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Author(s): Hughes, H. Grady III

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Enhanced Electron-Photon Transport in MCNP6

H. Grady Hughes [1*]

[1]*Los Alamos National Laboratory, Los Alamos NM 87545 USA*
[*]Corresponding Author, E-mail: hgh@lanl.gov

Improved methods for low-energy photon/electron transport have been developed for the Monte Carlo particle transport code MCNP6. Aspects of this development include a significant reworking of the MCNP coding to allow for consideration of much more detail in atomic relaxation processes, new algorithms for reading and processing the Evaluated-Nuclear-Data-File photon, electron, and relaxation data capable of supporting such detailed models, and extension of the electron/photon transport energy range below the traditional 1-kilovolt limit in MCNP, with the goal of performing transport of electrons and photons down to energies in the few-electron-volt range.

KEYWORDS:* *photon/electron transport; Monte Carlo; MCNP; single-event electron transport

I. Introduction

The Los Alamos Monte Carlo transport code MCNP6(1) is a major step forward for the MCNP family of codes. MCNP6 is the culmination of several years of work to combine the capabilities of MCNP5(2) and MCNPX(3), to improve the resulting code system, and to include a number of new features. Among these features is a significant enhancement of the coupled electron/photon transport capability. This work is based on the introduction of most of the electron/photon/relaxation data from release ENDF/B VI.8 of the Evaluated Nuclear Data File(4) into MCNP6, and the development of transport methods to make use of these new data. In this paper we shall give an overview of this work, discussing photon enhancements, improvements in atomic relaxation, and a new single-event electron transport method.

II. Photon enhancements

The new data and methods for MCNP6 include extensions of photon cross sections to lower energies than previously available, addition of entirely new data specific to atomic electron subshells, and completion of the form factor data for coherent and incoherent photon scattering.

The ENDF/B VI.8 database includes, for elements 1–100, tabulations of total cross sections as functions of photon energy for the four fundamental photo-atomic transport processes that have traditionally been considered in MCNP: coherent and incoherent scattering, photoelectric absorption, and electron/positron pair production. For the last of these, pair production, the data are essentially unchanged from previous MCNP libraries. The other three processes also remain unchanged for the energy range above 1 keV. The important difference is that data for these three processes are now available to the code in the low-energy range from 1 keV down to 1 eV. This is a significant extension of the energy range over which useful calculations can be done.

In addition to extending pre-existing data to lower energies, the ENDF/B VI.8 database also includes several kinds of data that have not previously appeared in MCNP. The first such enhancement is the presence of subshell photoelectric cross sections. Previously only a total photoelectric cross section (as a function of energy) was given for each element, to be used in the selection of a distance to collision and a sampling of the collision process. With the improved data, the sampling of a photoelectric event can be followed by the detailed, statistically realistic, energy-dependent sampling of an individual subshell, leading to a completely correlated sampling of secondary photoelectron energy, vacated shell, and subsequent atomic relaxation.

To sample the angular distribution from photon coherent and incoherent scattering the Thompson and Klein-Nishina cross sections, respectively, are modified by tabulated form factor functions, and the photon scattering angle is determined by sampling from the products of the resulting probability distributions. In earlier versions of the code and cross section libraries, both form factor functions were tabulated only over a limited set of values so that representation of the scattering over the full angular range was complete only for a rather modest range of photon energies. The ENDF/B VI.8 database extends both tabulations to values large enough to guarantee full angular coverage over the entire energy range of the new data, up to 100 GeV. The modification to the ACE-format libraries supplying these data to MCNP6 follows earlier work(5), but the algorithm is enhanced by the replacement of the previous linear interpolation of the form factors, no longer adequate for higher energies or larger scattering angles, by a correct logarithmic method.

III. Enhancements in atomic relaxation

A very significant addition to the photon/electron data in MCNP6 is a detailed compilation of information about atomic electron subshells. The data now include the identities of all subshells that can play any non-negligible role in the atomic relaxation process for energies down to the new 1-eV lower limit, their binding energies, ground-state electron populations, and number of possible relaxation transitions. In contrast to the previous model, which considered only relaxations to the K shell and to a weighted average of the L shells and allowed a maximum of five distinct transitions to these shells, the new data can consider as many as 29 subshells and can include almost 3,000 distinct transitions among them. These transitions include both radiative (photon-producing) and non-radiative (Auger or Coster-Kronig electron-producing) channels. With some code enhancements, the new database allows the code to perform detailed simulations of the atomic relaxation cascade, and offers the possibility of complex spectroscopic simulations beyond the previous capabilities of MCNP.

IV. Electron enhancements

The ENDF/B VI.8 database provides microscopic cross sections and secondary distributions appropriate to the four fundamental electro-atomic transport processes: atomic excitation, electron elastic scattering, subshell electro-ionization, and bremsstrahlung. In all cases, tabulations of cross sections are given for energies between 10 eV and 100 GeV, and appropriate forms of tabulated distribution functions for secondary particles or energy loss are also provided. To use these new data, we adopt a completely different approach from the condensed-history method[6] that previously was the only available algorithm for electron transport in MCNP. In this new “single-event” method we dispense with the multiple-scattering theories, substep-based approximations, uncorrelated processes, and other aspects of the condensed-history approach, in favor of direct sampling of microscopic data distributions. At the present stage of development, the new method is not intended to replace the condensed-history method in any energy range in which the traditional approach can be used, but only to extend electron transport below the previous lower limit of 1 keV. However the possibility of using single-event electron transport at higher energies is intriguing, and will eventually be explored.

For atomic excitation, two energy-dependent tables are provided for each element: a tabulation of the cross section for an excitation event, and a tabulation of average energy loss due to excitation. This representation allows a detailed sampling of the occurrence of excitation, but only a deterministic average of the electron energy loss. Since the range of energies lost to excitation is quite narrow, this is likely a good approximation for all but the lowest electron energies. This process involves no angular deflection of the electron and no production of secondary particles.

Electron elastic scattering is an energetically simple process involving no secondary particles and no energy loss by the electron. However the representations of the data for angular distributions and the sampling algorithms are somewhat complex. In addition to the usual tabulation of the energy-dependent cross section for elastic scattering, ENDF/B VI.8 provides a doubly-differential cross section $\sigma_{elas}(E,\mu)$ in the form of a set of tables for various electron energies from 10 eV to 100 GeV, covering the range of scattering angles $\mu = \cos\theta$ from $\mu = -1$ to a final angle $\mu = \mu_N = 1 - 10^{-6}$, about 1.4 milliradian from the forward direction. The intention of the evaluators is that the tabulated probabilities should be used for angles away from the peak and an analytic function $f(\mu) \propto 1/(\eta + 1 - \mu)^2$ for angles near the peak, where $\eta(E,Z)$ is proportional to a screening angle given by Seltzer[6]. This method has been installed into the current version of MCNP6 and provides an adequate representation of elastic scattering, especially in the low energy range that is the initial intended application for the single-event electron transport model. There are data issues limiting the resolution of the elastic peak, so that this topic is still under investigation for applications at higher energies.

For electroionization ENDF/B VI.8 provides a large amount of data new to MCNP. In addition to the usual tabulated energy-dependent total ionization cross section, there are sets of data for each of the atomic electron subshells discussed earlier in connection with photoelectric absorption and atomic relaxation. For each set, a subshell-specific ionization cross section is given and a doubly-differential distribution $\sigma_{knock}(E, E_\Delta)$ allows sampling of a secondary electron (“knock-on”) energy E_Δ for a given incident energy E. As a result, the sampling of the electroionization process achieves the same level of detail as the newly enhanced algorithm for photoelectric ionization. Furthermore, all channels of ionization and relaxation are now treated with a consistency previously absent in MCNP.

V. Conclusion

With ENDF/B VI.8 data and new methods, MCNP6 has benefited from a significant advance in electron/photon transport capability. With these enhanced capabilities there is now a greatly expanded range of potential applications newly subject to Monte Carlo exploration with MCNP6.

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