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The Monte Carlo Method Applied to a
Problem in γ -ray Diffusion

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The Monte Carlo Method is, by now, a well known and widely used statistical technique for obtaining numerical solutions to problems in applied mathematics. It has, for instance, been applied successfully to the evaluation of multiple integrals, the inversion of matrices, and to the solution of differential and integral equations of various types. The method was originally proposed by Dr. S. Ulam of Los Alamos and formalized by Dr. J. von Neumann, early in 1948, as a method for solving neutron diffusion problems. The mathematical description of such problems usually takes the form of an integro-differential equation. Rather than solve this equation directly, a very difficult task even in simple cases, one would, using the Monte Carlo technique, "follow" a large number of neutrons, collect the appropriate statistics, and, from the latter, extract the solution. It was evident from the beginning that the success of the method would be closely connected with the development of high speed computing machines. Nevertheless, much work was done by hand, using graphical aids and desk calculators, and, as calculators of moderate speed, such as the 604 and CPC, became available, work of this kind increased considerably.

In this paper, an example of a Monte Carlo calculation performed on the 701 will be presented to illustrate the principal techniques involved; those relating to the method, as well as those connected with the best utilization of the 701. A problem in the diffusion of γ -rays in an electron gas will be considered for this purpose. The details of this problem will be discussed later.

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It might be mentioned now that the 701 performed this particular problem elegantly and with impressive speed, at least 1000 times faster than possible on the punch-card equipment mentioned, without, however, entirely suppressing one's desire for still faster and more versatile calculators; for we are handling and anticipating far more elaborate applications of the Monte Carlo Method.

The Geometry of Diffusion.

A particle may be specified as to location and direction by six variables, the position by the coordinates x , y , and z , and the direction by the cosines α , β , and γ , where $\alpha^2 + \beta^2 + \gamma^2 = 1$. In addition, a number of parameters may be attached to the particle, such as its energy or velocity. A particle may be followed from one collision through the next by prescribing three numbers, the prescription depending on the physical laws involved. One quantity ℓ , the path length to the next collision, is required to find the new location, $x' = x + \alpha\ell$, $y' = y + \beta\ell$, and $z' = z + \gamma\ell$. Two quantities, $\nu \equiv \cos \theta$ and $\delta \equiv \cos \phi$, defining the direction of scattering, are required to find the new direction. Here θ and ϕ represent the deflection and azimuthal angles, respectively. Using the tools of spherical trigonometry, the following formulae were derived for the new direction cosines: $\alpha' = \alpha\nu + \delta \sqrt{1 - \alpha^2} \sqrt{1 - \nu^2}$,

$$\beta' = \left[\beta(\nu - \alpha\alpha') \pm \gamma \sqrt{1 - \alpha^2} \sqrt{1 - \nu^2} \sqrt{1 - \delta^2} \right] + (1 - \alpha^2), \text{ and}$$

$$\gamma' = \left[\gamma(\nu - \alpha\alpha') \pm \beta \sqrt{1 - \alpha^2} \sqrt{1 - \nu^2} \sqrt{1 - \delta^2} \right] + (1 - \alpha^2),$$

where the upper signs are chosen if $0 \leq \phi < \pi$, the lower if $\pi \leq \phi < 2\pi$.

If spherical, rather than Cartesian coordinates are used, it is convenient to take r^2 and $r\mu$ as position and direction variables where μ is the direction cosine of the particle with respect to the radius r . In this case, the new location is given by $r'^2 = r^2 + \ell^2 + 2\ell r\mu$. The direction $r\mu$ is replaced by $\bar{r}\mu$ in the process where $\bar{r}\mu = \ell + r\mu$.

The direction after scattering is given by $(r\mu)' = \nu \overline{r\mu} + \delta \sqrt{1 - \nu^2} \sqrt{r^2 - \overline{r\mu}^2}$.

Random Numbers and Random Variables.

The quantities ℓ , ν , and δ are determined with the aid of random numbers biased according to the physical laws involved in the problem. There are several methods for generating random numbers, or, at least, reasonable facsimiles thereof. Two methods are in general use. In the middle square method, a 34-bit (referring to the 701) fraction λ_1 is selected and squared and the middle 34 bits (λ_2) of the 68-bit product regarded as a random number. A chain of such numbers $\{\lambda_1\}$ is then generated by subjecting λ_2 and its successors to the same procedure. In the method described in a letter by Dr. D. P. Wall to Dr. C. C. Hurd, as a variation of the method due to Dr. D. H. Lehmer, a fixed 35-bit fraction λ_0 ending with the bits 101 is multiplied by a selected 35-bit fraction λ_1 ending with 1, and the last 35 bits (λ_2) of the product are regarded as a random number. By repeating this procedure, multiplying λ_2 and its successors by λ_0 , a chain of 33-bit random numbers $\{\lambda_1\}$ is generated. The last two bits are always the same and must, therefore, be excluded. The number λ_1 must, in each case, be selected so that a chain of sufficient length for the problem is generated.

A variable x , $a \leq x \leq b$, is said to be a random variable, if to x corresponds a probability density function $p(x)$, $a \leq x \leq b$, such that $\int_a^b p(x)dx = 1$. For random numbers generated by one of the methods mentioned above, $0 \leq \lambda < 1$ and $p(\lambda) \equiv 1$. If we now want to relate two random variables λ and x , and if $p(\lambda) \equiv 1$ and $p(x)$ subject to the integral condition stated, we have $d\lambda = p(x)dx$, hence, by integration, $\lambda = \int_a^x p(x)dx \equiv P(x)$, and, by inversion, $x = P^{-1}(\lambda)$. To amplify this, note that the probability of λ being in the range (λ_1, λ_2) equals $\lambda_2 - \lambda_1 = P(x_2) - P(x_1)$, which is precisely the probability that x be

in the range (x_1, x_2) . The above concepts may be generalized to the case where the variable is discrete and to the case where p is a function of several variables. Now, it may not always be possible to perform the integration and inversion analytically, but numerical procedures exist which accomplish the same thing, precisely or approximately. We shall return to this subject later.

The probability of a particle penetrating a distance ℓ is, in many cases, given in the form $p(\ell) = \sigma e^{-\sigma \ell}$ where σ is a function of the particle parameters, as well as the scattering material. In this case, the integration of $p(\ell)$ gives $\lambda = P(\ell) = 1 - e^{-\sigma \ell}$ and the inversion $\ell = -\frac{\ln(1 - \lambda)}{\sigma}$. The values of the azimuthal scattering angle are, in many applications, equally likely, hence $p(\phi) = \frac{1}{2\pi}$, $P(\phi) = \frac{\phi}{2\pi}$, and $\phi = 2\pi \lambda$.

Scattering and Absorption of γ -rays.

The Monte Carlo Method was applied to the problem of finding the emerging energy spectrum at the surface of a sphere of radius a due to a central source of γ -rays of initial energy e_0 , with e_0 in the MEV range. The scattering material was, in this particular case, taken to be tungsten ($Z = 74$). The processes of scattering and absorption of γ -rays by the electrons were considered, the former defined by the Klein-Nishina formula, and the latter by a $1/e^{7/2}$ law. This is not a realistic treatment of the problem, since, in this e and Z range, (1) the absorption law given is only an approximate one, and (2) processes other than those mentioned are not unimportant. Nevertheless, this furnishes us with a good test problem.

The quantities ℓ and δ are determined, using random numbers, as described previously with $\sigma = \sigma_a + \sigma_s$, where:

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$$(1) \begin{cases} \sigma_a = C_a / e^{7/2}, \\ \sigma_s = C_s \frac{3}{8e^2} \left[\frac{2e^2(1+e)}{(1+2e)^2} + 4 + (e - 2 - \frac{2}{e}) \ln(1+2e) \right], \end{cases}$$

with $C_a = 1.475$ and $C_s = 3.063$ for tungsten. Note that both σ_a and σ_s are functions of the γ -ray energy e , $e \leq e_0$. The direction ν is calculated from $\nu = 1 - \frac{1}{e'} + \frac{1}{e}$ where e and e' are the energies before and after scattering. The probability function associated with e' , $\frac{e}{1+2e} \leq e' \leq e$, is given by:

$$(2) p(e', e) = \frac{\frac{e}{e'} + \frac{e'}{e} + (1 - \frac{1}{e'} + \frac{1}{e})^2 - 1}{\frac{2e^2(1+e)}{(1+2e)^2} + 4 + (e - 2 - \frac{2}{e}) \ln(1+2e)}.$$

These formulae may be found in a text by W. Heitler¹⁾ or in the collection of tables prepared under the direction of H. Mayer²⁾.

Calculation of Functions by Approximate Methods.

Although $p(e', e)$ can be integrated analytically, it cannot be so inverted. The inverted function is, however, tabulated in the report by H. Mayer. We, therefore, chose to approximate it by a rational expression which could be easily calculated. We obtained:

$$(3) e' = P^{-1}(\lambda, e) = \frac{e}{1 + s\lambda + (2e - s)\lambda^3},$$

where $s = e/(1 + .5625e)$, a formula which was regarded as sufficiently accurate for the problem at hand. It could, however, easily be improved upon, if necessary.

This brings up an important point. Since the final result will be statistical in nature, and hence appear with a probable error which one

1) W. Heitler: The Quantum Theory of Radiation.

2) H. Mayer: Tables of the Compton Effect Cross Sections and Energies, LANS-1199.

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cannot normally afford to bring below, say, the 1% level, it is not worthwhile calculating functions appearing as part of calculation to excessive accuracy. The table look-up method is, therefore, used extensively. The functions $-\ln x$, $\cos \pi x$, and $\sqrt{1-x^2}$ were, for instance, stored in the 701, each function occupying 128 half-word locations, x being $n/256$ in each case, $n = 1, 3, 5, \dots, 255$. Similarly, $\sigma_a + \sigma_s$ and $\sigma_a / (\sigma_a + \sigma_s)$ were calculated just once and stored for the arguments $e = e_0 - \frac{n}{32}$, $n = 1, 2, \dots$ down to $e = \frac{11}{32}$, the cut-off energy for which the probability of absorption is about 97%. A square root routine was required, and this was based on the approximate formula:

$$(4) \quad \sqrt{x} = \frac{.16022 + x}{.70719 + .45303x}, \quad \frac{1}{4} \leq x \leq 1,$$

which is good, on the average, to 1/4%. Similar formulae have been derived for $-\ln x$ and $\sin \frac{\pi}{2} x$ with average absolute errors of .001 and .0002, respectively:

$$(5) \quad \begin{cases} -\ln x = \frac{1 - x}{.42135 + .6x}, & \frac{1}{2} \leq x \leq 1, \\ \sin \frac{\pi}{2} x = x \frac{11 - 3x^2}{7 + x^2}, & 0 \leq x \leq 1. \end{cases}$$

These formulae were, however, not used in the problem we are now discussing.

Details and Results of the Calculation.

We have now outlined the techniques and stated or derived the formulae required for the problem. The logical structure of the calculation is best visualized with the aid of a flow diagram. Some of the notations have to be explained. N represents the number of initial particles, n the number, i the accumulated track count, and $\sum \ell$ the accumulated path length of escaping particles. The random numbers $\lambda_1, \lambda_2, \lambda_3$, and λ_4 were generated all in one cycle by the second method mentioned, λ_1 being the first 7 bits,

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λ_2 the next 10, λ_3 the next 8, and λ_4 the last 8; a total of 33 bits. Two print-outs were provided for, one printing the data obtained for an individual escape, the other printing a table of results.

The problem was coded in fixed-point with the use of regional programming and the absolute code obtained by using Assembly Program 607. These topics are discussed in a paper by D. Sweeney. The de-bugging was done using Tracing Program 795, discussed by E. Voorhees in another paper. About 300 orders were required for the problem, plus 300 full-words of storage for constants and tables, plus a print program.

The results of a calculation with $e_0 = 3 \text{ mc}^2$ units (1.533 MEV) and $a = 5.13 \text{ cm}$ (4.17 mean free path units) are given in the table and represent about 20 minutes of 701 time. Thus, an average of 2100 particles was processed per minute, or about a track length every 10 milliseconds, a very satisfactory speed.

Certain integral results are of primary interest, such as the percentages of escaping particles (T_n) and of escaping energy (T_e). The correct value of T_0 , the number of particles escaping without collisions, is given in parentheses at the bottom of the table. This number is, of course, equal to $e^{-\sigma(e_0)a}$ and gives us a gross check on the randomness of the "random numbers" generated.

A quantity which is of particular interest is the average path length which a particle traverses in the sphere before escaping. Note that this average is only 2% longer than the radius. A calculation similar to the one reported on here was performed to verify that the calibration procedure associated with a certain experiment was satisfactory. This procedure assumed, in fact, that the path length correction was small.

In conclusion, I would like to mention that a solution of this problem can also be obtained by solving a certain integro-differential

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equation numerically, but this would be a far more time-consuming approach than the one discussed here. Neither approach is very practical without a calculator comparable in speed to the 701. Nevertheless, much work has been done in this field using semi-analytical methods developed for the purpose, in conjunction with less powerful computing equipment.

Flow Diagram.

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TableLeakage Spectrum for a Central Source of γ -rays in a Sphere.

$$e_0 = 3.0 \text{ mc}^2 (1.533 \text{ MEV}), a = 5.13 \text{ cm.}$$

$e(\text{mc}^2)$	No. of escapes	Av. no. of collisions	Av. length of path
3.00	649	0	5.13
2.75-3.00	185	1.06	5.14
2.50-2.75	245	1.25	5.17
2.25-2.50	231	1.41	5.21
2.00-2.25	220	1.67	5.26
1.75-2.00	209	2.02	5.31
1.50-1.75	198	2.04	5.38
1.25-1.50	157	2.35	5.40
1.00-1.25	100	2.62	5.52
.75-1.00	47	3.13	5.52
.34-.75	11	3.55	5.47
.34-3.00	2252	1.26	5.24
$N = 43176, T_0 = 1.50\% (1.54), \sigma(e_0) = .813$ $T_e = 3.53\%, T_n = 5.22\%$			

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The Monte Carlo Method Applied to
a Problem in γ -ray Diffusion.

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The basic geometrical and statistical concepts will be outlined, the physical problem stated and the computational methods discussed in detail in relation to the 701. The calculation time on the 701 will be compared to the corresponding time for other relevant computing equipment.

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