Research Article

MONTE CARLO METHODS IN NUMERICAL ANALYSIS AND THE PENELOPE CODE

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ABSTRACT

Monte Carlo Codes are based on a common numerical procedure called the Monte Carlo Method. This method relies on the use of stochastic processes in the solution of problems. PENELOPE – is a Monte Carlo Code developed for the purpose of the study of transport of electrons, photons and their resultant showers in materials. Simulation is achieved via basic events of photoelectric, or pair-production or Compton scattering interactions with their attendant energy-loss through matter. PENELOPE 2001 uses a simulation algorithm based on scattering models that combines numerical data- base with analytical cross-section and material libraries for the different interaction models. Fundamental concepts in the development of this code and a pictorial demonstration of ^{60}Co(1332.502keV) photon transport through lead and air are hereby presented. This code is an alternative to many physical laboratory experiments.

**Keywords: numerical analysis,** monte carlo, code, PENELOPE, photon transport, lead, air

INTRODUCTION

Fast computers which are indispensable tools for both computational and analytical research, are now available due to the recent progress in information technology. This feat has revolutionized scientific research and made physical experimentation faster and much easier. At its inception, the Monte Carlo method was first applied on the MANIAC computer at Los Alamos National laboratory [1] to predict the rate of neutron chain reaction in fission devices in mid 1946 during the Manhattan Project of World War II. Today, recent developments, modification and applications of the code have resulted in significant technological break-through in nuclear instrumentation [2-4]. The Monte Carlo Method, now applied in several areas of research has given rise to several codes of which PENELOPE is one of them. Basically, Monte Carlo calculation makes use of random numbers and has been found useful in predicting stochastic events giving rise to various forms of input data for simulating and modeling of experiments [3,4]. Application of the Monte Carlo techniques is mostly desirable in nuclear science and technology where it becomes needful to have an *a priori* data or information before risking the experimentation process, as is the case with fission related experiments. This paper is aimed at introducing the basic concept of the Monte Carlo Method, beginning with the numerical aspects behind the code and simulation of radiation transport problems as is the case with PENELOPE. The generic aspects of the Monte Carlo Method will be discussed, and its consequent application in the PENELOPE code will be highlighted.

THE MONTE CARLO METHOD

The Monte Carlo method could be studied by focusing on the problems of estimating the probability of a particle (photon) interacting on a shield (matter), undergoing successive collisions with scattering centres and perhaps escaping if possible (Fig.1).
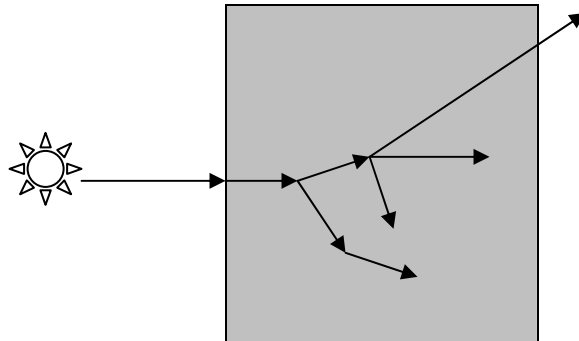
Figure 1: Scattering of particles as they interact with matter

The physics of the problem on a microscopic level involves collision kinematics where both elastic and non-inelastic scattering will prevail on the fate of the photon as the direction of motion and energy of the incoming photon will all come to bare on the trajectory of the scattered photons [1].

The knowledge of the reaction cross-sections and succession of free path-lengths will all contribute in the rubrics of the particle history. In order to attain a lower uncertainty in the Monte Carlo Method from an optimum particle history a variance reduction technique has to be applied which will include truncation as well as population control of the events.

Transport of particles (electrons or photons) in matter and centers that generate them can be regarded as sequences of random events. Flights of these particles occur in straight-line paths defined randomly by the geometry cross-sections and scattering centers of the media in which they traverse.

The outcome of these interactions such as the type of radiation emanating, its energy, direction, and other relevant variables are random events. A Monte Carlo simulation of such events can be constructed if one knows *a priori* the probability distribution function (pdf) that governs each step which could either be described by a physical system or a mathematical formulation of both. The pdfs could be assayed through the differential cross-sections. Essentially the Monte Carlo simulation process therefore has the following basic components:

- Probability distribution function (pdf) that describes the physical or mathematical system
- Random number generator that gives random numbers uniformly distributed on the unit interval
- Sampling rule from the specified pdfs, on the unit interval
- Scoring (or tallying) whose outcome must be accumulated into overall tallies or scores for the quantities of interest
- Estimation of the statistical error (variance) as a function of the number of trials (runs)
- Variance reduction techniques for reducing the variance in the estimated solution which is needful in the reduction of the computational time for the simulation and
- Parallelization or vectorization used in the algorithms to allow Monte Carlo methods be implemented efficiently on advanced computer architectures.

MONTE CARLO METHODS AND NUMERICAL ANALYSIS

The fundamental basis for the Monte Carlo method is the use of random numbers and random variables.

Consider x to be a random variable with values in the interval:

$$x_{min} \leq x \leq x_{max} \tag{1}$$

The probability of having x in the interval (a,b) is given as:

$$P\{ x | a < x < b \} \tag{2}$$

which is defined as the ratio n/N of the number n of values x that fall within that interval and the total number $N \rightarrow \infty$.

Assuming there exists a differential interval of length dx about x_1 The probability of obtaining x will then be :

$$P\{x | x_1 < x < x_1 + dx\} = p(x_1)dx \tag{3}$$

where $p(x)$ is the probability distribution function (pdf) of x. We therefore seek normalization due to two conditions:

1)   Negative probabilities may not have any meaning in real situations

2)   Values obtained for x must lie between x_{min} and x_{max} hence, we therefore normalize the pdf to unity since it must be defined in the positive sense thus:

$$p(x) \geq \text{ and } \int_{x_{min}}^{x_{max}} p(x_1)dx = 1 \tag{4}$$

Equation 4 is the condition for the definition of a pdf for any given function. Monte Carlo uses the uniform distribution function of the form:

$$U_{x_{min} x_{max}}(x) \equiv \begin{cases} 1/(x_{max} - x_{min}) \ if \ x_{min} < x < x_{max} \\ \qquad 0 \qquad \qquad otherwise \end{cases} \tag{5}$$

Such a function is discontinuous and could also include the Dirac delta $\delta(x - x_0)$ property defined for the limits a,b thus:

$$\int_a^b f(x)\, \delta(x - x_0)\, dx = \begin{cases} f(x_0) & if \quad a < x_0 < b, \\ 0 & if \quad x_0 < a \quad or \quad x_0 > b \end{cases} \tag{6}$$

for any function $f(x)$ continuous in x_0.

MONTE CARLO INTEGRATION

James [5] has shown that Monte Carlo calculations are equivalent to integrations. Consider a one-dimensional integral of the form:

$$I = \int_a^b F(x)dx \tag{7}$$

Consider a pdf as defined in the form $p(x)$, drawn from a sequence of samples x_i , $i = 1,2,…,N$ then we recast the integral in equation 7 to take into account our pdf and rewrite the integral with an expectation value thus:

$$I = \int_a^b f(x)p(x)dx \equiv \langle f \rangle \tag{8}$$

thus, setting $f(x) = F(x)/p(x)$ and assuming that $p(x) > 0$ in (a,b) and $p(x) = 0$ outside this interval.

Monte Carlo evaluation of the integral proceeds by generating a large number N of random points x_i from the pdf given as $p(x)$ and accumulate the sum values $f(x_i)$ in a counter. At the end of the calculation, the expected value of f is estimated as:

$$\overline{f} = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \tag{9}$$

The law of large numbers requires that if N becomes very large then

$$\overline{f} \rightarrow 1 \text{ (Probability law)}. \tag{10}$$

Statistically the above condition implies that the Monte Carlo result in the form $\overline{f}$ is a consistent estimator of the integral in equation 8 and valid for any function $f(x)$.

ESTIMATION OF VARIANCE

Recall the law of large numbers

$$\overline{f} \equiv \frac{\lim}{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} f(x_i) \qquad (11)$$

By definition, the variance of a function *f(x)* is thus:

$$Var\{f(x)\} = \int f^2(x)p(x)dx - \langle f \rangle^2 \qquad (12)$$

Using equations 8 – 12 we obtain the variance as:

$$var\{f(x)\} = \frac{\lim}{N \to \infty} \left\{ \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2 - \left[\frac{1}{N} \sum_{i=1}^{N} f(x_i) \right]^2 \right\} \qquad (13)$$

which is a measure of the dispersion of the pdf. This implies that the outcome of the Monte Carlo trials

(runs) with independent sequences of *N* random numbers x_i from *p(x)* will yield different estimates of the

random variable from the pdf.

If we recall the definition of the standard deviation as:

$$\sigma_f \equiv \sqrt{var(\overline{f})} = \sqrt{\frac{var\{f(x)\}}{N}} \qquad (14)$$

we obtain a measure of the statistical uncertainty of the Monte Carlo estimate $\overline{f}$. The implication of this is

that in order to reduce the statistical uncertainty by a factor of 10 we have to increase the sample size (runs)

by a factor of 100. This therefore sets a limit to the accuracy attained to the available computer power. The

statistical uncertainties can be lowered by the variance reduction techniques [6,7].

EXPERIMENTAL

PENELOPE is a Monte Carlo code devised to simulate PENetration and Energy LOss of Positrons and
Electrons in matter in the energy range of 100 eV to 1 GeV. Data bases include tables of physical
properties, interaction cross-sections, materials, etc, which are read when the program is on. The material
data file is created by an auxiliary program MATERIAL, known to extract atomic interaction data from the
data-base. The program PENSLAB simulates electron/photon showers within a material slab and generates
detailed information and many quantities of physical interest [8] some of which include:
- (i)   Fractions of primary particles that are transmitted, backscattered and absorbed and a number
of average quantities (track length within the sample; number of events of each kind per
particle; energy, direction and lateral displacement of particles that leave the sample; etc.)
- (ii)   Energy distribution of transmitted and backscattered primary particles
- (iii)   Angular distribution of transmitted and backscattered particles
- (iv)   Depth-dose distribution (i.e deposited energy per unit depth)
- (v)   Depth distribution of deposited charge and
- (vi)   Distribution of energy deposited in the slab.

When using PENELOPE it is pertinent to be aware of the simulation parameters. These parameters to
an extent will invariably affect the results notably the speed and accuracy of the simulation of the electrons

and positrons. The parameters include the absorption energy, elastic scattering parameters which are usually limited to the interval (0, 0.2); the cutoff energies and the allowed step length that defines the number of events. These are all user-selected parameters. The versatility in simulating quick computerized results makes PENELOPE very useful in shielding calculations.

RESULTS AND DISCUSSION

A simulated shower of photons from a source ([60]Co-1332.502 keV) on a lead and air shields of the same thickness were examined. Diagrams obtained from PENELOPE version 2001 using some of the main programs like PENSLAB are hereby shown as Figs. 2 and 3.

The absorption energies were set equal to 10 keV (for all kinds of particles) while the cut-off set at W_{cr} = 10 eV thus disregarding the emission of soft bremsstrahlung (i.e for all W < 10 eV).

PENELOPE's material definition file used was **lead.mat** and **air.mat.** The under listed parameters are defined in each of these files for lead and air respectively.

    Mass density
    Number of elements in the molecule
    Molecular density
    Plasma energy
    Mean excitation energy
   Number of oscillators and
    Cross-section tables.
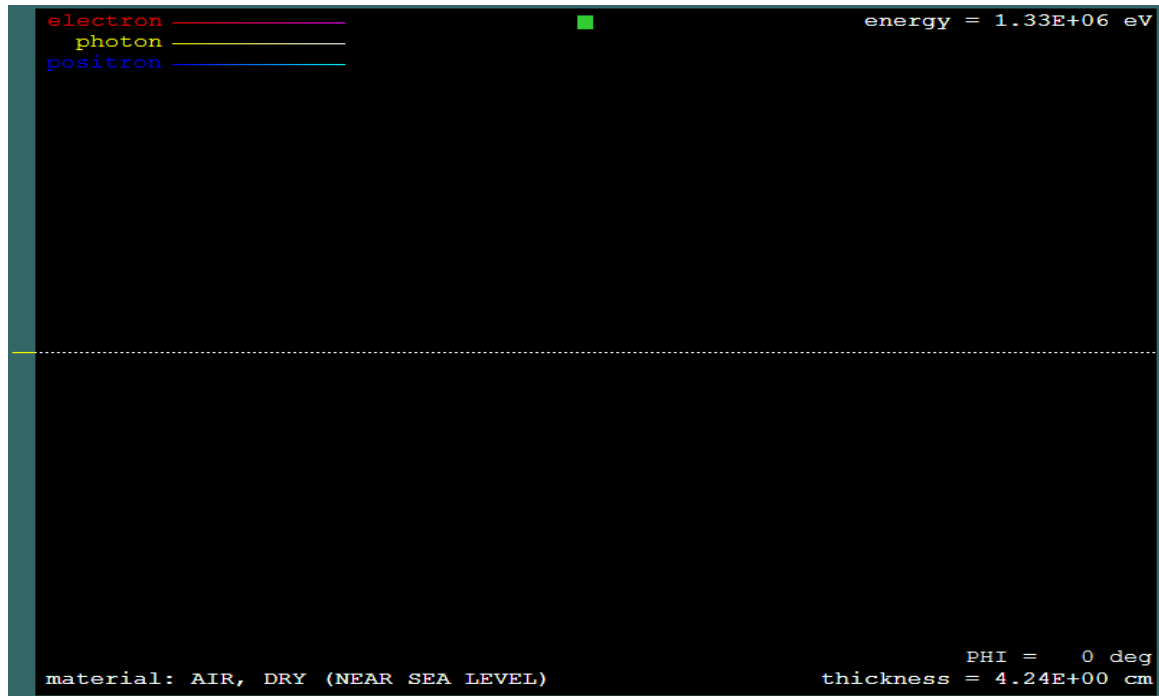Slab thickness = 4.237 cm
Maximum step length = 0.004 cm
Number of showers to be simulated = 2147483647
Computation time = 300 sec
Figs. 2 and 3 are pictorial representation of the Monte Carlo simulated results of the program MAINSLAB. The figures show the simulated pictures of the particle tracks through lead slab and an air medium respectively, of the same thickness, 4.237 cm. It is a shower resulting from primary photons simulated. It shows the actual trace of each particle's path, within the slab, from initiation to the end of its history. The shower shows
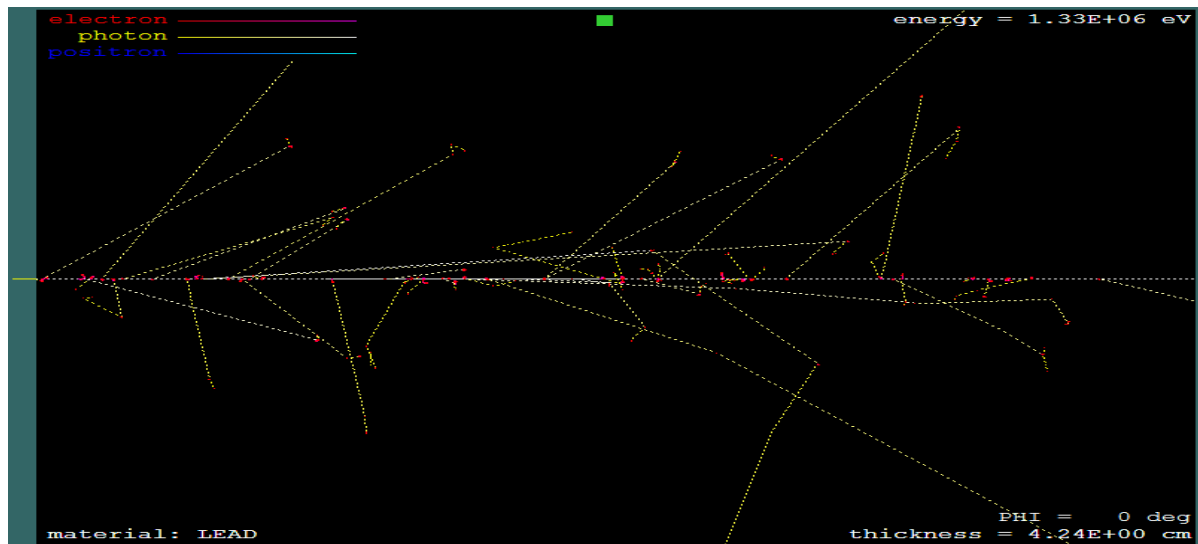
Figure 2: Scattering tracks of transmitted particles on a Lead slab of thickness 4.237 cm

Figure 3: Linear transmission of photons on an air slab of thickness of 4.237 cm

how photons as the primary particles from ^{60}Co(1332.502keV) generates secondary particles. The computer output depicts electrons (in red), photons (in yellow) and positrons (in blue). It is interesting to see that photons transmitted through air are not scattered (they traverse in a straight line) while scattering of particles were observed for the Lead slab. This result can assist us in predicting an appropriate Lead thickness that will shield completely (stop the photon tracks within the lead material) a given photon energy.

CONCLUSION

Photon interaction in lead and air has been investigated using the PENELOPE Code. The pictorial representation of gamma ray transport in lead and air has been demonstrated by the application of this code. One can use this alternative method to determine or predict a shielding thickness that will stop photons of particular energies. The scientific community can take advantage of the capabilities of the PENELOPE code for the investigation of radiation transport in matter, as it can be applied where many physical laboratory experiments are not possible or inaccessible, especially in a reactor core.

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