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The EGSnrc System, a Status Report

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Abstract. EGSnrc [1] is a general-purpose package for the Monte Carlo simulation of coupled electron-photon transport that is based on the popular EGS4 system but incorporates a variety of improvements in the class II implementation of the condensed history technique and the modelling of the underlying physical processes. This paper gives a status report on the EGSnrc system and presents several examples demonstrating the importance of the improvements in the underlying cross sections undertaken recently.

1 Introduction

Code systems for the Monte Carlo (MC) simulation of coupled electron-photon transport, such as EGS4 [2], ITS [3] and MCNP [4] (the latter two being largely based on the ETRAN system [5] in their treatment of electromagnetic showers), have been extensively benchmarked and are known to reproduce experimental data well in a variety of situations. There are, however, situations where all these systems fail to produce reliable results. An excellent example of such a situations is the comparison between MC simulations and measurements of the response of a plane-parallel ionization chamber with a replaceable back wall as a function of the atomic number of the back wall, shown in Fig. 1. Experimental data are from [6], the front wall is aluminum and the curves are normalized to unity at aluminum ($Z = 13$). The two different EGSnrc simulations will be discussed later in the text. The up to 10% difference between measurements and EGS4/PRESTA and ITS simulations is rather striking and difficult to understand in view of differences between the underlying cross sections and in the implementation of the condensed history technique for electron transport (see *e.g.* the pioneering work by M. Berger who introduced the technique and coined the terminology [7]). Such large differences between measurements and calculations, together with the well known step-size dependence of simulation results and the failure of EGS4/PRESTA to converge to the correct answer for small step-sizes for certain type of situations [8], have prompted us to undertake a substantial rework of the EGS4 system. This paper gives a brief status report on the resulting MC package called EGSnrc.

2 EGSnrc

The work on the various changes of the EGS4 system that were implemented in EGSnrc can be grouped into two main phases:

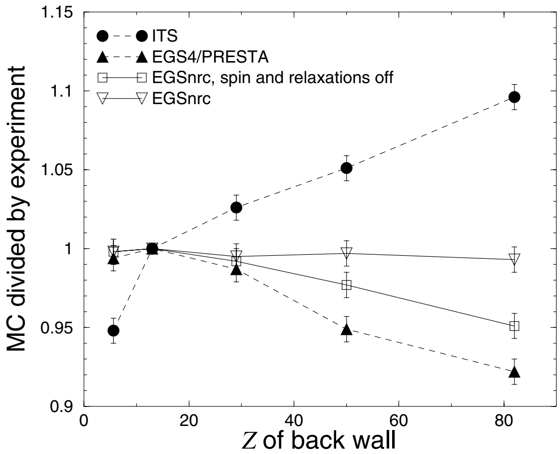

Fig. 1. MC simulations of a plane parallel chamber response in a broad parallel ^{60}Co beam as a function of the atomic number of the replaceable back wall. Results are divided by the experimental data of [6] (which has an uncertainty of 0.5%) and normalized to unity at $Z = 13$

1. Improved implementation of the condensed history (CH) technique
2. Improvements in the treatment of the various physical processes

Phase 1, which can be considered as completed, involved the following modifications

1. A new electron-step algorithm [9] with second order energy loss corrections as described in [10,11]
2. A new, any angle, any step, multiple elastic scattering theory based on the screened Rutherford cross section [12] with energy loss corrections discussed in [10,11]
3. Exact boundary crossing algorithm in single elastic scattering mode [10,11]
4. Correct implementation of the fictitious cross section method [10,11]
5. Exact evaluation of energy loss due to sub-threshold processes [10,11]

After completion of phase 1, EGSnrc was shown to produce step-size independent and artifact-free results at the 0.1% level when benchmarked against its own cross sections [10,13]. However, when applied to the plane-parallel chamber response situation described in the Introduction, phase 1 EGSnrc produced the curve labelled as "EGSnrc, spin and relaxations off" in Fig. 1. Although closer to the experiment than EGS4/PRESTA and ITS, there was still a significant difference between measurements and calculations for high atomic numbers (5% for lead). As artifacts due to the use of the CH technique can be excluded as a reason for the disagreement, the difference is clearly due to not sufficiently accurate cross sections which EGSnrc had inherited from the EGS4 system. The improvement of various cross section was undertaken in phase 2 which is still not completed. The current status can be summarized as follows:

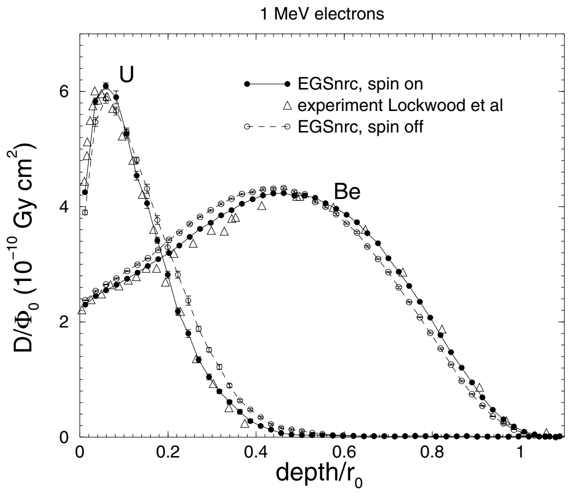

Fig. 2. Depth-dose curves for a broad parallel beam of 1 MeV electrons incident on a Beryllium or Uranium target as a function of depth expressed as a fraction of the CSDA range. The experimental data are from [22]

1. Electron elastic scattering is based on partial-wave analysis (PWA) cross section which take into account relativistic spin effects and are different for electrons and positrons. Sampling of multiple elastic scattering angles on the basis of the PWA cross sections requires one additional rejection loop in the sampling algorithm. For more details the reader is referred to [11]. To facilitate comparisons with EGS4 and in order to be able to study the effect of more accurate electron elastic scattering cross sections, the user is given the possibility to "turn off" spin effects.
2. In addition to the Bethe-Heitler cross sections for electron/positron bremsstrahlung used in EGS4, the possibility to use the NIST bremsstrahlung cross section data base [14,15], which is the basis for the radiative stopping powers recommended by the ICRU [16], has been implemented. In addition, sampling the angular distribution by the fixed angle approximation has been removed and is done either using equation 2BS from the article by Koch and Motz [17] (with a slight modification concerning the kinematics at low electron energies) or using the leading term of the distribution.
3. Binding effects and Doppler broadening in incoherent photon scattering are taken into account in the impulse approximation [18]. Shell-wise Compton profiles necessary for the sampling algorithm are approximated according to the formula suggested by the PENELOPE group [19]. The sampling algorithm makes use of the fictitious cross section method in order to avoid re-evaluation of total incoherent scattering cross sections. For more details see [11].
4. The sampling algorithm for photo-electric absorption has been modified (i) to explicitly sample the element in case of interactions with mixtures and (ii)

to explicitly sample the shell in the selected element absorbing the photon. In addition, the angular distribution of photo-electrons is modelled according to the Sauter distribution [20].
5. Atomic relaxations via the emission of characteristic X-rays, Auger and Coster-Kronig electrons are treated in a separate routine that can be called from any process generating inner shell vacancies (currently photo-electric absorption and incoherent scattering). Transition probabilities for the various de-excitation channels were taken from the Evaluated Atom Data Library (EADL) [21]. In order to keep the amount of data held in the memory at a reasonable level, transitions to and transitions from M and N shells are treated in an average way, see [11].

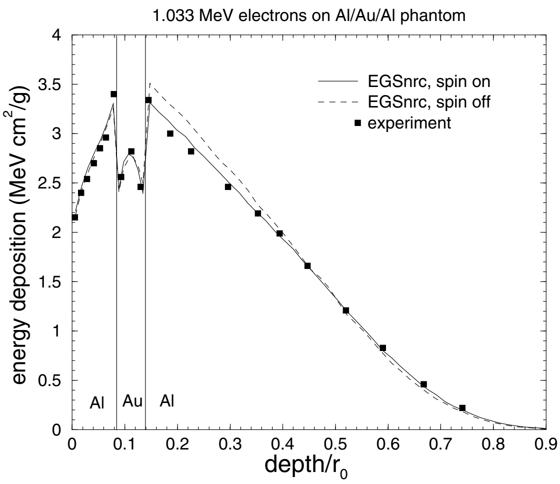

Fig. 3. Depth-dose curves for a broad parallel beam of 1 MeV electrons incident on an aluminum-gold-aluminum phantom as a function of depth expressed as a fraction of the CSDA range. The experimental data are from [22]

Simulation of the plane-parallel chamber situation described in the Introduction with EGSnrc in its current stage yields the curve labelled as "EGSnrc". The agreement with the measurement is within 0.7% which is comparable with the stated experimental uncertainty of 0.5%. It is worth noticing that half of the simulated response increase for lead (compared to the simulation using EGS4 cross sections) was due to the inclusion of relativistic spin effects for electron elastic scattering, the other half resulted from the proper treatment of photo-electric absorption and the production of Auger electrons.
Improvements of the modelling of the underlying physical processes in the near future will concern
1. Better treatment of electron/positron inelastic scattering at low energies. In particular the creation of inner shell vacancies (electron impact ionization) will

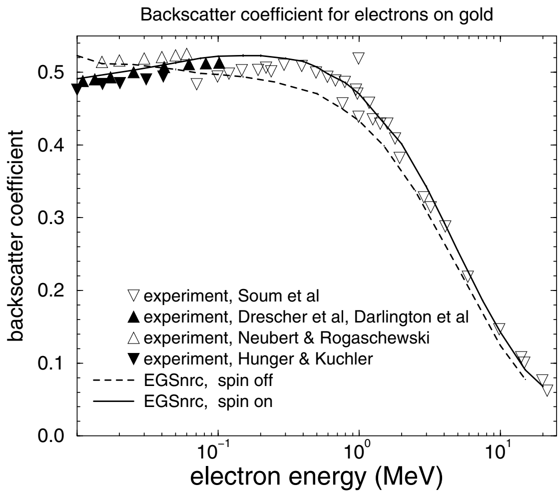

Fig. 4. Backscatter coefficients for electrons perpendicularly incident on a semi-infinite gold target

be taken into account
2. Implementation of energy loss straggling due to sub-threshold inelastic collisions. Although this could be considered to be part of the CH implementation, the precise shape of the straggling distribution depends on the small energy transfer inelastic cross section. Energy loss straggling can therefore be implemented only after completion of point 1.
3. Better modelling of coherent photon scattering.

Longer term goals could concern
1. Less important (at least from the point of view of the general user) cross section modifications such as differences between electron/positron bremsstrahlung cross sections, explicit treatment of triplet production, single and triple photon positron annihilation, etc.
2. Development of a general purpose geometry package for use with EGSnrc
3. Development of a general purpose source package

3 Examples

Perhaps the most important modification of cross sections in EGSnrc compared to EGS4 is the inclusion of spin effects for e^-/e^+ elastic scattering as it has an effect on the simulated results not only in the sub-MeV energy range. Figure 2 shows a comparison of calculated depth-dose curves in Beryllium and Uranium to measurements by Lockwood *et al* [22]. Both, the calculations and the measurements are absolute. The calculations with "spin on" are in much better agreement with the experiment. The effect of including spin is to make the effective range of electrons longer for low-Z materials and shorter for high-Z materials. It is also present for the energy range relevant for radiation therapy. Fig. 3 shows comparisons of depth-dose curves in an aluminum-gold-aluminum phantom to experimental data from [22]. Again, the inclusion of spin effects leads to a much better agreement with the measurements. As a final example Fig. 4 presents a comparison between the calculated backscatter coefficients for electrons impinging on a semi-infinite gold target as a function of the incident electron energy and experimental data from various measurements.

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