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IMPROVED LOGIC FOR SAMPLING LANDAU STRAGGLING IN MCNP5

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ABSTRACT

Previous versions of the MCNP Monte Carlo transport code have relied on a Class I approach to electron energy-loss straggling. Parameters of the Landau theory were calculated for a predetermined set of energy groups and for the average ranges associated with those energy groups. During transport, energy-loss fluctuations were sampled based on these pre-computed parameters, and the energy loss for the actual transport step was interpolated from the sample appropriate to the selected energy-group range. The particular choice of energy group for a given transport step could be made in two ways, one originally developed for MCNP, and the other based on logic found in the Integrated TIGER Series codes. For electron transport in sufficiently large geometric regions, these interpolations cause few problems, but in small zones, artifacts begin to appear. In this paper, we describe an improved logic by which the sampling of straggling can be done for the specific energy and path length of the electron step without interpolation. We illustrate this improvement with a set of test calculations suitable for showing the artifacts found in the previous methods.

KEYWORDS: electron transport, Landau straggling, MCNP

1.   INTRODUCTION

The electron transport algorithms of the MCNP5 Monte Carlo transport code [1] are based on those of the ETRAN codes [2] and the Integrated TIGER Series (ITS) [3]. These methods have been extensively compared to experimental results [4], and have been satisfactorily used for a wide variety of applications [5-6] in their intended domains of validity. Applications in very small geometric regions, however, tend to stress the limits of the current condensed-history methods. In this paper we shall describe in detail the implementation of one aspect of the electron transport algorithm, Landau energy-loss straggling, and explore an improved logic that helps to eliminate some unphysical artifacts in the treatment of small geometric zones.

The collisional energy-loss processes in MCNP5 are treated using a Class I (in the sense of Berger [7]) condensed-history model. All energy-loss calculations are based on a pre-computed set of energy groups bounded by energies E_n chosen so that $E_{n+1} = k\,E_n$ with the conventional value of $k = 2^{-1/8}$. For each energy group $E_n > E \geq E_{n+1}$ a range S_n is calculated so that on the average, an electron of energy E_n traversing a step of length S_n will lose an energy $E_n - E_{n+1}$. The

actual condensed-history steps taken by the electron are smaller than the ranges S_n. As a function of the average atomic number of the material, a number M of angular substeps per energy step is defined, and a set of substep ranges $R_n = S_n / M$ is calculated. Within each energy group, the corresponding substep range acts as an upper limit on the length of the individual condensed-history step that an electron may take. This length will be the typical substep distance traversed by the electron, but may be shortened by an encounter with a geometric boundary.

In the standard treatment of energy-loss straggling, an appropriate energy group n is selected for an electron and the Landau straggling distribution [8] (with the enhancements described by Seltzer [2]) is sampled under the assumption that the electron actually has energy E_n and will traverse a step S_n. Call this sampled energy loss ΔE. For each of the expected M substeps of range R_n, the interpolated value $\Delta E / M$ is used for the substep energy loss. The user may choose between two available algorithms by which the energy group n is chosen for the M substeps. After a brief review of Landau straggling theory, we shall describe the two existing algorithms and the new approach, which obviates the need for a choice of energy group.

2. LANDAU ENERGY-LOSS STRAGGLING

The theory of Landau [8] describes the probability distribution $f(s,\Delta)d\Delta$ for energy loss Δ by an electron traversing a path of length s in terms of a universal function $\varphi(\lambda)$ of a dimensionless variable λ:

$$f(s, \Delta) \, d\Delta = \varphi(\lambda) \, d\lambda \ , \tag{1}$$

where λ corresponds to energy loss by

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

Here m and v are the mass and speed of the electron, β is v/c, I is the mean excitation energy of the medium, δ is the density effect correction, and C is Euler's constant. The parameter ξ is

$$\xi = \frac{2\pi \, e^4 N \, Z \, z^2}{mv^2} \, s , \tag{3}$$

where e is the charge of the electron, NZ is the number density of atomic electrons, and z is the charge of the projectile. The universal function

$$\varphi(\lambda) = \frac{1}{2\pi \, i} \int_{x-i\infty}^{x+i\infty} \exp\left(\mu \log \mu + \lambda \mu\right) d\mu , \tag{4}$$

for positive real x, can be sampled using a combination of a tabulation and a large-λ asymptotic form. One *ad hoc* adjustment must be made: the Landau distribution does not have a finite mean, since no maximum individual energy transfer was accounted for in the theory. In order to recover

a finite (and correct) mean energy loss, a pre-computed material- and energy-dependent limit on the allowed sampled value of λ is used in a rejection technique in the sampling.

Following the work of Blunck and Leisegang [9], Blunck and Westphal [10], Chechin and Ermilova [11], and Seltzer [12], we attempt to account for the second moment of the distribution by sampling the convolution of $f(s,\Delta)$ with a Gaussian,

$$f^*(s,\Delta) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma}\int_{-\infty}^{\infty} f(s,\Delta')\exp\left[-\frac{(\Delta-\Delta')^2}{2\sigma^2}\right]d\Delta' \; , \tag{5}$$

with the Gaussian width

$$\sigma = \frac{(10\,eV\cdot Z^{4/3}\,\overline{\Delta})^{1/2}}{1+3\left[\dfrac{10\xi}{I}\left(1+\dfrac{\xi}{10\,I}\right)^3\right]^{-1/2}} \tag{6}$$

in terms of the mean sampled energy loss $\overline{\Delta}$.

Let us symbolize this complex sampling process by imagining a straggling sampling operator $L\left(E,s,\overline{\Delta}\right)$ which returns a suitable sample of energy loss for an electron of energy E traversing a path length s with expected mean energy loss $\overline{\Delta}$.

3.   SAMPLING LOGIC FOR LANDAU STRAGGLING

In previous versions of MCNP, all parameters needed for sampling straggling were pre-computed and associated with the standard energy boundaries E_n and the corresponding ranges S_n. In effect the code was restricted to calculations based on discrete arguments of the operator $L\left(E_n,S_n,\overline{\Delta}_n\right)$. As a result, the proper assignment of an electron transport step to an energy group n required a rather subtle logic. Eventually, two algorithms for apportioning straggled energy loss to electron substeps were made available.

3.1. MCNP Energy Indexing Algorithm

The first energy indexing algorithm (also called the "bin-centered" treatment) developed for MCNP is arguably the less successful of the two existing algorithms, but for historical reasons remains the default option. It was an attempt to keep the electron substeps aligned as closely as possible with the energy groups that were used for their straggling samples. Somewhat simplified, this is the MCNP algorithm. An electron of energy E is assigned to the group n such that $E_n > E \geq E_{n+1}$. A straggled energy loss Δ is sampled from $L\left(E_n,S_n,\overline{\Delta}_n\right)$. The electron attempts to traverse M substeps, each of which is assigned the energy loss Δ/M. If M substeps are completed, the process starts over with the assignment of a new energy group. However, if the electron crosses a cell boundary, or if the electron energy falls below the current group, the loop

over *M* is abandoned, even if fewer than *M* substeps have been completed, and the energy group is reassigned.

Since the straggling parameters are pre-computed at the midpoints of the energy groups, this algorithm does succeed in assigning to each substep a straggled energy loss based on parameters that are as close as possible to the beginning energy of the substep. However, there are two problems with this approach. First, there is a high probability that the electron will not actually complete the expected range S_n for which the energy loss was sampled, in which case the energy loss relies on a linear interpolation in a theory that is clearly nonlinear. Second, the final substep of each sequence using the sampled energy loss from $L(E_n, S_n, \overline{\Delta}_n)$ will frequently fall partially in the next-lower energy group $n+1$, but no substep using the sample from $L(E_n, S_n, \overline{\Delta}_n)$ will ever be partially in the higher group $n-1$. This results in a small, but potentially significant systematic error. (See for example the investigations of Schaart *et al* [13] and references therein.)

3.2. ITS Energy Indexing Algorithm

Developed for the ITS codes earlier than the MCNP algorithm, this method (also called the "nearest-group-boundary" treatment) was added to the MCNP code in order to explore some of the energy-dependent artifacts of the condensed history approach, and in order to offer more consistency with the TIGER Series codes. This algorithm differs from the default treatment in two ways. First, the electron is initially assigned to a group *n* such that $(E_{n-1} + E_n)/2 > E \geq (E_n + E_{n+1})/2$. In other words, the electron is assigned to the group whose upper limit is closest to the electron's energy. Second, although the electron will be reassigned when it enters a new geometric cell, it will not be reassigned merely for falling out of the current energy group. These differences serve to reduce the number of times that unwanted imposition of linear interpolation on partial steps occurs, and to allow more equal numbers of excursions above and below the energy group from which the Landau sampling was made. As Ref. [13] shows, these advantages make the ITS algorithm a more accurate representation of the energy loss process, as indicated in comparisons with reference calculations and experiments. Nevertheless, although the reliance on linear interpolation and the systematic errors are reduced, neither is completely eliminated. It is straightforward to create example calculations that show unphysical artifacts in the ITS algorithm as well as in the MCNP logic, as we shall soon see.

3.3. New Energy- and Step-Specific Method

It is easy to express what we would like to see in the straggling logic. For an electron with energy *E* about to traverse a step of length *s*, we would like to sample the straggling from the operator $L(E, s, \overline{\Delta})$ without regard to the prearranged energy boundaries E_n. In the actual MCNP5 code, we have now brought this situation about. A new FORTRAN90 module has been installed to deal with straggling data. Those parameters that are separate from the individual straggling events are still pre-computed, but each electron transport step can now sample its energy loss separately from adjacent steps, and specifically for its current energy and planned step length. Using this approach, we largely eliminate the linear interpolations and energy misalignments of the earlier algorithms. Along with those previous algorithms, this new logic will be available in the forthcoming update to MCNP5 as a user option.

4. TESTING THE ALGORITHMS

Guided by the foregoing discussions, we would expect to see unphysical artifacts in the two earlier straggling algorithms for cell dimensions smaller than standard energy steps, and we would hope to see those artifacts disappear in the new logic. To test and illustrate these ideas, consider a monoenergetic beam of 10-MeV electrons normally incident on a 15-mm slab of water. We tally the emerging energy spectrum of transmitted electrons. In order to concentrate on the energy-loss mechanisms, we turn off angular deflections, and the production of electron-induced X-rays and knock-on electrons. We describe the geometry in three physically-equivalent ways: as a single 15-mm slab, as 15 adjacent 1-mm slabs, and as 150 adjacent 0.1-mm slabs. These dimensions can be compared to the initial energy-step (4.091 mm) and to the angular substep (1.364 mm). We would expect that a well-behaved transport method should be reasonably insensitive to the differences in geometric description. Fig. 1 shows the results for the MCNP (bin-centered) logic.
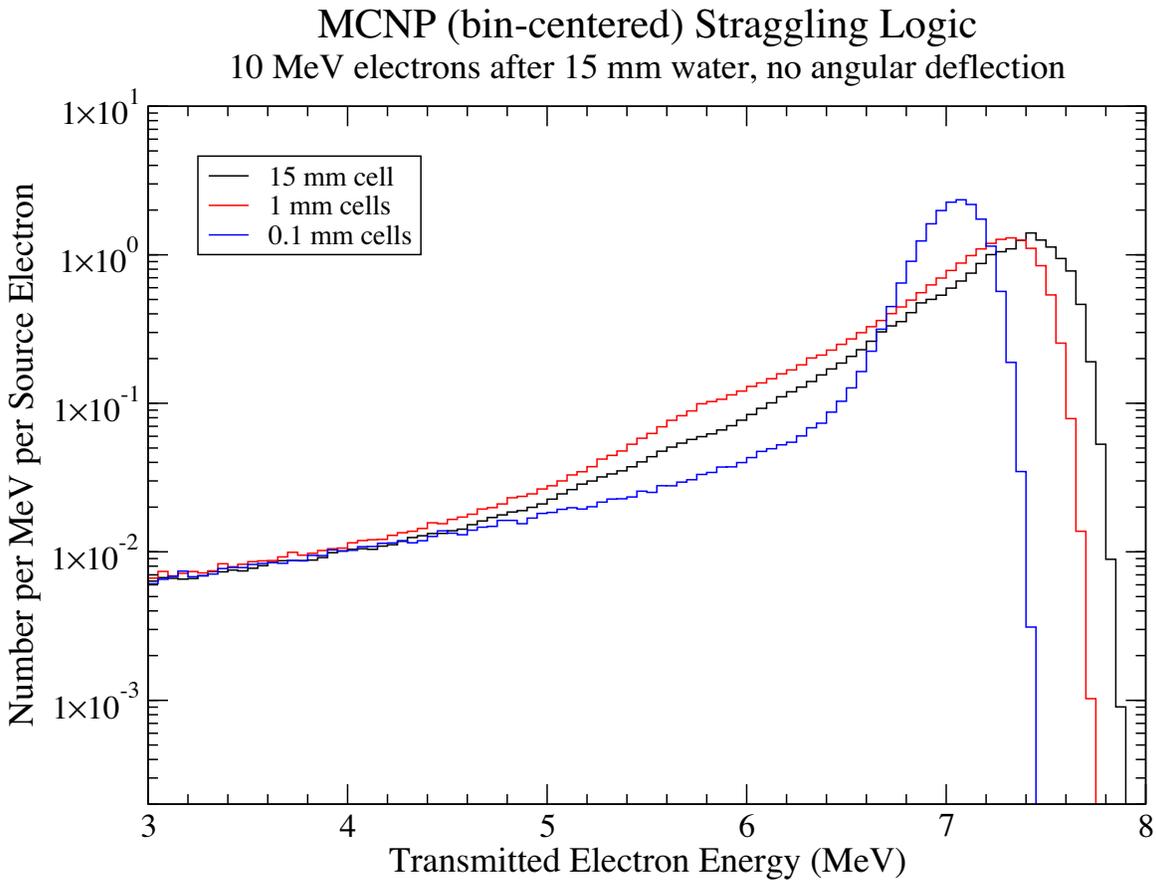

Figure 1. Results of the bin-centered straggling logic for three equivalent geometries showing unphysical step-size artifacts.

For clarity, error bars are omitted from the figure; however almost all bins have been computed to better than 5% 1-σ Monte Carlo standard relative error for the 15-mm and the 1-mm cases, and to better than 10% for the 0.1-mm case. Clearly the differences in the three calculations are unacceptably large, and far exceed any uncertainties in the tallies. Attempting the same set of calculations with the ITS (nearest-group-boundary) logic provides no relief from these artifacts. Fig. 2 shows the corresponding results using that algorithm.
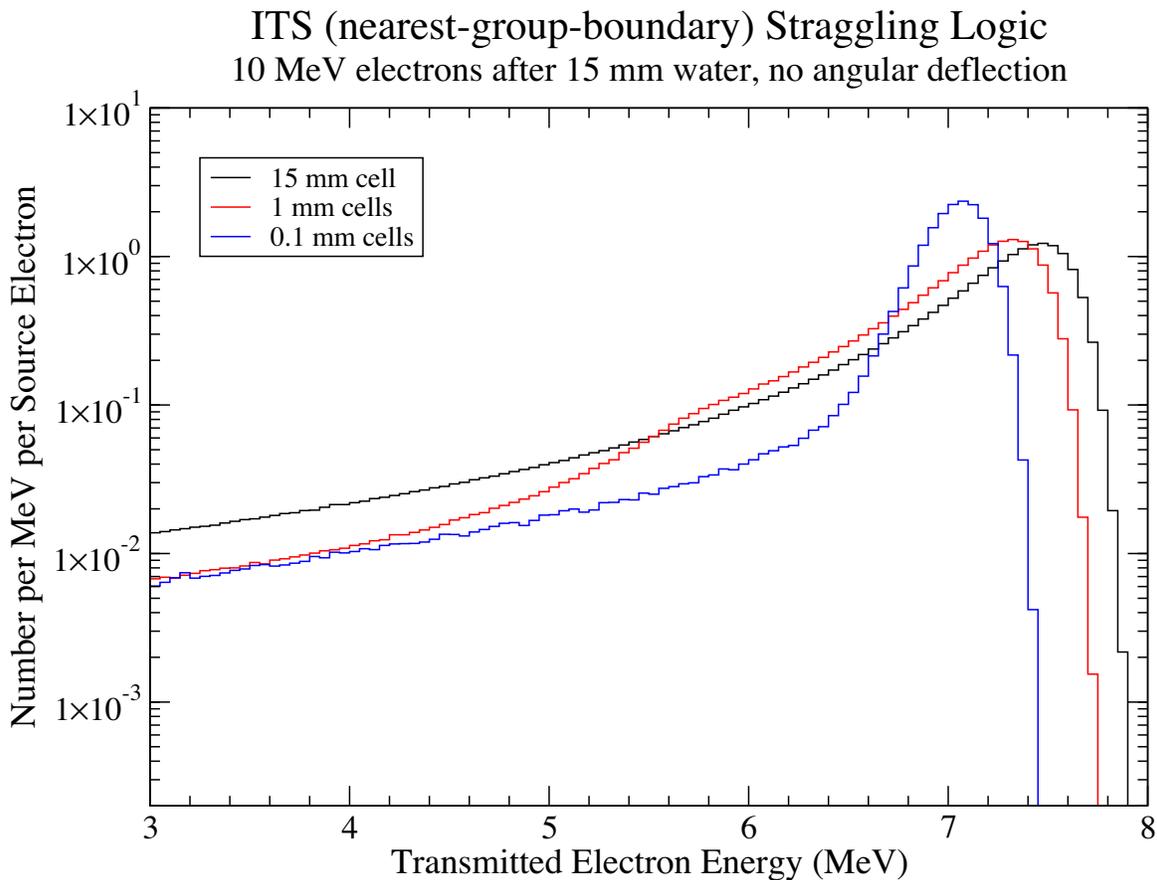

Figure 2. Results of the nearest-group-boundary straggling logic for three equivalent geometries again showing unphysical step-size artifacts.

We may note that these simple problems provide quite a severe test of the straggling algorithm, since in the 1-mm case the minimum cell dimension is already smaller than an energy step, and in the 0.1-mm case it is smaller than an angular substep by more than a factor of 13. It is for the latter case that we have turned off angular deflections for these calculations, since we know that the angular interpolation procedures for partial substeps also need the scrutiny and improvement that we are giving to the energy-loss methods.

Turning at last to the new step-specific straggling logic, we repeat the calculations for the same three representations of the geometry, with Fig. 3 showing a very satisfactory result. The step-size artifacts are now gone, even for the smallest cells in the test.

Step-Specific Straggling Logic
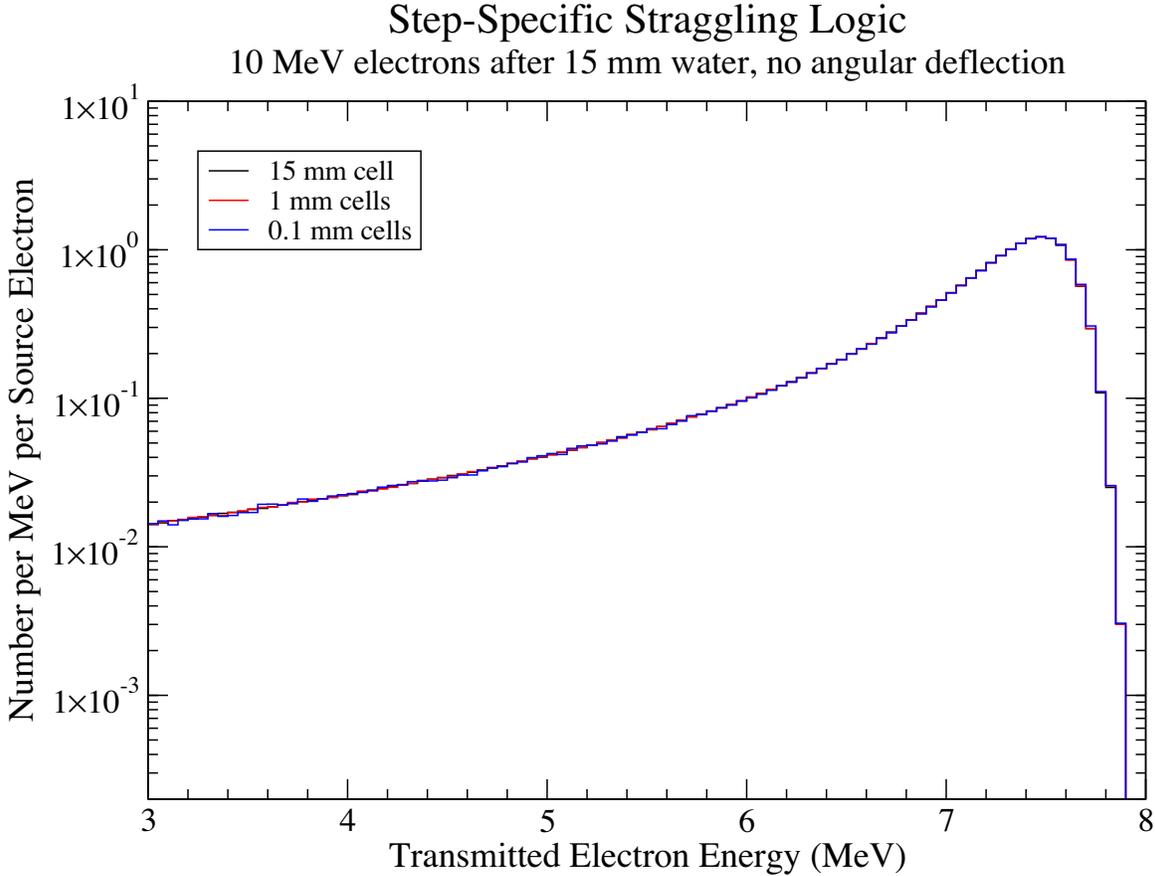### 10 MeV electrons after 15 mm water, no angular deflection

Figure 3. Results of the new step-specific straggling logic for three equivalent geometries now showing the elimination of unphysical step-size artifacts.

5. CONCLUSIONS

We have developed a new approach to the application of the Landau model to electron transport in MCNP5. The new logic is simpler than earlier methods, is specific to energy and step size for the transport step to be traversed, and is successful in eliminating severe step-size artifacts in very small geometric zones. The new treatment will be available as a user option in a forthcoming update to MCNP5.

ACKNOWLEDGMENTS

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