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MODELING CHARGED-PARTICLE ENERGY-LOSS STRAGGLING

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Abstract

We present the current forms of the algorithms used to model collisional energy-loss straggling for electrons and for heavy charged particles in MCNP5 and MCNPX. We also describe a recent improvement in the logic for applying the straggling models for heavy charged particles, and show illustrative results for the improved logic.

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Introduction

Monte Carlo simulation of charged-particle transport is a difficult matter. In contrast to neutral particles, whose transport can be regarded as a series of free flights between isolated, localized interactions, charged particles in matter experience very large numbers of small, long-range Coulomb interactions with atomic electrons and with the screened charges of nuclei. This circumstance makes the cost of a direct Monte Carlo simulation of charged-particle transport prohibitive for most situations of practical interest, even with present-day computers. In order to achieve a manageable Monte Carlo capability, it has been necessary to rely on a variety of analytic and semi-analytic multiple scattering theories which attempt to use the fundamental cross sections and the statistical nature of the transport process to predict probability distributions for significant quantities, such as energy loss and angular deflection. These theories are limited by a variety of approximations and constraints; in particular they are generally invalid unless the energy loss of the charged particle is small compared to its starting energy. Therefore multiple scattering theories must be applied for sufficiently short paths along the charged particle's trajectory. The technique of dividing the charged particle's trajectory into segments that are large compared to the microscopic mean free path, but small enough for the application of multiple scattering theories is called the "condensed history" method. This approach to Monte Carlo for charged particles was essentially invented by Martin J. Berger, whose 1963 paper [1] described the techniques that have guided Monte Carlo code development ever since. Based on the methods of that work, Berger and Stephen M. Seltzer developed the ETRAN series of electron/photon transport codes [2]. These codes have been maintained and enhanced for many years at the National Institute of Standards and Technology, and are the basis for the Integrated TIGER Series [3,4] (ITS), a system of general-purpose, application-oriented electron/photon transport codes developed by John A. Halbleib, Ronald P. Kensek, and others at Sandia National Laboratories. The electron transport physics of the MCNP code [5] is largely based on that of the Integrated TIGER Series. In this paper we will concentrate on two of the multiple scattering theories important to MCNP and to its high-energy version MCNPX [6]. These are the Landau [7] theory for energy-loss straggling of electrons and the Vavilov [8] theory applicable to heavy charged particles. We will also discuss a recent improvement in the detailed logic of heavy charged particle transport relevant to the application of the Vavilov model.

Landau theory for electron energy-loss straggling

For the mean collisional energy loss of electrons, MCNP uses an analytic representation given by Berger [1] based on a combination of the Bethe-Bloch stopping power [9–11] and the Møller [12] cross section for electron-electron scattering. Because an electron step represents the cumulative effect of many individual random collisions, fluctuations in the energy loss rate will occur. Thus the energy loss will not be simply the mean collisional energy loss $\overline{\Delta}$; rather there will be a probability distribution $f(s,\Delta)d\Delta$ from which the energy loss Δ for the step of length s can be sampled. Landau [7] studied this situation under the simplifying assumptions that the mean energy loss for a step is small compared with the electron's energy, that the energy parameter ξ defined below is large compared with the mean excitation energy of the medium, that the distribution of energy losses ε from individual collisions can be adequately represented (above some minimum related to the mean ionization energy) by

$$w(\varepsilon) = \frac{\xi}{s\varepsilon^2}, \tag{1}$$

based on the Rutherford [13] cross section, and that the formal upper limit of the individual energy losses ε can be extended to infinity. With these simplifications, Landau found that the energy loss distribution can be expressed as

$$f(s, \Delta)d\Delta = \phi(\lambda)d\lambda ,$$

in terms of $\phi(\lambda)$, a universal function of a single scaled variable

$$\lambda = \frac{\Delta}{\xi} - \log\left[\frac{2\xi mv^2}{(1-\beta^2)I^2}\right] + \delta + \beta^2 - 1 + C . \tag{2}$$

Here m and v are the mass and speed of the electron, δ is the density effect correction, β is v/c, I is the mean excitation energy of the medium, and C is Euler's constant ($C = 0.5772157\ldots$). The parameter ξ is defined by

$$\xi = \frac{2\pi e^4 NZz^2}{mv^2} s ,$$

where e is the charge of the electron, NZ is the number density of atomic electrons, and z is the charge of the projectile ($z = -1$ for electrons). The universal function is

$$\phi(\lambda) = \frac{1}{2\pi i}\int_{x-i\infty}^{x+i\infty} e^{\mu\log\mu + \lambda\mu} d\mu , \tag{3}$$

where x is a positive real number specifying the line of integration.

For purposes of sampling, $\phi(\lambda)$ is negligible for $\lambda < -4$, so this range is ignored. Börsch-Supan [14] originally tabulated $\phi(\lambda)$ in the range $-4 \le \lambda \le 100$, and derived for the range $\lambda > 100$ the asymptotic form

$$\phi(\lambda) \approx \frac{1}{w^2 + \pi^2} , \tag{4}$$

in terms of the auxiliary variable w, where $\lambda = w + \log w + C - 3/2$. The developers of the ITS code have extended Börsch-Supan's tabulation, keeping the same range, but increasing the resolution. Sampling from this tabular distribution accounts for approximately 98.96% of the cumulative probability for $\phi(\lambda)$. For the remaining large-λ tail of the distribution, ITS uses the approximate form $\phi(\lambda) \approx w^{-2}$, which is easier to sample than Eq. 4, but is still quite accurate for $\lambda > 100$. Currently, MCNP follows the same procedures as ITS for the sampling of straggling.

Blunck and Leisegang [15] have extended Landau's result to include the second moment of the expansion of the cross section. Their result can be expressed as a convolution of Landau's distribution with a Gaussian distribution:

$$f^*(s,\Delta) = \frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} f(s,\Delta')\exp\left[-\frac{(\Delta-\Delta')^2}{2\sigma^2}\right]d\Delta' .$$

Blunck and Westphal [16] provided a simple form for the variance of this Gaussian:

$$\sigma_{BW}^2 = 10\text{eV}\cdot Z^{4/3}\bar{\Delta} .$$

Subsequently, Chechin and Ermilova [17] investigated the Landau/Blunck-Leisegang theory, and derived an estimate for the relative error

$$\varepsilon_{CE} \approx \left[\frac{10\xi}{I}\left(1+\frac{\xi}{10I}\right)^3\right]^{-1/2}$$

due to the neglect of higher-order moments. Based on this work, Seltzer [18] describes and recommends a correction to the Blunck-Westphal variance:

$$\sigma = \frac{\sigma_{BW}}{1+3\varepsilon_{CE}} .$$

This completes the purely theoretical description of the Landau straggling model as it is used in ITS and essentially identically in MCNP and MCNPX. However, examination of Eq. 2 and Eq. 4 shows that unrestricted sampling of λ will not result in a finite mean energy loss. Therefore, a final *ad hoc* adjustment to the sampling algorithm must be made. In the initialization phase of the codes, a material- and energy-dependent cutoff λ_c is computed subject to the condition that the integral of the energy-loss distribution up to λ_c gives the correct mean energy loss. During the transport phase, this cutoff is imposed as an upper limit on the sampled value of λ. In this way, the correct mean energy loss is preserved.

Vavilov theory for heavy charged-particle straggling

For heavier charged particles losing energy through collisions with atomic electrons, a more realistic theory is needed. In particular the assumption of unlimited energy losses from individual collisions is no longer valid, and a maximum possible individual energy loss ε_{max} must be introduced. For an unrestricted theory (typical of Class I condensed history models in the sense of Berger), this maximum is known from relativistic kinematics:

$$\varepsilon_{max} = \frac{2mc^2\beta^2\gamma^2}{1+2\gamma(m/M)+(m/M)^2} ,$$

where $\beta = v/c$ and $\gamma = (1-\beta^2)^{-1/2}$ are the usual relativistic parameters for the projectile, and M and m are the rest masses of the projectile and the electron, respectively. In terms of ε_{max} the single-collision energy-loss cross section of Eq. 1 now becomes [19]

$$w(\varepsilon) = \frac{\xi}{s\varepsilon^2}\left(1 - \frac{\varepsilon\beta^2}{\varepsilon_{max}}\right), \quad \varepsilon \le \varepsilon_{max}; \qquad w(\varepsilon) = 0, \quad \varepsilon > \varepsilon_{max}.$$

Working from these assumptions, Vavilov [8] developed a more general theory of energy straggling. In terms of previously defined quantities and the new dimensionless parameter

$$\kappa = \frac{\xi}{\varepsilon_{max}},$$

Vavilov defines a new form for the scaled energy-loss variable:

$$\lambda_v = \frac{\Delta - \bar{\Delta}}{\varepsilon_{max}} - \kappa(1 + \beta^2 - C).$$

Now the probability distribution for energy loss becomes

$$f(s, \Delta)d\Delta = \frac{1}{\xi}\phi_v(\lambda_v, \kappa, \beta^2)d\lambda_v,$$

where the new function to be sampled for the energy-loss variable is

$$\phi_v(\lambda_v, \kappa, \beta^2) = \frac{\kappa}{\pi}e^{\kappa(1+\beta^2 C)}\int_0^\infty e^{\kappa f_1(y)}\cos(y\lambda_v + \kappa f_2(y))dy, \tag{5}$$

written in terms of two auxiliary functions

$$f_1(y) = \beta^2\{\log y + \mathrm{Ci}(y)\} - \cos y - y\,\mathrm{Si}(y)$$

$$f_2(y) = y\{\log y + \mathrm{Ci}(y)\} + \sin y + \beta^2\,\mathrm{Si}(y)$$

which are themselves written in terms of auxiliary special functions, the sine integral Si(y), and the cosine integral Ci(y).

This analytic representation is obviously a difficult one, consisting of combinations and integrals of quite complicated functions. However, from a theoretical point of view, its real difficulty lies in the fact that the distribution to be sampled, Eq. 5, depends explicitly on the projectile energy (through the factor β^2) and on the energy- and material-dependent parameter κ. By contrast the distribution function in Eq. 3 can be sampled without regard to the energy of the projectile or the characteristics of the medium; those quantities appear only in the translation from the scaled variable λ to the actual energy loss Δ by Eq. 2. The additional complexity of Eq. 5 makes the practical application of the Vavilov theory in Monte Carlo a challenging problem. This situation has been addressed by a variety of investigators (see Ref. 20–25 for an introductory sample). In MCNP5 and MCNPX, we currently use a version of an algorithm described by Rotondi and Montagna [26], and we are evaluating several other methods as well. This topic is an active area of investigation in recent new MCNP development.

An improvement in condensed-history logic

Guided by earlier success in the simulation of electrons by the modified Class I algorithms of the Integrated Tiger Series, the initial versions of MCNPX exploited a similar distinction between "energy steps" and smaller "angular substeps," and relied on similar logic for associating the sampling of energy-loss straggling with the energy steps. For heavy charged particles, this system often works well, but has been found wanting in some cases, especially in the calculation of straggled energy spectra when thin regions are important. In this section we will briefly describe the old and new versions of the condensed-history transport logic for heavy charged particles, and show some computational tests to illustrate improvements from the new logic.

In earlier versions of MCNPX, the transport logic was essentially as shown in the following somewhat simplified pseudocode:

```
For charged particle with energy E, find initial energy interval J, with E_J > E ≥ E_J+1.
Begin CELL LOOP.
    Get  N = preset number of substeps per energy step  (N > 1).
    Begin ENERGY LOOP.
        Sample straggled energy deviation Δ for step size p = (E_J – E_J+1)/q_J,  where q_J
                                                    is the mean stopping power in energy interval J.
(*)     Define an effective stopping power Q_J = q_J + Δ/p for substeps within interval J.
        Set default substep size = p/N.
        Begin SUBSTEP LOOP  n = 1, N.
(*)         Find distances to time and energy cutoffs
            Find distances to possible interaction, and to surface crossing.
            Select d = the minimum of all of these and the default substep.
            Advance the particle by d and scatter the direction based on d and E.
(*)         Set E = E – Q_J d   (adjust J if necessary).
            Select appropriate case:
                Process energy or time cutoff (terminate track).
                Process inelastic interaction (make secondaries and terminate track).
                Process elastic interaction (decrease E and adjust J if necessary).
                Process surface crossing. Cycle CELL LOOP.
                Process uneventful end of substep.
            If (energy group has changed) cycle ENERGY LOOP.
        End SUBSTEP LOOP.
    End ENERGY LOOP.
End CELL LOOP.
```

The three steps marked with an asterisk (*) above involve unnecessary approximation. The second of these (concerning cutoffs) is not particularly damaging, since it affects only the very end of the particle track. However, the first and last represent a more severe approximation. The problem is that the

sampling of the straggling is done for a step (p) that is always longer than the actual step to be taken by the particle. Since the straggling theory is not linear in step size, this interpolated sampling is generally not accurate. The situation is exacerbated when there are many small zones or thin foils in the problem. Furthermore, the straggling sample is always related to the energy interval containing the beginning of the step, even if the particle falls into a lower energy interval by the end of the step. This produces a small, but systematic error. Finally, this logic is unnecessarily complex, since the SUBSTEP loop can be ended either by its normal count, or be the energy group having changed. This is the well-known MCNP *vs.* ITS step-counting issue, which has been studied and discussed [27] in the context of electron transport.

In recent versions of MCNPX and in the developmental version of MCNP5, we have replaced this transport logic with a more straightforward approach that largely avoids these approximations. The new logic is essentially represented by the following pseudocode:

For charged particle with energy E, find initial energy interval J, with $E_J > E \geq E_{J+1}$.
Begin CELL LOOP.
  Get N = preset number of substeps per energy step (N > 1).
  Begin ENERGY LOOP.
    Set default substep size = p/N, as before.
    Begin SUBSTEP LOOP
      Find distances to possible interaction, and to surface crossing.
      Select d = the minimum of these and the default substep.
      Sample straggled energy change δE_d for actual substep size d.
      Set $E = E - \delta E_d$ (adjust J if necessary).
      Check for energy cutoff (adjust endpoint and terminate track).
      Check for time cutoff (adjust endpoint and terminate track).
      Select appropriate case:
        Process inelastic interaction (make secondaries and terminate track).
        Process elastic interaction (decrease E and adjust J if necessary).
        Process surface crossing. Cycle CELL LOOP.
        Process uneventful end of substep.
      If (energy group has changed) cycle ENERGY LOOP.
    End SUBSTEP LOOP.
  End ENERGY LOOP.
End CELL LOOP.

These seemingly minor changes in logic can make a significant difference for situations in which the shortcomings of the previous approach were important. The principal improvement with the new logic is that the sampling of straggling is now almost always done based on the step size that is actually traversed by the particle. The only exception is the last substep of a track that is terminated (and adjusted after the straggling sample) by time or energy cutoff. This generally represents a negligible fraction of the total substeps in the problem, and is not certain to occur at all. A secondary benefit is that the treatment of the energy and time cutoffs is handled more naturally and more accurately.

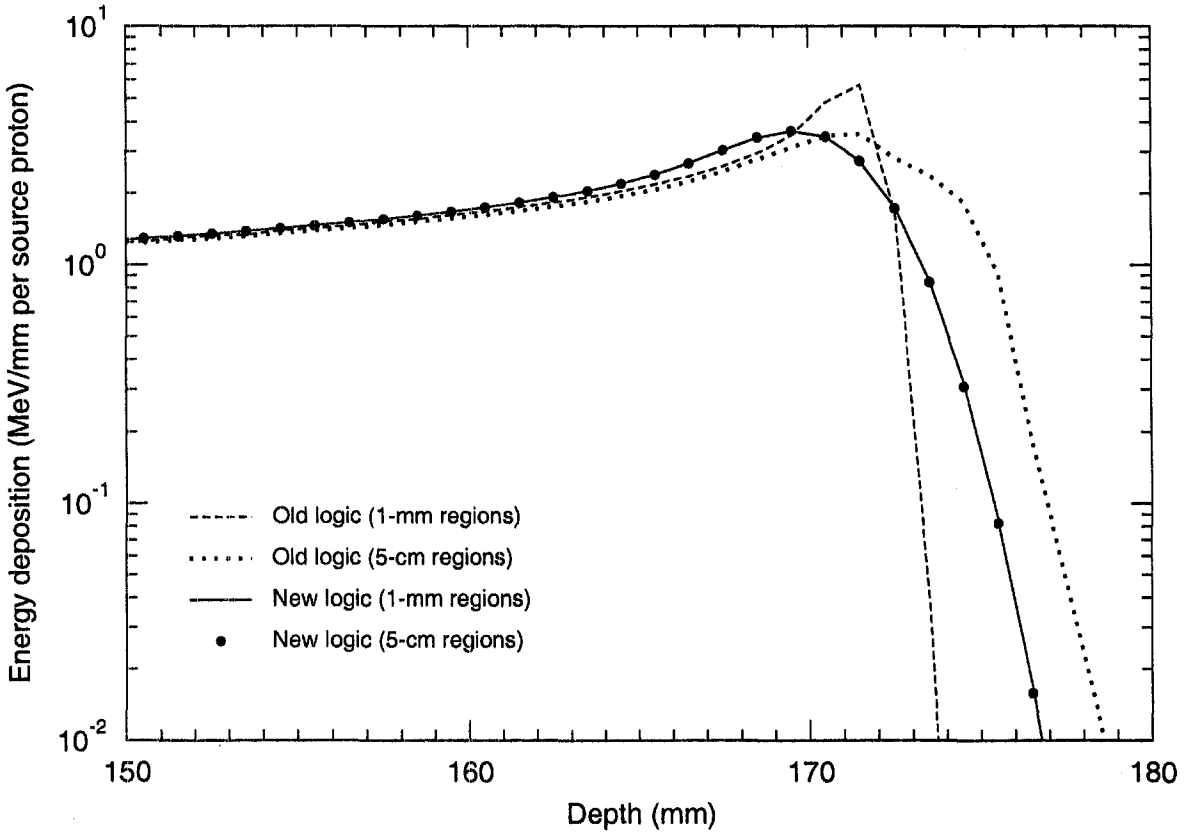

Figure 1. Energy deposition as a function of depth for 157.2-MeV protons normally incident on water.

In order to illustrate the considerable difference that the new logic can make, we have compared the two algorithms for the case of a mono-energetic, mono-directional beam of 157.2-MeV protons on a uniform water target. (This problem is based on a user's application whose strange results motivated us to re-examine the straggling logic [28].) The average energy deposition as a function of depth and the energy spectrum of the proton flux at a specific depth (15 cm) were calculated using the old and the new condensed-history algorithm. The problem was simulated twice. In the first case, the target was divided into slabs 1 mm thick, so that a large number of interruptions of the natural substep were encountered. In the second case, only the region deeper than 15 cm was divided into 1-mm slabs; the first 15 cm were divided into three 5-cm-thick slabs. This allowed us to test the sensitivity of the two algorithms to differences in the geometry specification. Fig. 1 shows details of the energy-deposition peak for both simulations. Results from the simulation with uniform 1-mm slabs are marked as "1-mm regions" in this figure, while those from the mixed 5-cm/1-mm simulation are marked as "5-cm regions," The old algorithm exhibits an un-physical sensitivity to the details of the geometry specification, as well as a noticeable artifact at the peak for the coarsely-resolved 5-cm case. By contrast, the new method produces a smoother profile for the peak, and shows essentially no sensitivity to the details of the representation of the geometry. Fig. 2 shows the energy spectrum of the proton flux at a depth of 15 cm in the water target, calculated with the old and new algorithms and for the same two physically equivalent representations of the geometry. With the old logic, the severe sensitivity to the geometry model and the presence of strange artifacts are even more apparent in these results. The new logic again

shows a more realistic profile and a satisfactory insensitivity to the geometric representation. Although we do not show the results here, we have also compared the new calculations with LAHET results and have found good agreement. We conclude that the new transport logic for heavy charged particles is an unambiguous improvement, and we have implemented this treatment as the default model in recent versions of MCNPX and in the new developmental version of MCNP5.

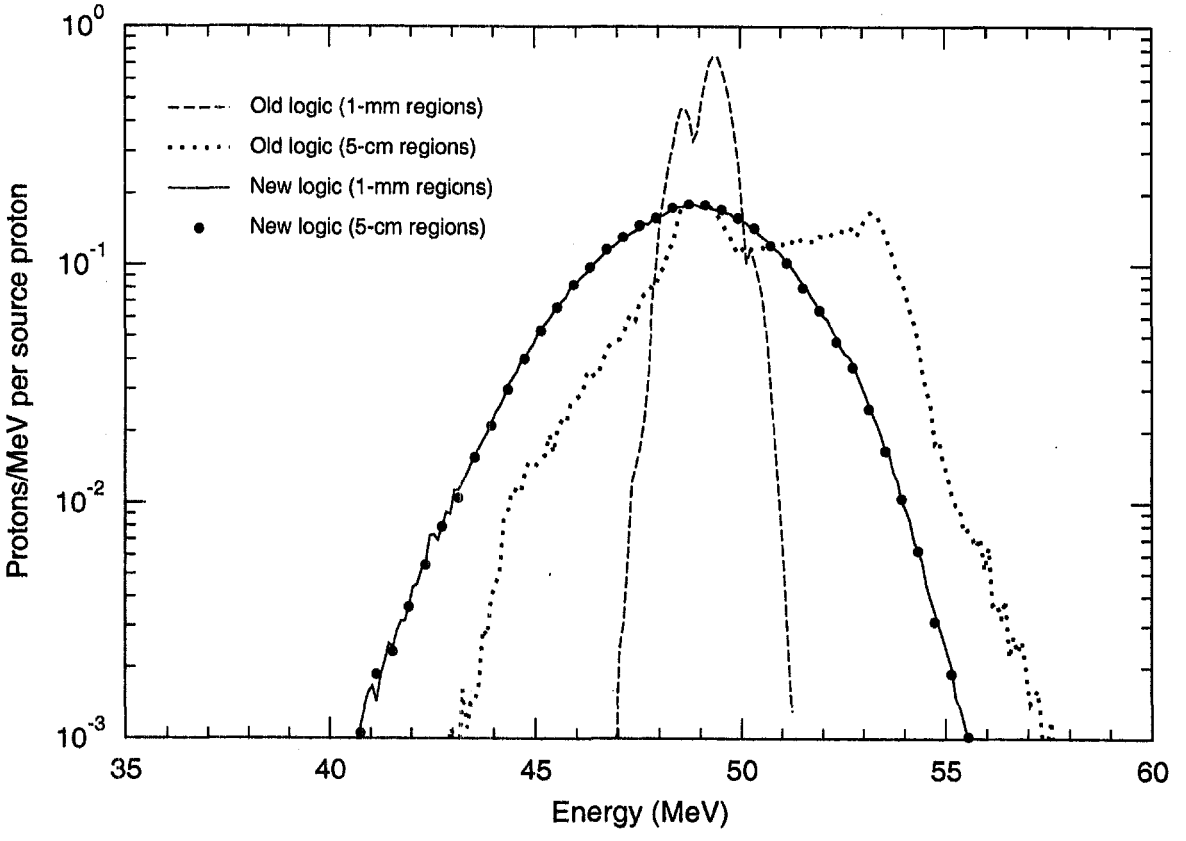

Figure 2. Proton energy spectrum at 15 cm depth for 157.2-MeV protons normally incident on water.

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