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# Evaluation of computational models and cross sections used by MCNP6 for simulation of electron backscattering

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ABSTRACT

This work evaluates the accuracy of the single-event (SE) and condensed-history (CH) models of electron transport in Monte Carlo simulations of electron backscattering from thick layers of Be, C, Al, Cu, Ag, Au and U at incident electron energies from 200 eV to 15 MeV. The CH method is used in simulations performed with MCNP6.1, and the SE method is used in simulations performed with an open-source single-event code MCNelectron written by the author of this paper. Both MCNP6.1 and MCNelectron use mainly ENDF/B-VI.8 library data, but MCNelectron allows replacing cross sections of certain types of interactions by alternative datasets from other sources. The SE method is evaluated both using only ENDF/B-VI.8 cross sections (the "SE-ENDF/B method", which is equivalent to using MCNP6.1 in SE mode) and with an alternative set of elastic scattering cross sections obtained from relativistic (Dirac) partial-wave (DPW) calculations (the "SE-DPW method"). It is shown that at energies from 200 eV to 300 keV the estimates of the backscattering coefficients obtained using the SE-DPW method are typically within 10% of the experimental data, which is approximately the same accuracy that is achieved using MCNP6.1 in CH mode. At energies below 1 keV and above 300 keV, the SE-DPW method is much more accurate than the SE-ENDF/B method due to lack of angular distribution data in the ENDF/B library in those energy ranges. At energies from 500 keV to 15 MeV, the CH approximation is roughly twice more accurate than the SE-DPW method, with the average relative errors equal 7% and 14%, respectively. The energy probability density functions (PDFs) of backscattered electrons for Al and Cu, calculated using the SE method with DPW cross sections when energy of incident electrons is 20 keV, have an average absolute error as low as 4% of the average PDF. This error is approximately twice less than the error of the corresponding PDF calculated using the CH approximation. It is concluded that the SE-DPW method is sufficiently reliable to be used as an alternative of the CH method in MCNP6 at electron energies up to the order of 100 keV, including energies from 200 eV to 1 keV, where CH approximations are not applicable in principle.



## 1. Introduction

The phenomenon of electron backscattering is important in various experimental applications, such as electron probe microanalysis and scanning electron microscopy. Consequently, there is a constant interest both in experimental investigations of electron backscattering and in its theoretical analysis. An extensive subset of theoretical research in this area is based on Monte Carlo simulations. Several general-purpose Monte Carlo simulation codes are available for such computations: MCNP [1,2], Geant4 [3,4], EGS5 [5], PENELOPE [6] and others. In all of them, electron transport is simulated using a combination of two methods – single-event (SE) and condensed-history (CH). The SE method simulates individual electron collisions separately, whereas the CH approximation is based on breaking the electron's path into many steps, chosen long enough to encompass many collisions, which are treated by multiple-scattering theories [1,7–12]. The need for the CH approximation arises from the fact that an electron with energy of the order of 10 keV experiences several thousand inelastic collisions with small energy transfers and with small-angle deflections [13], plus an even greater number of elastic collisions, before coming to a halt. As electron energy is increased, the number of collisions increases proportionally. This large number of collisions can make the detailed event-by-event simulation prohibitively long when simulating interaction of high-energy electrons with thick targets. The CH approximations make it possible to shorten the simulation significantly while preserving the essential physical features of the simulated process.

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Since the multiple-scattering theories are based on the assumption that the total energy loss and angular deflection of an electron is a result of many collisions, each characterized by small energy transfer and small angular deflection, they cannot be applied in a situation where electron's energy or direction is determined by a small number of so-called "hard" or "catastrophic" collisions, characterized by large energy transfers or large angular deflections. Consequently, some Monte Carlo codes treat such collisions on an event-by-event basis by detailed simulation, using single-event cross sections. For example, EGS5 and PENELOPE use threshold energies ($W_c$) and threshold polar deflection angles ($\theta_c$) such that events with energy loss $W$ greater than $W_c$ or with angular deflection $\theta$ greater than $\theta_c$ are treated by a detailed simulation, whereas the "soft" events (characterized by $W < W_c$ or $\theta < \theta_c$) are treated as contributing to the continuous processes of energy loss and deflection of the electron in between relatively infrequent discrete (or "hard") events [5,6]. Using the terminology proposed by Berger [10], such approach is categorized as "Class II" or "mixed" scheme. In contrast, the implementation of the CH approximation in MCNP belongs to "Class I" group of methods, where the collisions are not divided into "soft" and "hard" ones, whereas the net energy loss, the net angular deflection and production of secondary particles are sampled statistically from relevant multiple-scattering distributions [12].

In addition to sampling the particle energies and directions after "hard" collisions (in Class II codes), single-event cross sections are used for constructing the angular distributions of multiple scattering [7,12]. The Goudsmit–Saunderson multiple-scattering distribution [7] is usually written as a Legendre series with coefficients expressed in terms of weighted integrals of the single-event differential cross section (e.g., see Eq. (7.3) and Eq. (7.4) in [12], or Section 4.1 of [6]). Consequently, various additional approximations are applied in order to simplify the calculations (see [12] and references therein).

Any implementation of multiple scattering theories involves defining so-called "major steps" and "sub-steps" [12]. In MCNP, a "major step" (also called an "energy step") is a part of the electron's path where its energy decreases from one predefined energy value to another (typically, the average relative energy loss per one such step is $1 - 2^{-1/8} = 8.3\%$ [2,12]). The cross sections and angular distributions, which are used throughout one major step, are evaluated at the mid-energy for each step, in order to minimize errors associated with the use of a constant energy [12]. In order to increase accuracy of calculated angular deflections and numbers of produced secondary particles, each major step is further broken down to $m$ "sub-steps" of equal length. Angular deflections and the production of secondary particles are sampled at the level of these sub-steps [2]. The number of sub-steps ($m$) depends only on material (average atomic number $Z$). Appropriate values for $m$ have been determined empirically [2] and increase with increasing $Z$: $m = 2$ for Be ($Z = 4$), 3 for C ($Z = 6$), 5 for Al ($Z = 13$), 7 for Cu ($Z = 29$), 8 for Ag ($Z = 47$), 13 for Au ($Z = 79$), 15 for U ($Z = 92$). As a rule of thumb, an electron should make at least ten sub-steps in any material of importance to the transport problem [2]. In EGS5 and PENELOPE, energy steps and sub-steps are of random length [5,6].

All versions of MCNP up to MCNP5 did not possess the capability to apply the single-event method for simulations of electron transport. MCNP6 introduced a user-adjustable energy boundary, below which all electron interactions are simulated using the SE method, whereas electrons with energies above that boundary are transported using the CH model [14]. If that boundary energy exceeds the largest possible energy encountered in the simulated system, electron transport is entirely simulated using the SE method. Then motion of an electron is simulated by repeating those four steps:

(1) Calculate the total cross section and use it to calculate distance to collision.
(2) Select target (if there are several types of atoms in the material).
(3) Select the type of interaction.
(4) Calculate energies and directions of the primary and secondary particles after the interaction event.

This scheme is always applied to photons, because photon transport is faster than electron transport, i.e., the number of photon collisions is typically much less than the number of electron collisions. In the case of electrons, however, adopting such a scheme is generally considered impractical [2,6,12], except in the case of thin geometries or low-energy electrons, because otherwise it would cause a major performance hit. That is one of the reasons why the SE method is intended at the present stage of development of MCNP6 to be used only at electron energies below 1 keV (which is both the default value of the mentioned energy boundary and its lowest recommended value [15]). As stated in [14], large amount of validation and verification must be done before the application of the SE method in MCNP6 for higher electron energies can be considered reliable. The present paper is a contribution to the mentioned validation process.

As it is obvious from the above description of the single-event method, it is conceptually much simpler than the condensed-history approximation. Since the SE method is less dependent on implementation-specific theoretical assumptions than the CH approximation, the SE method is potentially more accurate. Its accuracy is mainly determined by accuracy of cross sections used for the simulation. In fact, all purely single-event codes that share the cross section data should yield identical results, because probability distributions of random variables sampled in each of the mentioned four steps are completely defined by the corresponding cross sections. Thus, when evaluating suitability of a particular cross section dataset (such as the ENDF/B library) for single-event simulations, a particular code (e.g., MCNP6) is irrelevant. On the other hand, CH approximations use various theoretical assumptions and simplifications, which are implemented in the code itself, rather than in cross section data. This leads to a number of adjustable parameters (such as the lengths of the mentioned "energy steps" and numbers of sub-steps), which are different in different codes. Consequently, each code has its own implementation of the CH approximation.

In this work, the accuracy of CH and SE methods is evaluated by comparing Monte Carlo simulation results with experimental data on electron backscattering. The main quantitative characteristic of electron backscattering is the backscattering coefficient ($\eta$), which is conventionally defined as the ratio of the number of backscattered electrons with energy above 50 eV to the number of incident electrons. The mentioned threshold energy is needed to ensure that the majority of detected electrons are multiply scattered "primary" electrons, rather than low-energy "secondary" (or "knock-on") electrons ejected from atoms during ionizing collisions. Under those conditions, a comparison of the measured values of $\eta$ with those obtained from Monte Carlo simulations is a sensitive tool for validating the physical models and simulation methods used for simulating elastic and inelastic electron scattering. In experimental studies of electron backscattering, it is customary to present the values of $\eta$ obtained from Monte Carlo simulations along with experimental data (some of those studies will be cited in the "Simulation results" section below). In particular, if CH approximations are used, this comparison can be used to evaluate the implementations of multiple scattering theories in the simulation codes. Such approach has been recently applied for an extensive analysis of the accuracy of electron scattering algorithms implemented in six Geant4 versions released between December