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A MONTE CARLO CODE FOR DEEP PENETRATIONS OF GAMMA RAYS

by

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This code employs special techniques for the express purpose of trying to obtain reasonable estimates of deep penetrations of gamma rays in an infinite medium emitted from a point monoenergetic source. The code is presently in the "debugging" stage and will be tested against well known standards before it is used for production.

The problem this code is concerned with is determining the angular and energy distributions of gamma rays at a point detector emitted from a monoenergetic, point isotropic or point monodirectional source embedded in an infinite, uniform, homogeneous isotropic medium. Monodirectional is used here in a loose sense; the emission directions are in a half-cone specified by a polar angle, where the source-detector axis is the polar axis, and are uniformly distributed in the azimuthal angle. The status of this code is "debugging" on the IBM 704 electronic data processing machine. It is hoped that by using special techniques it will be useful for deep penetrations, say as much as twenty mean free paths. In its final form the code can be used for neutron penetration also, provided a differential cross section for scattering is given.

The purpose of this code is twofold. First, it is hoped that it will shed some light on the discrepancy between calculational and experimental energy distributions from a Co^{60} source in water. The chief difficulty being the magnitude of the distributions. The calculational method mentioned is the "moments method"¹⁻⁴ and the experimental method being that of Maienschein, et al.⁵ Secondly, there is merit in experimenting with these special Monte Carlo techniques in order to see when and where they can be applied.

The techniques mentioned above are the following: importance sampling on the first collision distribution coupled with double systematic sampling, statistical estimation, splitting and Russian Roulette, and a special form of output.

The importance sampling will be discussed from the viewpoint of a point isotropic source. The technique for the monodirectional source is simpler and straightforward.

One is attempting to estimate in this code:

$$\bar{Z} = \int dx \int dy \int dw \dots \int dt h(x,y,w,\dots,t) Z(x,y,w,\dots,t)$$

One assumes the probability distribution function can be written:

$$h(x,y,w,\dots,t) = f(x,y) g(w,\dots,t)$$

and defines:

$$\overline{Z(:x,y)} = \int dw \dots \int dt g(w,\dots,t) Z(x,y,w,\dots,t)$$

$$\overline{Z^2(:x,y)} = \int dw \dots \int dt g(w,\dots,t) Z^2(x,y,w,\dots,t)$$

$f(x,y)$ is the probability distribution function for the first collision. X , say, is the cosine of the angle between the direction of emission and the source detector axis and y is the number of mean free paths to the first collision. One desires to sample from $f^*(x,y)$ instead of $f(x,y)$ (importance sampling) and has,

$$\int dx \int dy f^*(x,y) \overline{Z(:x,y)} \frac{f(x,y)}{f^*(x,y)} = \bar{Z}$$

However the variance is not the same in general when importance sampling is employed. The probability distribution function for the first collision that gives the minimum variance is of the form:

$$f^*(x,y) = f(x,y) \sqrt{\overline{Z^2(:x,y)}} N$$

where

N = normalizing constant.

Kahn⁶ shows this for importance sampling with one variable and his argument can easily be extended to two variables. The code will begin with the task of estimating $\overline{Z^2(:x,y)}$. $\overline{Z^2(:x,y)}$ will be estimated by performing an auxiliary Monte Carlo calculation. Instead of sampling from a first collision distribution, x and y will be fixed and $\overline{Z^2(:x,y)}$ will be estimated. This will be done for a number of points (x,y) . This will then provide estimates for the functions $f^*(x,y)$, $G(y:x)$, $F(x)$ which will be placed in tabular form in the machine

where:

$$G(y:x) = \frac{\int_{-\infty}^y d\eta f^*(x, \eta)}{\int_{-\infty}^{\infty} d\eta f^*(x, \eta)}$$

$$F(x) = \int_{-\infty}^x d\xi \int_{-\infty}^{\infty} d\eta f^*(\xi, \eta)$$

Once the auxiliary Monte Carlo problem is completed and the importance distribution functions have been calculated, the main Monte Carlo routine begins.

The importance distribution for first collision is sampled using double systematic sampling as follows:⁷

$$F(x_i) = \frac{i + \frac{1}{2}}{N} \quad i = 0, 1, 2, \dots, N-1$$

$$G(y_i:x_i) = \frac{j + \frac{1}{2}}{N} \quad j = 0, 1, 2, \dots, N-1$$

$N = 2^\alpha$ = number of histories; α is a positive integer ≥ 0 . The point (x_i, y_i) is then found by interpolation in the tables. The j 's must be randomized since they shouldn't be correlated to i . This can be done using the periodicity of the pseudo-random numbers generated by the congruence method. Each binary bit in a pseudo-random number has a certain period as illustrated below

$$\begin{array}{cccccccccccc} 2^6 & 2^5 & 2^4 & 2^3 & 2^2 & 2^1 & 2^0 & 2^0 & & \text{period} \\ \dots & x & x & x & x & x & 0 & 1 & & \text{bit} \end{array}$$

Suppose one is interested in obtaining all the even integers, 0, 2, $\dots, (2^{\alpha+1} - 2)$ then by logical computer operations one can obtain from a pseudo-random number the following number

$$\begin{array}{cccccccccccc} 2^\alpha & 2^{\alpha-1} & \dots & 2^3 & 2^2 & 2^1 & 2^0 & & \text{period} \\ 000 & \dots & 0 & x & x & \dots & x & x & x & 0 & \text{bit} \end{array}$$

Generating 2^α random numbers in succession will provide the 2^α integers desired in random order. Thus the random correspondence $i \longleftrightarrow j$ is obtained. Of course, a separate random number generator must be provided which has the same basic random number but an initial random number deep in the series. When a first collision point is chosen by the sampling technique the initial weight must be modified by the factor $f(x_i, y_i)/f^*(x_i, y_i)$.

The technique of statistical estimation will be used at every collision, that is, the probability of the radiation reaching the detector after the collision will be calculated and used to estimate the flux at the detector.

It is planned to sample the direction after collision from an isotropic distribution, rather than the Klein-Nishina differential cross section, and "weight" with the Klein-Nishina distribution. This is chiefly due to simplicity and saving in calculational cost. It is certainly biased sampling. For small separation distances this is probably the better method. For large separation distances the variance of the estimated flux will increase but intuitively may be compensated for by the use of importance sampling and splitting.

The techniques of splitting and Russian Roulette are to be used with the splitting occurring at the collision point rather than at a splitting boundary. In other words, if the particle crosses "b" boundaries with the boundaries successively closer to the detector, it will be split into 2^b particles at the final collision point. If a particle crosses "b" boundaries with the boundaries successively farther away from the detector, it then has a probability of 2^{-b} of surviving. If it survives, its weight is increased by 2^b . The splitting boundaries are concentric spheres with the detector as their center. Again the reason for this technique of splitting at the collision point is chiefly simplicity. In all cases the statistical estimation is performed before either splitting or Russian Roulette. Although one may argue that splitting at the collision point will introduce biasing, it remains to be shown whether it is serious enough to warrant the increased calculational cost.

Other features in the code are an energy cut-off, a weight cut-off, and cut-off for distance from the detector.

The output will be of a special form. There will be no histograms! The usual process is to estimate the flux at the detector and determine the angular and energy distributions from the total flux arriving in an angular and energy sector; this provides histograms. This code makes use of the expansion:

$$\phi(D, \omega, \tau) = \sum_{k=0}^{\infty} \sum_{\ell=0}^{\infty} A_{k\ell}(D) \frac{2k+1}{2} \frac{2\ell+1}{2} P_k(\omega) P_{\ell}(\tau)$$

$$A_{k\ell}(D) = \int_{-1}^1 d\omega \int_{-1}^1 d\tau P_k(\omega) P_{\ell}(\tau) \phi(D, \omega, \tau)$$

where

$$\tau = 2 \frac{E - E_c}{E_0 - E_c} - 1,$$

E = energy of radiation,

E_c = cut-off energy,

E_0 = initial energy,

ω = cosine of angle between source detector axis and direction of radiation,

D = separation distance,

P_k, P_{ℓ} = Legendre Polynomials,

$\phi(D, \omega, \tau)$ = flux at D per unit ω per unit τ .

At each collision statistical estimates are made of the $A_{k\ell}(D)$ ⁸ rather than simply $A_{00}(D)$, which is easily seen to be the total flux. Single scattering is treated separately from multiple scattering. The code allows $k, \ell \leq 15$ for single scattering and $k, \ell \leq 7$ for multiple scattering. Of course, the coefficients for single scattering and multiple scattering are completely additive.

One may have the choice of any combination of the following output: number flux, energy flux, energy deposition in the medium (ergs/gm), and energy deposition in carbon (ergs/gm) at the detector, which is the standard material for dose-rate calculations or measurements. Also the variance of the estimated coefficients ($A_{k\ell}$) will be automatically calculated.

The code will be tested against three standards. First, problems with no energy degradation and isotropic scattering will be checked against the exact solutions given by Case, deHoffman, and Placzek.⁹ Secondly, problems with a medium other than water will be checked against the energy distributions of energy flux furnished by the "moments method."¹⁻⁴ Thirdly, problems with water as a medium will be checked against the experimental work of Maienschein, et al.⁵ and the "moments method."¹⁻⁴

In conclusion, if the code survives all these tests mentioned above and the heavy hand of "father time," it may provide brighter prospects for Monte Carlo.

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