **Barnett, U. D.,** The behaviour of pseudo-random sequences generated on computers by the multiplicative congruential method, *Meth. Comp.,* **16,** 63 (1962).
3. **Carter, L. L. and Cashwell, E. D.,** Particle-Transport Simulation with the Monte Carlo Method. ERDA Critical Review Series, National Technical Information Service, Springfield, MA, 1975.
4. **Coveyou, R. R.,** Serial correlation in the generation of pseudo-random numbers, *J. Assoc. Comput. Mach.,* **7,** 72 (1960).
5. **Coveyou, R. R. and MacPherson, R. D.,** Fourier Analysis of Uniform Random Number Generators, *J. Assoc. Comput. Mach.,* **14,** 100 (1967).
6. **Ermakov, S. M. and Mikhailov, G. A.,** Course of Statistical Modelling (in Russian), Nauka, Moscow (1976).
7. **Everett, C. J. and Cashwell, E. D.,** A Monte Carlo Sampler. LA-5061-MS Report, Los Alamos Scientific Laboratory, Los Alamos (1972).
8. **Everett, C. J. and Cashwell, E. D.,** A Second Monte Carlo Sampler. LA-5723-MS Report, Los Alamos Scientific Laboratory, Los Alamos, CA, (1974).
9. **Everett, C. J. and Cashwell, E. D.,** A Third Monte Carlo Sampler. LA9721-MS Report, Los Alamos National Laboratory, Los Alamos, CA, (1983).
10. **Forsythe, G. E.,** Generation and Testing of Random Digits at the National Bureau of Standards. Applied Mathematics Series, No. 12, U.S. Government Printing Office, Washington, D.C. (1951), 34.
11. **Gruenberger, F.,** Tests of random digits, *Math. Tables Aids Comput.,* **4,** 244 (1956).
12. **Halton, J. H.,** A retrospective and prospective survey of the Monte Carlo method, *SIAM Rev.,* 12, 1 (1970).
13. Radiation Quantities and Units. Report 33, International Commission on Radiation Units and Measurements, Washington, D.C. (1980).

14. **Irving, D. C., Freestone, R. M., Jr., and Kam, F. B. K.,** 05R, A general-purpose Monte Carlo neutron transport code. ORNL-3622 Report, Oak Ridge National Laboratory, Oak Ridge, TN (1965).
15. **Kahn, H.,** Applications of Monte Carlo. AECU-3259 Report, Rand Corporation, Santa Monica, CA (1954.)
16. **Kendall, M. G. and Babington-Smith, B.,** Randomness and random sampling numbers, *J. R. Statist. Soc.* A, **101,** 147 (1938).
17. **Kendall, M. G. and Moran, P. A. P.,** *Geometrical Probability,* Hafner Publishing Co., New York (1963).
18. **Kinderman, A. J. and Ramage, J. G.,** Computer generation of normal random variables, *J. Am. Statist. Assoc.*, **71,** 893 (1976).
19. **Lehner, D. H.,** Mathematical methods in large-scale computing units, in *Proc. Symp. on Large-Scale Digital Calc. Mach.*, Harvard Univ. Press, Harvard, MA (1949), 141.
20. **Lux, I.,** A special method to sample some probability density functions, *Computing,* **20,** 183 (1978).
21. **Lux, I.,** Generation of random numbers by iterative rejection technique (in Hungarian). Alkalmazott Matematikai Lapok, **1,** 347 (1975).
22. **Lux, I.,** HEXANN-EVALU — a Monte Carlo Program System for Pressure Vessel Neutron Irradiation Calculation. VTT Report 210, Technical Research Centre of Finland, Espoo (1983).
23. **Marsaglia, G.,** Generating Exponential Random Variables, *Ann. Math. Stat.*, **32,** 899 (1961).
24. **Marsaglia, G. and Bray, T. A.,** A convenient method for generating normal variables, *SIAM Rev.*, **6,** 260 (1964).
25. **MacLaren, M. D., Marsaglia, G., and Bray, T.,** A fast procedure for generating exponential random variables, *Comm. ACM,* **7,** 298 (1964).
26. **MacLaren, M. D. and Marsaglia, G.,** Uniform random number generators, *J. Assoc. Comput. Mach.*, **12,** 83 (1965).
27. **McGrath, E. J. and Irving, D. C.,** Random Number Generation for Selected Probability Distributions. ORNL-RSIC-38 Report, *Techniques for Efficient Monte Carlo Simulation,* Vol. II., Oak Ridge National Laboratory, Oak Ridge, TN (1975).
28. **Mikhailov, G. A.,** On modelling random variables for one class of distribution laws, (in Russian), *Teoriya Veroyatnostei i ee Primeneniya,* **10,** 749 (1965).
29. **Neumann, J.,** Various Techniques Used in Connection with Random Digits. National Bureau of Standards Applied Mathematics Series, No. 12, U.S. Government, Printing Office, Washington, D.C. (1951), p. 36.
30. **Rhoades, W. A. and Mynatt, F. R.,** The DOT III. Two-dimensional Discrete Ordinates Transport Code. ORNL-TM-4280 Report. Oak Ridge National Laboratory, Oak Ridge, TN (1973).
31. **Shreider, Y. A., Ed.,** *Metod statisticheskih ispytani Monte Carlo* (in Russian) Fizmatgiz, Moscow (1961). — German translation: *Die Monte Carlo Methode und ihre Verwirklichung mit elektronischen Digitalrechnern* B.b. Teubner Verlagsgesellschaft, Leipzig (1964). — English translation: *The Monte Carlo Method,* Pergamon Press, New York (1966).
32. **Sobol, I. M.,** *The Monte Carlo Calculational Method,* (in Russian), Nauka, Moscow (1973).
33. **Spanier, J. and Gelbard, E. M.,** *Monte Carlo Principles and Neutron Transport Problems,* Addison-Wesley, Reading (1969).
34. **Taussky, O. and Todd, J.,** Generation of Pseudo-random Numbers. Symp. on Monte Carlo Methods, University of Florida 1954, H.A. Meyer, Ed., John Wiley & Sons, New York (1956), 15.
35. **Wood, J.,** *Computational Methods in Reactor Shielding,* Pergamon Press, Oxford (1982).

Chapter 3

DIRECT SIMULATION OF THE PHYSICAL PROCESSES

"Life" of a neutron or photon, from its birth to its death is governed by nature via many *random processes*. Just at the very beginning: there is only a *certain probability* that a particle is "born" at all in the source in a given short time interval. The initial direction of flight of a particle is also a random variable and such is its energy (if the source is not mono-energetic) and its location (if the source is not so small in spatial extension that can be represented by a point).

In addition, randomness remains with the particle throughout its further history. Neither the distance traversed up to its next collision site nor the type of the subsequent interaction can be determined in advance for an individual particle. Instead, probability distributions of them are known. Similarly, random variables are the energy and the direction of the scattered particles and even the number of the secondaries created in a multiplicative interaction.

The same uncertainty characterizes the detection: only a certain fraction of the particles crossing the receptor region will interact in that volume. Again, only the interaction probabilities and not the reactions of any individual particles can be predicted even if all the physical parameters of both the particle and the receptor are known.

As a consequence of these inherent stochastic processes all observed results will be accompanied by smaller or larger fluctuations, this is why, e.g. measured count rates are generally given together with their standard deviations. In measurements carried out under time-independent (steady-state) conditions, the easiest way to decrease the statistical uncertainties is the increase of the observation time. The alternative — but seldom realizable in practice — way is the increase of the source intensity. Anyhow, in most experiments the product of the source intensity and the observation time can be set to as large as 10^6 particles, or even higher by several orders of magnitude.

If the reader compares the definition of Monte Carlo methods we gave at the beginning of Chapter 2 and the random nature of the neutron and photon migration outlined in the previous paragraphs, one cannot but wonder that many people got the idea to connect the two phenomena: to try to simulate the particles' random walk on computers. The word *simulation* here means the as accurate as possible realization of the coordinates of the particles — in a computer.

At first sight one might think that the accuracy of the computer simulation depends on the answers to two questions:

1. How precisely do we know the probability distributions governing the physical processes, and
2. How correctly can we select random samples from these distributions?

And really, lack of satisfactory knowledge of the distributions or application of incorrectly selected procedures may draw systematic errors into the computations. By using a terminology more familiar in Monte Carlo: the results will be *biased.*

There is, however, another source of error. It is the statistical uncertainty which is — at least in the one-to-one simulation — completely analog — or even equivalent — to the random fluctuation observed at measurements. The origin of this uncertainty is theoretically the same for the physical processes and their computer simulations. Nevertheless, in practice they differ — unfavorably for the Monte Carlo technique — in their extent. The random walk simulations are very time-consuming and therefore an increase of the simulation number (the computational counterpart of the product of the source intensity and the measuring time) over about 10^5 is seldom realizable.

Thus, in most Monte Carlo programs, special techniques are introduced to decrease the statistical uncertainties. The introduction of such techniques leads to deviations from the one-to-one simulations, to so-called nonanalog games. Appropriate selection of the nonanalog procedures is of major importance and will be discussed many times, in different levels throughout this book.

Now, however — in spite of all its disadvantages — let us turn back and investigate in detail the analog simulation, from which the idea of Monte Carlo application for particle transport originated in the 1940s. Still now, a deep understanding of the simplest analog procedures is the basis for understanding the more advanced techniques.

In the same way as the life of a physical particle starts by its emission from some sort of source, in an analog Monte Carlo game first the initial coordinates have to be selected. The next step is the free flight of the neutron or photon up to its next collision, consequently, in the simulation, a path length has to be selected. From the starting point coordinates and the direction of flight, the site of the subsequent interaction is to be determined.

At the collision site, a large variety of interactions with the different atoms constituting the material at that point can take place. Accordingly, in the numerical simulation, first the types of both the collided atom and the interaction have to be selected. If the actual collision does not lead to absorption the particle goes on its way with a new energy and direction — both of them are to be selected. In multiplicative events, or e.g. (n,γ) reactions, new particles are also created, the parameters of which are generally immediately selected but temporarily stored and handled as coordinates of particles from secondary sources. The histories of these "secondaries" are followed after the termination of the "primary" particle. (For correctness it must be noted here that in, e.g. an (n,2n) reaction there is no physically correct distinction between the two outcoming neutrons as to which one is the primary and which is the secondary. The decision is arbitrary from the point of physics and is governed by practical consideration.)

After the simulation of a scattering event, the process is followed by a next path selection. The repetition of this two step (transition + collision) cycle is terminated by one of the following three events:

- An absorption takes place
- The particle leaves the system investigated in such a way that there is no possibility to return
- The energy of the particle falls out of the range of interest

If the event, whose frequency is just studied, occurs, the actual contribution is calculated either in the transition or in the collision phase. The sum of the contributions collected during the simulation of the history of a single primary source particle is called the score. And the average of an appropriately large number of scores is the Monte Carlo estimate of the physical quantity investigated.

In the consecutive sections of this Chapter, the basic procedures used during these steps (source selection, transition and collision simulations, and scoring) are discussed, several specific procedures, frequently used in neutron and photon transport processes, are collected in the Appendices of this Chapter.

I. ANALOG SIMULATION OF THE RANDOM WALK

A. SELECTION OF SOURCE PARAMETERS

There are six fundamental parameters of a particle emitted from a source, viz:

- The three spatial coordinates: $\mathbf{r} = (x,y,z)$, in a Cartesian system
- Two coordinates of the direction of flight: $\boldsymbol{\omega} = (\omega_x,\omega_y,\omega_z)$, $|\boldsymbol{\omega}| = 1$ and
- The energy (E) of the particle

The list presented above is not the only possible specification, one can use, e.g., spherical coordinates instead of Cartesian, or replace the energy of the photons by the wavelength, or prefer to describe the state of a neutron by the velocity vector instead of the energy and the unit length direction vector.

However, in any representation, the number of the mutually independent parameters is six and simple transformation rules can help to change from one representation to another, if needed.

Any set of the six parameters can be considered as the coordinates of a point in a six-dimensional phase-space.

In nearly all practical cases the source density $Q(\mathbf{r},\boldsymbol{\omega},E)$ can be factorized as:

$$Q(\mathbf{r},\boldsymbol{\omega},E) = Q_r(\mathbf{r}) \cdot Q_\omega(\boldsymbol{\omega}) \cdot Q_E(E)$$

reflecting the physical fact that the spatial, directional, and energy distributions are mutually independent from each other.

From the point of view of Monte Carlo selection, it means that one can select separately the $\mathbf{r}$, $\boldsymbol{\omega}$, and E coordinates.

To simplify the description of the selection procedures, we assume — for this Section — that the source is normalized to unity, i.e.,:

$$\int Q(P)dP = 1$$

moreover:

$$\int Q_r(\mathbf{r})\,d\mathbf{r} = 1$$

$$\int Q_\omega(\boldsymbol{\omega})\,d\boldsymbol{\omega} = 1$$

and

$$\int Q_E(E)\,dE = 1$$

If these conditions are not fulfilled and

$$\int Q(P)\,dP = Q_o \neq 1$$

then the only correction that has to be made is the multiplication of all results by Q_o since the transport processes are linear with respect to the absolute source intensity.

1. Space Coordinates Sampling

For *point-like sources,* the random selection is replaced by an assignment:

$$\mathbf{r}_i \equiv \mathbf{r}_o \qquad \text{for} \qquad i = 1,2, \ldots, n$$

i.e., all the n simulations start from the source point $\mathbf{r}_o$.

If the source is uniformly distributed along a *straight line* (or rod of negligible radius)

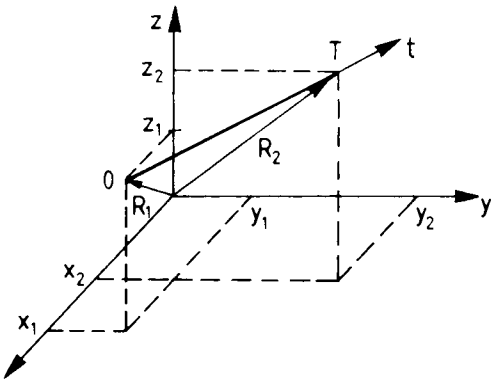

FIGURE 3.1. Selection of a random point from a line source.

then let us put this line into the coordinate system as given in Figure 3.1, and define the axis t along the source line. Then

$$Q(t)\,dt = p(t)\,dt = \frac{1}{T}\,dt$$

if $t = 0$ at $\mathbf{R}_1$ and $\mathbf{R}_2 = \mathbf{R}_1 + T(\mathbf{R}_2 - \mathbf{R}_1)$.

Now the i-th source point is selected as:

$$\mathbf{r}_i = \mathbf{R}_1 + \rho_i T(\mathbf{R}_2 - \mathbf{R}_1)$$

More complicated, one-dimensional sources (or more precisely sources that can be approximated by one-dimensional curves) seldom occur in practice. But if they do occur, the best approach is to describe the curve in a parametric form, then select the parameter t from p(t) and determine the Cartesian coordinates by transformation.

After, the zero- and one-dimensional forms let us continue with sources that can be described by *surfaces*.

If the surface is a region of a plane, let us fix a (ξ,η) coordinate system to the plane. Points from sources that have simple boundaries can be easily selected. Recipes to pick-up points from a square (or from a rectangle, after linear transformations) and a circle are given in Sections 2.I.I and 2.I.J, respectively. For other surfaces with complicated boundaries, the application of the *rejection technique* is recommended — if the user cannot find a special, efficient tricky method for his problem. In the application of the rejection method the source region is to be covered by a rectangle (Figure 3.2.a) from which tentative coordinates are selected. The points lying out of the region of interest are to be rejected.

If the area of the covering rectangle is much larger than that of the source, it is expedient to cover the source region by several smaller rectangles (Figure 3.2.b). In this case, first one of the rectangles is to be selected. The i-th one is chosen with a probability of

$$p_i = \frac{t_i}{T}$$

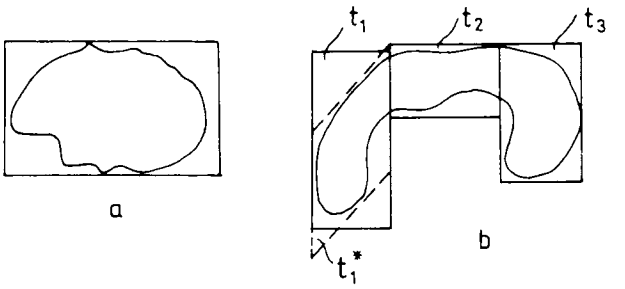

FIGURE 3.2. Covering plane sources with rectangles — for sampling by the rejection method.

if t_i is its area and

$$T = \sum_{i=1}^{T} t_i$$

then the coordinates are selected from the i-th rectangle — by the rejection method.

The covering surface is not necessarily a rectangle. (The reader should remember that in the general description of the rejection technique in Section 2.I.C we have also started with a majorant constant and subsequently proceeded to majorant functions.) Any geometrical figure which is easy to sample can be used. For example, in Figure 3.2.B the first covering rectangle should, generally, be replaced by a parallelogram, if the t_1/t_1^* efficiency gain overcompensates for the time increase brought in by the more complicated sampling procedure needed.

Surfaces extended into three dimensions seldom occur in practice. If the source is uniformly distributed on the surface of a sphere then the method given in Section 2.I.J for the selection of three dimensional unit vectors can be applied — with two additional transformations: first all the three Cartesian coordinates have to be multiplied by the actual radius, then the points have to be shifted by the coordinates of the actual center of the source.

Most sources are extended into *three dimensions.* (Physically there are only three-dimensional sources, the representations of them by points, curves, or surfaces are only approximations.)

The ideas of random sampling *in three dimensions* are the same as in two dimensions. For simple regions (rectangular blocks, circular cylinders, spheres, etc.) direct procedures can be developed by establishing the appropriate PDFs and using the inverse distribution method (Section 2.I.A). Points from source zones limited by complex boundary surfaces can be selected by the rejection technique: now the zones (or separate parts of it) are to be imbedded in rectangular boxes — or sometimes into other volumes still easy to handle.

2. Sampling of Initial Directions

In the great majority of problems the particles are emitted by *isotropic distribution,* in which case, the method for selecting the direction cosines of random vectors described in Section 2.I.J may be used.

Sometimes a *parallel beam* of particles enters the system of interest. In such a case, the random sampling of the direction cosines is replaced by assignments of the actual values.

A *cosine distribution* is achieved if a plane is placed into an isotropic field (i.e., into

the infinite space where isotropic sources are distributed uniformly). Let us fix the coordinate system's [x, y] plane parallel to the plane of interest. Then the outer normal to the plane has the following direction cosines:

$$\omega_{x,n} = \omega_{y,n} = 0$$

and

$$\omega_{z,n} = 1$$

The cosine distribution has the PDF:[6]

$$p(\omega_z) = 2\omega_z, \qquad \omega_z \geqslant 0$$

Thus, according to Equation 2.2

$$\rho = \int_0^{\omega_z} 2\omega_z d\omega_z$$

and the

$$\omega_z = \sqrt{\rho}$$

sampling rule can be used. (The reader should remember Theorem 2.6 and replace the execution of a square root by selecting the maximum of two random numbers.) Since the azimuth is uniformly distributed over $(0,2\pi)$, in the formulae

$$\omega_x = \sqrt{1 - \omega_z^2} \cdot \cos\varphi$$

and

$$\omega_y = \sqrt{1 - \omega_z^2} \cdot \sin\varphi$$

$\cos\varphi$ and $\sin\varphi$ can be selected either directly ($\varphi = \rho_1 2\pi$), or by the Neumann method given in Section 2.I.J, Equation (2.15).

3. Selection of the Initial Energies

The simplest — and not too rare — case is if one has a *monoenergetic source* and can, therefore, replace the energy selection by an assignment. There are many gamma sources that emit photons of different discrete energies with different intensities (probabilities). The sampling from such *line spectra* can be carried out as described in Theorem 2.1.

More skillful techniques are needed to pick-up energies from *continuous spectra.* A relatively easy, though not exact, method is to approximate the spectrum with either a step function or by a broken line. In both cases the inverse distribution method (Section 2.I.A) is applicable. If the continuous spectrum is described by an analytical formula, the task is to find the best of the methods discussed in Section 2.I, but the rejection technique is the only one that always works.

Two source types have special importance in neutron transport calculations. Methods for selecting neutron energies from the Watt-fission spectrum and from the Maxwellian distribution describing the energy distribution of the thermal neutrons are given in Appendices 3B and 3C, respectively.

B. PATH LENGTH SELECTION

As has been introduced in Section 2.II.E the path (R) traversed between two collisions has a PDF of:

$$p(R) = \sigma(R)\exp\left[-\int_0^x \sigma(R')dR'\right] \tag{3.1}$$

If the medium is *homogeneous:*

$$\sigma(R') \equiv \sigma_o$$

then

$$p(R) = \sigma_o e^{-\sigma_o R}$$

and an actual path length can easily be selected by the inverse distribution method (see Equation (2.2) and Equation (2.6) with the transformation $x = \sigma_o R$):

$$R = -\frac{1}{\sigma_o}\ell n\rho \tag{3.2}$$

Naturally, the fast methods listed in Section 2.I.G can replace the execution of the logarithm in Equation (3.2).

The selection is more complicated if the medium is inhomogeneous. In practical problems, the cross-sections (or the compositions of the materials) are generally constant within extended zones.*

Let us consider n regions with cross-sections $\sigma_1, \sigma_2, \ldots \sigma_n$. If the particle crosses the distances $R_1, R_2, \ldots, R_n$ in these regions (see Figure 2.7) then the PDF (3.1) becomes:

$$p(R) = \sigma_j\exp\left[-\left(\sum_{i=1}^{j-1}\sigma_i R_i\right) - \sigma_j\left(R - \sum_{i=1}^{j-1} R_i\right)\right],$$

$$\text{if} \quad \sum_{i=1}^{j-1} R_i \leq R \leq \sum_{i=1}^{j} R_i$$

Thus, the path length selection can be carried out by determining j from the inequalities

$$\sum_{i=1}^{j-1}\sigma_i R_i < -\ell n\rho \leq \sum_{i=1}^{j}\sigma_i R_i \tag{3.3}$$

and then, calculating:

$$R = \sum_{i=1}^{j-1} R_i + \frac{1}{\sigma_j}\left(-\ell n\rho - \sum_{i=1}^{j-1}\sigma_i R_i\right) \tag{3.4}$$

The difficulty in solving Equations (3.3) and (3.4) lies not in the summations but in the

* Though it is beyond the scope of this book it should be noted here that in the transport of *charged* particles the cross-section changes quasi-continuously even within a homogeneous medium, since the energy of the particle changes (decreases) quasi-continuously.

determination of the R_i distances, i.e., in the determination of the coordinates, where the particle trajectories cross the boundaries separating the different homogeneous zones. This procedure may be extremely complicated in complex geometries thus another technique[48] is suggested instead of the "straightforward" method described above.

The method is the following:

1. Define a majorant cross-section: $\sigma_o \geq \sigma(\mathbf{r})$, for all $\mathbf{r}$-s along the path;
2. Select a distance R by Equation (3.2) and determine the *tentative* next collision site ($\mathbf{r}'_k$):

$$\mathbf{r}'_k = \mathbf{r}_{k-1} + R\boldsymbol{\omega}_{k-1}$$

if $\mathbf{r}_{k-1}$ is the starting point and $\boldsymbol{\omega}_{k-1}$ is the direction of flight;

3. Play a rejection game:

- with a probability of $\sigma(\mathbf{r}'_k)/\sigma$ *accept* this point as a real collision site ($\mathbf{r}_k = \mathbf{r}'_k$);
- with a probability of $1 - \sigma(\mathbf{r}'_k)/\sigma_o$ *do not accept* $\mathbf{r}'_k$ as a real collision site but select a new path starting from $\mathbf{r}'_k$ with the unchanged direction $\boldsymbol{\omega}_{k-1}$, again taking the total cross section to σ_o (i.e. set $\mathbf{r}_{k-1} = \mathbf{r}'_k$ and return to step 2).

A mathematically correct proof of this procedure (even for continuously varying cross-sections) is given in Reference 10, but there is a very easy-to-follow method to understand its validity:

Let us introduce an imaginary scattering event which changes neither the energy nor the direction of the particle. This definition implies that such imaginary scatterings are not physically observable, i.e. they can be introduced with any cross-section at any point. Now if we assume that the majorant cross-section (σ_o) is a sum of the real (σ) and imaginary (σ_i) cross-sections, then in the procedure outlined above there is no acceptance and rejection, but in a fraction of:

$$1 - \frac{\sigma(\mathbf{r}'_k)}{\sigma_o} = \frac{\sigma_i(\mathbf{r}'_k)}{\sigma_o}$$

the collisions an imaginary interaction is simulated.*

The advantage of the method is clear: only the locations of the tentative collision sites have to be determined independently from the boundary crossings up to those points.

The majorant cross-section method is trivially applicable for paths going through cavities (regions filled with vacuum). Tentative collision sites lying in vacuum are, per se, never accepted. (Those who like curious statements can say that there are solely imaginary scattering events in regions filled with no material.)

The selection of the path length leads to termination of the simulation if the particle leaves the system and has no chance to return. Such situations never exist in physical reality. However, if the system investigated is surrounded by a low density material (most probably air) and even the nearest reflectors (e.g., walls of the room) are so far that the contribution of backscattering is negligible then placing the volume of interest into an infinite vacuum space is a reasonable approximation.

* The imaginary or hypothetical collisions are called "delta-scatterings".[44] Delta scattering will be examined more closely in Chapter 5.IV. A proof of the unbiasedness of the selection procedure above will also be given there.