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MONTE CARLO APPLICATIONS TO PHOTON RADIATION PROTECTION AND DOSIMETRY AT ENEA

R. GUARALDI, F. PADOANI, K. W. BURN and G. F. GUALDRINI

Abstract: A new version of the MCNP Monte Carlo Code has been written that transports electrons, besides neutrons and photons, incorporating the EGS4 electron modules. The code, which is currently being benchmarked, is intended for use in the field of radiation protection and dosimetry.

1. INTRODUCTION

Monte Carlo has demonstrated its capability in solving many problems in the field of health physics, radiation protection and dosimetry especially in determining radiation quantities which are difficult to measure. In the field of photon dosimetry an extensive use has been made of Monte Carlo (e.g. Nelson and Chilton, 1983, Grosswendt et al., 1988, Dymbilow and Francis, 1984, Williams et al., 1985, and other authors) to determine radiation quantities as defined by the International Commission on Radiation Units (ICRU Report 33, 1980, ICRU Report 39, 1985). Most of these calculations have been performed in the so-called Kerma approximation which neglects the electron transport. In certain conditions this approach is not valid.

The correct modelling of electron transport coupled with photon transport is of particular relevance in the following applications:

- 1) Beta dosimetry.
- 2) Assessment of the energy deposition in the various organs of the human body due to photon irradiation, in particular at material interfaces (e.g. bone-muscle).
- 3) Calculation of photon detector responses through secondary electron energy deposition.
- 4) Calculation of radiation quantities.

For several years MCNP (LASL, 1981) has been widely used at ENEA both for photon and neutron transport especially in shielding problems. The code has demonstrated its ability to solve highly complex problems through its powerful geometry and the availability of many estimators (tallies), which allow the computation of a variety of physical quantities. Moreover the code has been found to be reasonably user oriented. For these reasons it was decided to incorporate the electron transport capabilities of the code EGS4 (Nelson and al., 1983) into MCNP with a minimum variation to the general characteristics of MCNP.

This paper summarizes the main features of the new version of the code, presenting some examples of its application to dosimetry problems.

2. SIMULATING ELECTRON TRANSPORT WITH MONTE CARLO

It is interesting to compare the transport of electrons with that of neutrons or photons:

- in neutron/photon transport, the interactions of the particles with matter involve short range nuclear forces. This has two consequences: 1) the interaction distance is negligible compared with the total distance travelled by the particle (thus the concept of 'cross-section' which implicitly separates the event of 'collision' from that of 'free flight' can be employed); 2) the distance between collisions is relatively large. The possibility then exists of simulating with Monte Carlo each individual physical event. Monodimensional sampling distributions may therefore be employed which facilitate the sampling and allow variance reduction, involving biased sampling distributions (with corresponding weight compensation), to be introduced relatively easily.

- in electron transport, the longer range electromagnetic force governs the interactions. The interaction distance may not then be negligible compared with the distance travelled and the concept of 'cross-section' is no more valid. Even if the interaction distance is negligible compared with the total distance travelled, the cross-section is very high and the electron experiences a multitude of collisions. In this case a simulation of each individual event becomes impossible.

Thus when modelling electron transport it is necessary to consider together a multitude

of events, be they microscopic collisions/free flights or deviations in some potential field. The distance/angle variables are not therefore separable and independent sampling of each may not be made.

Two models for the distributions of these variables are available: Goudsmit-Saunderson (G-S) used by the ITS code series (Halbleib and Melhorn, 1984) and Molière used by EGS. G-S employs an exact treatment involving expansion in a Legendre series and requires a fixed path (for reasons of quadrature). All possible electron interactions are included. Molière instead truncates the series expansion, assuming small values of some variables. Excluded therefore are 'catastrophic' events such as bremsstrahlung or delta ray production which involve large changes in the direction and energy of the primary electron.

Thus electron transport in the Molière model bears some analogy with neutron/photon transport. The collisions are the catastrophic events with their cross-sections. Free-flight between the collisions corresponds to transport using the Molière model which models a multitude of single elastic or inelastic scatterings of the electron ('multiscattering'). This analogy was the principal reason the Molière model was the one chosen for the electron transport. In extracting and adapting the EGS routines to MCNP the similar basic structure arising from the analogy between the two types of transport, allowed the programming to proceed 'with the grain' of MCNP rather than against.

As EGS is not directed at dosimetry applications (involving lower energy electron transport), improvements in the data and transport modelling appropriate to lower energy applications, were then planned to be inserted in the new code MCNPE.

3. MCNPE : A NEW VERSION OF MCNP FOR THE COUPLED TRANSPORT OF PHOTONS AND ELECTRONS.

The starting point was the program source of MCNP (version 3a) and the EGS4 routines dealing with electrons. The layout of the transport process for all tracked particles is based on the original MCNP structure and is driven by the HISTORY routine (see flow chart). The cross-section library for electrons is provided by PEGS, the pre-processing step of EGS4. It produces the total cross sections for delta ray production, bremsstrahlung radiation and positron annihilation, besides rejection functions for bremsstrahlung radiation. The photon cross section library used in MCNPE is the original pointwise MCNP cross section library. PEGS also produces a photon cross section file which was not used.

The major changes to MCNP3a were the introduction of the ELETOT and COLIDE subroutines that deal with electron collisions (total cross-section and post-collision phase space parameters), and the modification of the photon collision subroutine COLIDP (see

Although MCNPE in its coding differs considerably from MCNP, for the user the input changes are rather modest, so that a MCNP user can immediately run MCNPE. The changes in the MODE and TALLY cards are typical: card MODE:N, P, E, NP, PE, EP, NPE is analogous to the one in MCNP, the first letter indicating the source particle, card Fn:E is a new one for the electron tallies while Fn:EP is for the electron and photon tally for energy deposition only (i.e. $n=6, 16$, etc.).

4. SOME EXAMPLES OF MCNPE APPLICATIONS

4.1 Absorbed dose in air

The first test for MCNPE was a calculation of absorbed dose in free air, to be compared to available data (Dimbylow and Francis, 1983, and ICRP PUBLICATION 51, 1987) and to the results obtained with ACCEPT (of the ITS code series). Following Dimbylow and Francis we calculated the absorbed dose to a sphere of air surrounded by air in condition of full secondary electron equilibrium (SEE), for four different energies of a monodirectional photon source: 80keV, 300keV, 1MeV and 10MeV. The 15cm radius sphere is contained in a cylinder of radius R ; the photon source is at one end of the cylinder, $-z_0$, and has the same radius R , (see fig.1). z_0 was set equal to the maximum range of secondary electrons: for energies $\geq 300\text{keV}$ we considered the maximum energy of Compton electrons; at 80keV due to the presence of the photo-electric effect we assumed all the photon energy transferred to the electrons.

Fig. 1. Geometry of the system cylinder-sphere

Dimbylow and Francis used for the distance from the other end of the cylinder, z_1 , a constant value of 20cm, but we actually adopted $z_1=z_0$ to be sure to take into account all backscattered electrons and photons. The radius of the cylinder was found with a series of calculations at different R until we considered SEE to be reached, i.e. until the absorbed

flowchart). There follows a brief description of COLIDP and COLIDE.

COLIDE. This subroutine is similar to the subroutine ELECTR in EGS4. Depending on the reaction which has been selected in the branching, it calls:

- a) MSCAT: a multiple scattering has been selected. This routine uses Molière's theory.
- b) MOLLER: a knock-on by an electron with an electron .
- c) BHABHA: a knock-on by a positron with an electron.
- d) BREMS: a bremsstrahlung event.
- e) ANNIH: an annihilation, in the case of positron transport.

COLIDP: This MCNP routine, treating the photon collisions, has been modified as follows:

MCNP3a	MCNPE
a) COMPTON : incoherent scattering	the secondary electron is stored in the bank
b) RAYLEIGH : coherent scattering	no modification
c) PAIR : pair production	the EGS4 PAIR subroutine is called and the electron-positron pair is stored in the bank
d) PHOTO : photoelectric absorption	no modification

dose per unit fluence had reached a plateau. This maximum value should be the same as that obtained in the Kerma approximation, neglecting the energy loss from bremsstrahlung, and easily calculated by MCNPE with MODE:P (equivalent to the standard version of MCNP3a for photons).

The values of absorbed dose per unit fluence, pGy cm^2 , from MCNPE, ACCEPT and the references are given in figs. 2-5 for the different energies, as a function of the radius R of the air cylinder. The comparison is reasonably satisfactory at 80 and 300 keV but presents some anomalies at 1 and 10 MeV. The most evident is that MCNPE reaches SEE, i.e. the plateau, for a much smaller radius R of the cylinder compared with ACCEPT, even though the radius is greater than the one found by Dimbylow and Francis. The MCNPE values do not moreover reach the Kerma values as we expect they should and as ACCEPT does.

Fig. 2. Absorbed dose per unit fluence as a function of the radius of the cylinder for a 80keV parallel photon beam.

Fig. 3. Absorbed dose per unit fluence as a function of the radius of the cylinder for a 300keV parallel photon beam.

Fig. 4. Absorbed dose per unit fluence as a function of the radius of the cylinder for a 1MeV parallel photon beam.

Fig. 5. Absorbed dose per unit fluence as a function of the radius of the cylinder for a 10MeV parallel photon beam.

4.2 Calculation of Dose Equivalent near the Surface of the Tissue Equivalent ICRU Sphere

A second test of MCNPE was concerned with the calculation of shallow directional dose equivalent, which is defined at a depth of 0.07mm in the ICRU sphere. The ICRU sphere has 30 cm. diameter and is composed of a theoretical tissue equivalent material with density 1 g/cm³ and a mass composition of 76.2% Oxygen, 11.1% Carbon, 10.1% Hydrogen and 2.6% Nitrogen.

The calculations were performed in exactly the same geometry as in the previous example, with two different photon sources of Co-60 and Cs-137. The quantity to be investigated was the energy deposition (MeV/g) per unit source photon fluence in thin shells at different depths, in the part of the sphere facing the source bounded by a 60° cone. As

photons scattered in the air give a negligible contribution to the energy deposition compared with unscattered photons, the source was taken only over the central region of the disk with the same diameter as the sphere.

The results (fig.6) show a large overestimation, as expected, of the energy deposition using the Kerma approximation in the first layers of the ICRU sphere where electronic equilibrium has not yet been reached. At 0.07mm depth it is clearly necessary to include electron transport for lower energy photon sources than the two considered here. For higher energies at depths up to 0.3cm the dose equivalent should be determined with a coupled photon-electron calculation.

Fig. 6. Absorbed dose as a function of the depth from the surface for the ICRU sphere.

It should be borne in mind that a coupled photon-electron calculation is much more time consuming than a pure photon calculation (the ratio of efficiencies or figures of merit is nearly 300 for this problem), so that care has to be used when deciding whether to transport electrons or not.

5. MCNPE UPDATES

Future changes to the code to tune it better to low energy electron/photon transport may be divided into two categories although, for electrons, they are interrelated.

5.1 Physics and data

It is intended to recover the low energy physics present in the ACCEPT code and not present in EGS (i.e. X-ray emissions, straggling, the Auger effect) and insert into MCNPE. It is also intended to substitute in a step-by-step manner the current photon and electron data of MCNPE with the latest data from the Lawrence Livermore National Laboratory (see for example Cullen *et al.*, 1989).

5.2 Electron transport algorithm

A new multiple scattering algorithm has been developed that uses the Molière theory (as does the standard EGS algorithm or an improvement of the standard version called the PRESTA algorithm). We remind ourselves that the Molière distribution is expressed as $(f_0 + f_1/B + f_2/B^2)$. It is intended to incorporate the new algorithm into MCNPE.

Bearing in mind the range of application of the Molière model (the small angle approximation resulting in a condition on the maximum step length allowed; also a condition on the minimum step length; an only partially corrected screened Rutherford single scattering cross section; a lower limit on Molière's B parameter of 1.5 to avoid negative regions in the angular distribution; etc.), the differences between the new algorithm and the standard and PRESTA algorithms may be summarized in the following items:

- 1) The curve to straight path correction (PLC=path length correction) uses an algorithm similar in principle to the PRESTA one. The correction is computed starting from the integration along the path of the average cosine of scattering. Whilst in the PRESTA algorithm both the f_0 and f_1 terms of the Molière distribution are used for this, in the new algorithm only the f_0 (Gaussian) term is used; this because in the original theory (small angle approximation), the f_1 term is strictly divergent with any attempt to cut off its integration at a reasonable limit being extremely sensitive to physical effects that affect the low probability, large angle tail of the distribution (such as the spin-relativistic effect). Using only the f_0 term is usually sufficient because wherever the f_1 term becomes important, the whole theory is at, or beyond, its limit of applicability anyway. The f_0 term is integrated in a completely analytic manner, as opposed to PRESTA in which numerical approximations leading to divergence at small values of B have been applied. (The standard EGS algorithm uses a PLC based on the Fermi-Heyges-Yang theory which is well known to strongly overestimate the PLC correction and as a consequence to be strongly step-length, and therefore user, dependent. The stability of the new algorithm under large step-length variations has so far shown itself to be good, whilst PRESTA also apparently has an excellent stability.)

2) This item concerns the update of the particle's position after the step has been made. The standard algorithm simply moves the particle a distance in the straight-ahead direction determined by the PLC from the given curved path, and then applies the angular correction. Both PRESTA and the new algorithm apply a lateral deflection (that is, the end step position is not on the straight-ahead direction) and both correlate this lateral deflection to the sampled final scattering angle. However the way they compute this is different. PRESTA makes a simple approximation to get the lateral deflection as a function of the final scattering angle and applies a fixed longitudinal displacement equal to the average straight-ahead step for the given curved step as found by the PLC. Instead the new algorithm computes a polar, an azimuthal position angle and a straight line displacement, that are all correlated with the final scattering polar and azimuthal angles. With the new algorithm instead, the displacement "in depth" is correlated with the final scattering angle and the position vector and the final direction vector do not lie in the same plane. One advantage that it is hoped to obtain with this approach is to overcome the known problem of lack of backscattered particles in EGS. Now a particle undergoing a large angular scattering also undergoes a small straight-ahead displacement (and a large lateral one), resulting in an increased backscattering probability.

3) The original EGS angular sampling was abandoned as it behaves very poorly for low values of B . Instead the new sampling from the Molière distribution is accomplished in an original manner. The zero total integral of both the f_1 and f_2 terms is exploited to always sample from the Gaussian and then to move the sampled value from a negative part of a f_1 distribution to a corresponding value in a positive part of the same f_1 . The algorithm uses polynomials fitted to the Molière f_1 distributions to a high degree of accuracy (1 part in $1e6$ over the whole range of interest). Despite a certain coding complexity, the new sampling is fast, very accurate even for small B and samples with the exact weight also the tail of the distribution.

4) A dependence (absent in the standard and PRESTA algorithms) of the screening angle on the electron velocity β (arising as a correction to the simple Born approximation) has been inserted. This turns out to be important when assessing the minimum step size at low velocities (therefore affecting the range of validity of the algorithm).

Although an improvement on the standard EGS algorithm and possibly also on PRESTA, the new algorithm has still not solved the problem of boundary crossings and interface effects whose treatment in the framework of a condensed history Monte Carlo is not satisfactory with any of the present solutions.

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computational dosimetry.

Dr. A. Ferrari of 'Istituto Nazionale di Fisica Nucleare' (INFN), Milan, is working on the new electron transport algorithm. Section 5.2 represents a summary of a paper to be submitted by him to Nuclear Instruments and Methods (co-author P. Sala).

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