UCRL- 87745
PREPRINT
Conf-820668--2

UCRL--87745

DE82 017635

THE APPLICATION OF MONTE CARLO CODES TO NEUTRON DOSIMETRY

MASTER

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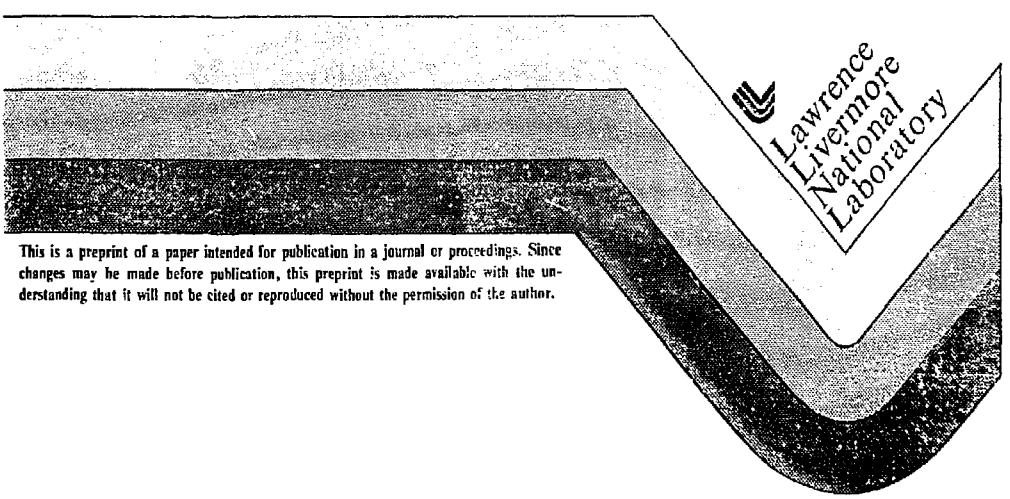
This paper was prepared for submittal
to the DOE Workshop on
Personnel Neutron Dosimetry,
Las Vegas, NV, June 24-25, 1982

June 15, 1982



Introduction

It is important for any research and development program that calculational tools be available to complement experimental efforts. In neutron dosimetry, calculations enable one to predict the response of a proposed dosimeter before effort is expended to design and fabricate the neutron instrument or dosimeter. Also, since the neutron spectrum is so important in determining how a particular dosimeter will respond, having the ability to calculate the neutron spectrum for a wide variety of source, moderator, and shield configurations is extremely valuable. The nature of these calculations requires the use of computer programs that implement mathematical models representing the transport of radiation through attenuating media. Numerical, and in some cases analytical, solutions of these models can be obtained by one of several calculational techniques.

Calculational methods include spherical harmonics, discrete ordinates, moments, Monte Carlo, diffusion theory, invariant imbedding, and kernels, plus a method which combines a removal kernel with diffusion theory. Except for the invariant bedding method, all of these techniques are either approximate solutions to the well-known Boltzmann equation or are based on kernels obtained from solutions to the equation. The Boltzmann equation is a precise mathematical description of neutron behavior in terms of position, energy, direction, and time.

The Boltzmann transport equation describes the general behavior of uncharged particles or quanta of electromagnetic radiation in terms of the seven-dimensional phase space $(\bar{r}, E, \bar{\Omega}, t)$. This space consists of three spatial coordinates, two direction-defining angles, the particle energy, and time. Knowledge of the radiation particle density over all phase space for some prescribed physical situation is in fact the complete solution to the transport equation. However, experience has shown that the particle flux density, which is simply related to the particle density, is a more convenient variable for analysis. Accordingly, particle flux density, rather than current, is used as the dependent variable in the Boltzmann equation.

The flux density quantity used is the angular flux, denoted by $\phi(\bar{r}, E, \bar{\Omega}, t)$ and defined as the number of particles that cross a unit area normal to the Ω direction per unit time with energies in dE about E and in a direction that lies in $d\bar{\Omega}$ about $\bar{\Omega}$. This function is more properly called the differential energy and angle spectrum of the number flux density, but the simple expression angular flux density has become standard terminology. Integrating the angular flux density over all directions yields the scalar flux density, given by

$$\phi(\bar{r}, E, t) = \int_{\Omega} \phi(\bar{r}, E, \bar{\Omega}, t)\, d\bar{\Omega}$$

and having the units neutron cm^{-2} sec^{-1} MeV^{-1}. This scalar flux density is sometimes referred to as a total flux, although it is differential with respect to energy. A second integration over some specified energy range will produce $\phi(r)$, which is truly a total flux density.

Derivation of the Boltzmann equation can be regarded as a bookkeeping process that sets particle losses equal to particle gains within a differential element of phase space (dr dE dΩ). One of the more familiar forms for the time-dependent problem is given by

$$v \cdot \bar{\Omega}\phi(\bar{r}, E, \bar{\Omega}) + \Sigma_t(\bar{r}, E)\,\phi(r, E, \bar{\Omega}) = S(\bar{r}, E, \bar{\Omega}) + \iint \Sigma_s(\bar{r}\ E' \to E, \bar{\Omega}' \to \bar{\Omega})\,\phi(\bar{r}\ E', \bar{\Omega}')\,dE'\,d\bar{\Omega}'$$

where

$v \cdot \bar{\Omega}\phi(\bar{r}, E, \bar{\Omega})\,dE\,d\bar{\Omega}$ = net convective loss at $\bar{r}$ of particles with energies in dE about E and with directions which lie in dΩ about Ω per unit volume per unit time,

$\Sigma_t(\bar{r}, E)\,\phi(\bar{r}, E, \bar{\Omega})\,dEd\Omega$ = collision loss at $\bar{r}$ of particles with energies in dE about E and directions which lie in dΩ about Ω per unit volume per unit time,

$S(\bar{r}, E, \bar{\Omega})\,dEd\bar{\Omega}$ = source particles emitted at $\bar{r}$ with energies in dE about E and directions which lie in dΩ about Ω per unit volume per unit volume per unit time,

$\iint \Sigma_s \phi(\bar{r}, E', \bar{\Omega}') \, dE' d\bar{\Omega}$ = inscattering gain at r of particles with energies in dE about E and directions which lie in $d\Omega$ about Ω per unit volume per unit time,

$\Sigma_t(\bar{r}, E)$ = total macroscopic cross section at r evaluated at the energy of the incident particle,

$\Sigma_s \, dE d\bar{\Omega}$ = differential scattering cross section which describes the probability that a particle with initial energy E' and an initial direction Ω' undergoes a scattering collision at r which places it into a direction that lies in $d\Omega$ about Ω with a new energy in dE about E.

The solution of the transport equation represents the average value of the particle flux density. Solutions of the transport equation are inherently complex due to its integradifferential forms, and exact solutions are limited to a few highly specialized problems. The most practical techniques are approximate and essentially numerical in nature, the more familiar ones being the sphereical harmonic method, the discrete ordinates (S_n) technique, and the moments methods. It is interesting to note that diffusion theory actually corresponds to a low-order approximation of the transport equation. Also, integral forms of the transport equation are generally regarded as the formal

basis for the Monte Carlo method, the results of which can in principle be made to approach the exact solution. For the remainder of this paper the focus will be on the Monte Carlo technique.

The Monte Carlo Method

The Monte carlo method is a mathematical technique used to approximate a desired quantity by random sampling from the probabilities describing the true stochastic processes that affect the magnitude of the quantity. With sufficient sampling it is assumed that the average value obtained is an accurate estimate of the quantity. For example, a game of chance may be played in which the probability of success P is a number whose value is desired. If the game is played N times with r wins, then r/N is an estimate of P.

Many types of problems in physics and mathematics can be solved successfully by random sampling or stochastic techniques. For simple problems, such as the evaluation of single or double integrals, the usual numerical integration schemes will give accurate results with less effort, but for four- or five-fold integrals, Monte Carlo becomes a practical tool.

The method can be demonstrated by considering the Monte Carlo evaluation of a single integral, for example the integral

$$J = \int_a^b g(x)\, f(x)\, dx$$

which generates the average of the function g (x) weighted by the function f(x). Let the values of the random variable x be sampled from f(x), a normalized probability density function (pdf); the normalization condition is

$$\int_a^b f(x)\, dx = 1$$

with this sampling procedure the integral can be rewritten as

$$J = \int_a^b g(x)\, dF(x),$$

with

$$F(x) = \int_a^x f(x')\, dx' \ .$$

The function F(x) is the cumulative distribution function (cdf) corresponding to f(x). With this transformation a selection of values of F(x) with uniform probability over the interval (0,1) is equivalent to the selection of values of x according to f(x) over the interval (a,b). Then for the ith selection there is a value $g(x_i)$, and an estimation for the value of J is given by

$$\bar{J} = \frac{1}{N} \sum_{i=1}^{N} g(x_i)$$

Where $\bar{J}$ is the Monte Carlo estimate of J and N is the arbitrary number of samples.

When generalized to multidimensional integrals Q, the above procedure gives

$$Q = \int g(r) f(P) dP,$$

Where P denotes the multidimensional phase space. The Monte Carlo estimate of Q is given by

$$\bar{Q} = \frac{1}{N} \sum_{i=1}^{N} g(P_i)$$

Where the P_i's are selected according to a complicated set of probabilities giving rise to the probability density function f(P).

In solving for the basic quantities mentioned above or for others determined by these quantities, the sampling in phase space is accomplished by following particle case histories from birth to death by absorption or leakage. This analogy to real particles has led some to call Monte Carlo a theoretical experiment.

When generating the sequence of events in the life of a case history, certain quantities of interest are selected or computed at each step of the random walk. Each step may be regarded as a collision or as a flight.

Termination of a history generally takes place when the particle is absorbed, reaches a portion of phase space not allowed, or is killed according

to some prescription such as Russian Roulette. The most common areas of phase space not allowed are spatial regions exterior to the system or energy regions below an arbitrary cutoff.

Selecting a sample from a distribution usually requires first the selection of one or more random numbers. Once a random number has been selected, there are a number of possible ways to select from a distribution. Consider the following examples:

1. Select a nuclide from N nuclides in a mixture. Each nuclide has a total macroscopic cross section Σ_n and the total macrascopic cross section for the medium, Σ, is given by

$$\Sigma = \sum_{n=1}^{N} \Sigma_n$$

Nuclide 1 is selected if a random number R is less than Σ_1/Σ, and the its nuclide is selected if

$$\sum_{n=1}^{i-i} = \frac{\Sigma_n}{\Sigma} < R < \sum_{n=1}^{i} \frac{\Sigma_n}{\Sigma}$$

Once the nuclide has been selected, a choice is made between an absorption or a scattering reaction. If a random number is less than Σ_s/Σ, where Σ_s is the scattering cross section, a scattering reaction will occur; otherwise, it will be an absorption.

2. Select a value of x from the pdf f(x), where

$$\int_{-\infty}^{\infty} f(x)\,dx = 1,$$

and define the cdf F(x):

$$F(x) = \int_{-\infty}^{x} f(x')\,dx'.$$

A value of x is selected by setting R = F(x) and solving for x:

$$x = F^{-1}(R)$$

As an example, pick the distance from one collision site to the next. The pdf is given by

$$f(x) = \Sigma e^{-\Sigma x}$$

and the cdf by

$$F(x) = \Sigma \int_{0}^{x} e^{-\Sigma x'}\,dx' = 1 - e^{-\Sigma x}$$

Let

$$R = 1 - e^{-\Sigma x}$$

then

$$x = -\frac{1}{\Sigma} \ln (1-R)$$

The quantity (1-R) is a random number and consequently can be replaced by the random number R', giving

$$x = -\frac{1}{\Sigma} \ln R'$$

Often it is difficult or impossible to solve for x explicitly, as was done in this example. A table can be constructed with $F(x)$ inverted; that is, x can be regarded as the dependent variable, and $F(x)$ (or R) as the independent variable. Thus, a value of x can be obtained from the table for any given value of R.

In any numerical integration scheme it is essential for accuracy that a sufficient number of points be processed in the phase-space regions where large contributions are made by the integral. In many Monte Carlo problems adequate sampling becomes a crucial problem. For example, in deep-penetration problems analog sampling may not yield any histories for particles traveling through the region of interest. Even when a few histories that make important contributions are obtained, the probable error may be too large, and increasing the number of histories decreases the error only slowly. A possible solution to the problem is to alter the sampling scheme to one which samples primarily from the important regions.

In importance-sampling techniques, the basic stochastic process is so modified that the event density of the basic process is multiplied by a chosen function (importance function) which measures the importance of an event at x on the quite reasonable basis that important regions of the phase space should be sampled most frequently. Important regions are those in which events contribute, directly or potentially, most heavily to the desired answer, the consideration of which provides some insight to the selection of the importance function.

When the sampling schemes are altered, the concept of statistical weight is introduced to correct for the altered or biased probability, so that the expected value of the mean will not be affected. For example, the information obtained from a case of history is increased (and thus the probable error is decreased), generally, by not permitting absorption. Absorption is accounted for by reducing the weight of each particle by the factor Σ_s/Σ_t or, to be more general, by the ratio of the average number of particles emerging from a collision to the number entering a collision.

If absorption is not allowed, the particle must eventually be killed by another means. The normal way is by Russian Roulette. Thus, when the weight becomes lower than some arbitrary value, a game is played in which a particle is killed if $R > c$, where c is the survival probability ($0 < c < 1$). If $R < c$, the particle survives and the weight is increased by the factor $1/c$. The surviving particle then represents all those particles killed in the game.

Russian Roulette can also be used to decrease the sampling in any region of phase space by arbitrary tests, in which case it is often coupled with the inverse-process splitting. That is, with certain criteria satisfied, a particle can split into two or more particles with the appropriate weight reduction. This is done when a particle crosses into an important region of phase space or at the first collision site in such a region.

In many cases the importance function is selected arbitrarily and intuitively. A more systematic approach is to use value functions. The value function, a solution of a transport equation adjoint to the Boltzmann transport equation, has been shown to be a very good, and sometimes an

optimum, important function for biasing the original Monte Carlo procedure. In most cases, a reasonable approximation to the actual value function will produce quite good results. A useful specialization of these techniques is the exponential transformation, which can be quite helpful if parameters for its use are obtained from a value function approximation.

Thus far only the generation of histories has been considered. At some point with each history, a score must be evaluated, a score being the contribution to the quantity of interest. (Typical quantities of interest are flux density, current, absorption, transmission, and dose.) For example, suppose that it is desired to estimate a reaction rate integrated over a volume V of phase space, where $\Sigma(x,E)$ is the macroscopic cross section for the reaction of interest. This rate is given by

$$\int_V \Sigma\ (P)\,\phi(P)dP.$$

One way of estimating it is to record $\frac{\Sigma(P)}{\Sigma_a(P)}$ for every particle absorbed in the volume V, where $\Sigma_a(P)$ is the macroscopic absorption cross section. Another commonly used estimator records $\Sigma(P)\cdot d$ for every flight of length d in the volume of interset, where it is assumed that $\Sigma(P)$ does not vary over the track d. It is possible to reduce the variance of the estimate by using computed means in connection with the basic collision data.

The mean is usually the quantity of most interest in a Monte Carlo problem, but a study of the statistical properties of the problem higher moments are often calculated, particularly the second moment, or the estimate of the variance. The sample variance is given by

$$S^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 = \frac{1}{n-1} \left[\sum x_i^2 - \frac{(\sum x_i)^2}{n} \right]$$

where

n = number of samples,

x_i = value of a sample,

$\bar{x} = \frac{1}{n} \sum x_i$ = mean value of n samples.

The estimate of the variance of the mean is

$$\text{var}(\bar{x}) = \sigma = \frac{S^2}{n}$$

There are some principles that should be kept in mind at this point. With adequate sampling of the important regions of phase space, the distribution of the mean might be expected to be close to the normal distribution, but there is a good possibility that it will be skewed, and the above interpretation of the sample variance will be far from correct. From a practical standpoint the above interpretations of the variance are overly optimistic. In many cases (especially in deep penetration problems) it is typical to undersample important regions of phase space and to obtain an underestimate of the mean. Then, the estimate of the variance is likely to be even worse and hence, completely unreliable. If the standard deviation approaches 30 to 50% of the mean, the mean itself should be regarded as unreliable.

Monte Carlo techniques may be designed to reproduce a physical model in as much detail as is necessary, and so provide a powerful tool to solve problems with very few compromises with the physics. The Monte Carlo method is capable

of incorporating any geometry. The successful use of Monte Carlo, however, generally requires a considerable investment in analysis, programming, and computer machine time. It is important for the user to keep in mind that a well developed theory exists which specifies, in principle, a near-optimum procedure for solving a given problem. This procedure consists of obtaining the best possible approximation to the value function for the problem and then using this function to obtain parameters for importance-sampling techniques or to guide development of new biasing techniques.

In general, Monte Carlo methods will not be applied to one-dimensional problems, since discrete ordinates codes are likely to be much faster than Monte Carlo codes. For two-dimensional problems, Monte Carlo and discrete ordinates methods are somewhat comparable, but for three-dimensional or time-dependent problems, there is no competitor to Monte Carlo for a rigorous solution of transport problems.

MORSE and TARTNP

At LLNL the two Monte Carlo codes which are applicable to neutron dosimetry problems are MORSE[1] and TARTNP[2]. Although these codes differ in many ways, which are unimportant, the special features of MORSE make it particularly suitable to the solution of deep penetration problems, problems with a large geometrical attenuation, and problems involving coupled neutron-gamma reactions. As such, it complements TARTNP which is particularly well-suited for the determination of dosimeter response functions.

MORSE solves the group integrated Boltzmann equation which implies the equation has been integrated over energy to form a series of energy groups. Input cross sections describe the average reaction in a group and is no longer point wise in nature. MORSE may be run with as few as one group or as many groups as desired within machine storage limitations. For deep penetration problems there are several techniques that can be used to modify the random walk process in order to spend more computing time on useful histories and less on those which are unimportant.

The easiest method to use is Russian Roulette. In this method, particles which have a low statistical weight undergo a Russian roulette. Those losing the game are killed, while those winning have their statistical weight increased. The choice of playing this game as well as the probability of survival are dependent upon the energy group of a particle coming out of a collision and the geometrical position of the collision. It is normal practice to play this game in the lower energy groups. It is also possible to kill off all particles in a geometrical position where random walk histories contribute nothing to the desired result.

Splitting provides a way of increasing the number of particles in the region of interest. Generally, splitting is used at high neutron energies.

Occasionally, problems are found where there is a high probability that most of the particles will not react and will simply leak from the defined geometry into space. It is possible to alter the problem so that leakage is not allowed. Meaningful histories are thus generated without the need to produce an excessive number of source histories.

Particles born in certain portions of phase space may be more important in their contribution than others. MORSE allows biasing to be made in all phases of the source description (position, energy, time and angle).

The most powerful technique available in MORSE for deep penetration problems is the exponential transformation. This method stretches the path of a particle which is headed toward a given point in space and shortens the path of a particle headed away from the point. This method tends to make the results move accurate at or around the given point while making answers at other points less accurate.

The only variance reduction techniques currently in TART are splitting and Russian Roulette which take place only as a particle crosses the boundary between two zones. However, TART does have the ability to calculate the energy deposition in a zone or the number of interactions which take place in a zone which are useful for detector evaluations.

Let us look at some examples which illustrate the usefulness of Monte Carlo calculations. At LLNL we use the Eberline PNR-4 remmeter for monitoring neutrons. Two questions which have arisen concern the $1/R^2$ dependence of the detection system and sensitivity of the calibration factor to the spectral shape. In order to address these questions, a series of TARTNP calculations have been made. The first set of calculations were made to determine the response function for the system. The results obtained do not agree well with previous calculations made by Hankins.[3] The results for the TARTNP calculations are given in Table I. A comparison to the results published by

Hankins is shown in Figure 1. Also shown is the neutron dose curve. The three curves were normalized at 2.2 MeV which is the mean energy of the group used for normalization by Hankins. TARTNP predicts a greater response to intermediate energy neutrons than predicted by Hankins the reason for this difference is not known. Using the TARTNP response function, a code was written to calculate the neutron dose rate per unit flux density for a given calibration factor. The code uses a given spectrum to calculate the tissue dose rate, and the dose rate measured by the PNR-4. This enables one to calculate the errors associated with using calibration factors obtained with various calibration sources. For example, for a source consisting of 50 percent fission and 50 percent PuBe moderated with approximately 5 cm of CH_2 the PNR-4 would over estimate the dose by 13 percent if calibrated with a ^{252}Cf source. If the calibration was done with a PuBe source, the error would be 31 percent.

A second set of TARTNP calculations were made to determine the response of the PNR-4 detector as a function of distance. This was done to see if it has a $1/R^2$ behavior. For a point source, an analysis of variance test of the TARTNP results showed that for distances greater than 25 cm, the PNR-4 at the 95 percent confidence level indeed has a $1/R^2$ dependence. This was done for 1 keV, 100 keV, 1 MeV, 100 MeV, and fission neutrons.

Most of the neutron dosimetry work at LLNL is performed using the neutron sources available in the calibration facility. These sources, when used with different moderators, provide a wide variety of neutron spectra. The dose rates at one meter have been calcuated using ANISN.[4,5] Since ANISN is a one-dimensional code, then one can not calculate the effects of such things as the hole in the moderator to allow insertion of the source and the asymmetry

of the scattering walls. MORSE does allow for the calculation of the effects produced by asymmetry. A MORSE calculation was made on the dose rate at one meter from ^{252}Cf in the 15 cm D_2O sphere using the same spherized geometry as was used in ANISN. The result was that MORSE predicted a dose rate 1.9% higher than ANISN.

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TABLE I TARTNP Calculated PNR-4 Response

E(MeV	R(Counts/n)
2.5×10^{-8}	2.95×10^{-5}
1.0×10^{-6}	3.57×10^{-5}
1.0×10^{-3}	5.81×10^{-5}
1.0×10^{-2}	7.50×10^{-5}
1.0×10^{-1}	9.32×10^{-5}
3.0×10^{-1}	1.53×10^{-4}
5.0×10^{-1}	2.07×10^{-4}
7.0×10^{-1}	2.24×10^{-4}
1.0	2.78×10^{-4}
2.0	3.06×10^{-4}
2.2	3.27×10^{-4}
3.0	2.82×10^{-4}
4.0	2.72×10^{-4}
6.0	2.51×10^{-4}
8.0	2.04×10^{-4}
10.0	1.73×10^{-4}
14.0	1.57×10^{-4}

FIGURE 1 PNR4 RESPONSE AND TISSUE DOSE RESPONSE AS A FUNCTION OF ENERGY