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A Theoretical Result for Moment-Preserving Approximations to the Landau/Vavilov Straggling Model

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ABSTRACT

A theoretical result is presented that explains the high accuracy of numerical results observed for moment-preserving approximations to the Landau/Vavilov straggling model. We show explicitly that a finite number of moments of the energy spectrum or flux can be exactly preserved if the same number of moments of the corresponding energy-loss differential cross section are also exactly preserved. This result provides confidence in the application of moment-preserving straggling theories to charged particle penetration in thin targets as well as to energy straggling in condensed history Monte Carlo methods.

Key Words: energy straggling, moment-preserving approximations

1. INTRODUCTION

It is well known that the accuracy of the condensed history Monte Carlo method for electron transport [1] can be significantly increased if attributes of so-called Lewis theory are faithfully incorporated into the method. Lewis [2] showed that, in an infinite medium and neglecting energy loss, i.e., assuming single energy particles, two transport problems with dissimilar differential scattering cross sections but with identical Legendre moments through order N will have identical space-angle moments of the angular flux also through order N. This theoretical observation has been used to increase the computational efficiency and accuracy of condensed history methods through the use of larger step sizes [3]. However, in recent years it has also facilitated the development of pseudo-transport formulations which can be efficiently simulated using single event Monte Carlo [4–7] and which have become viable alternatives to the condensed history method.

Recent numerical work has provided strong evidence for the existence of a Lewis-like theory underlying moment preserving approximations for energy straggling [7–9]. Specifically, it has been noted that approximate transport models for energy straggling that are explicitly constructed to preserve a finite number of energy-loss moments of the analog differential cross section yield more accurate dose distributions and energy spectra than those that fail to capture these moments. Moreover, the accuracy can be made to approach analog with increasing numbers of true moments retained and very accurate results can be realized with surprisingly few moments [7]. While these observations have general validity, we limit considerations in this summary to the Landau/Vavilov straggling model that is commonly employed in condensed history Monte Carlo to sample energy losses at the end of a step. The Landau/Vavilov model is also a useful paradigm for the analysis of experiments designed to investigate the energy spreading of an initially monoenergetic beam penetrating a thin layer. The advantage of using this model of straggling is that it enables us to derive a sharp theoretical result which provides an explanation for the observed accuracy of moment preserving approximations. The Landau/Vavilov straggling model is discussed in the next section after which we derive our key result regarding moment-preserving energy straggling theories.

2. ENERGY STRAGGLING AND THE LANDAU/VAVILOV MODEL

In the condensed history method, particle directions, positions, and energy losses are sampled at the end of fixed but short track segments or steps from precomputed distributions based on multiple scattering and multiple excitation/ionization theories that describe the cumulative effect of a large number of collisions. Larsen [10] has presented a rigorous derivation of the condensed history algorithm using operator split strategies to provide some justification for the application of independent angular deflection, energy loss, and transverse spatial displacement of the particle at the end of each step. The distributions used for sampling the particle state are obtained as solutions to reduced transport equations that are more easily solved than the original transport equation. Here we are concerned with energy straggling which is described by the solution to the following straight ahead transport equation:

$$\frac{\partial \psi(s,E)}{\partial s} = \int_0^\infty dE'\, \Sigma_e(E' \to E)\psi(s,E') - \Sigma_e(E)\psi(s,E), \quad 0 < s < T, \tag{1}$$

with monoenergetic incidence at $s = 0$ given by

$$\psi(0,E) = \delta(E_0 - E). \tag{2}$$

In Eq.(1), s is the path length variable, the distance traveled along the actual track, E is the particle energy and $\psi(s,E)$ is the flux which gives the energy distribution at s. The particle initially has energy E_0 and the step size corresponds to a total path length of T. Also $\Sigma_e(E' \to E)$ is the differential energy transfer cross section, and $\Sigma_e(E)$ the associated total cross section, for elastic collisions between the primary particle and the medium electrons. A distinguishing feature of charged particle interactions is that this differential cross section, given by the Moller cross section [11] for energetic electrons and by the relativistic Rutherford cross section [11] for protons and heavier ions, is highly peaked about small energy transfers. The collision mean free path $1/\Sigma_e(E)$, moreover, is extremely small. Kinematical considerations restrict the maximum energy transfer possible in a single collision while a minimum energy transfer is introduced to prevent a divergency in the cross section. An alternate characterization of interactions is through the energy-loss moments which play a vital role in straggling theories. Expressing the energy loss in a collision as $Q = E - E'$ and defining $\Sigma_e(E,Q)dQ$ such that

$$\Sigma_e(E \to E')dE' = \Sigma_e(E,Q)dQ, \tag{3}$$

the energy-loss moments are defined by:

$$Q_n(E) = \int_0^\infty Q^n\, \Sigma_e(E,Q)dQ. \tag{4}$$

Physically, $Q_1(E)$ is the mean energy loss per path length traveled or the stopping power, and $Q_2(E)$ is the mean-square energy loss per path length, also known as the straggling coefficient.

For sufficiently thick targets or for low enough energies, energy spectra and dose are dominated by these two moments and approximate models can be developed to exploit this fact. For thin targets or for high energies, however, the higher moments assume increasing importance and can strongly influence spectra and dose.

The solution to Eqs.(1) & (2) at $s = T$ gives the straggling distribution from which the starting energy for the next step is sampled. Closed form solutions of the analog problem do not exist and deterministic numerical solution approaches require extremely refined spatial and energy grids to resolve the sharply varying flux. Given the broad parameter space of energies, materials and particle types that must be considered, grid-based numerical solutions approaches are not practical and nor are they convenient for use with the condensed history method. In practice, condensed history codes use a solution to a simplified version of Eq.(1) that is accurate for small step sizes and was initially developed for electrons by Landau [12] and later refined and extended to ions by Vavilov [13]. The simplification amounts to assuming that the energy transfers in the step are small enough that the mean free path of the particle does not change appreciably from its value at the initial energy. This then enables the straggling equation to be solved by integral transform methods [12, 13]. The constant mean free path approximation is tantamount to replacing E by E_0 in the differential cross section $\Sigma_e(E, Q)$ and in the maximum energy loss possible in a collision. The resulting energy loss moments $Q_n(E_0)$ then also become independent of energy, a key simplification that makes possible the central result of this work. We refer to this theory of energy loss as the Landau/Vavilov straggling theory and its conditions of validity are that the step size must be large enough that sufficient collisions occur to justify the use of the multiple ionization and excitation collision model, yet it must be short enough that the mean energy loss is negligible compared to the initial particle energy.

We now motivate the work to be presented in the next section. It has been found in both condensed history [9] and pseudo-transport formulations [7] that the accuracy of approximate models of energy straggling is strongly correlated with the number of energy loss moments $\{Q_n,\, n = 1, 2 \cdots\}$ that are exactly preserved by these models. This is true for both thin targets [9], where the conditions of the Landau/Vavilov straggling model hold, and for thick targets [7, 9] where the energy dependence of the mean free path (and hence implicitly of the energy-loss moments) must be retained. This observation is suggestive of the existence of a sharp relationship between energy-loss moments of the differential cross section and energy moments of the flux that is analogous to the relationship between angular moments of the scattering cross section and the space-angle moments of the angular flux in Lewis theory. We demonstrate in the next section that a Lewis-type theory can indeed be formulated for Landau/Vavilov energy straggling.

3. MOMENT-PRESERVING THEORY

We introduce energy moments of the flux defined by:

$$I_n(s) = \int_0^\infty dE\, E^n\, \psi(s, E), \quad n = 1, 2, \cdots \tag{5}$$

We refer to these moments as the energy-flux moments. It follows that $I_0(s)$ is the total number of particles that have traveled a path length s, $I_1(s)/I_0(s)$ is the mean energy of the particles at s,

$I_2(s)/I_0(s)$ the mean-square energy, and so on. We make the strong hypothesis (supported by numerical evidence and inspired by Lewis theory) that there exists a direct relationship between the energy-loss moments Q_n and the energy-flux moments I_n. Our goal is to establish the conditions under which this hypothesis is true.

We begin by developing equations for the energy-flux moments. Multiplying Eq.(1) by E^n, integrating over all energies, and simplifying somewhat we get:

$$\begin{aligned}\frac{dI_n(s)}{ds} &= \int_0^\infty dE E^n \int_0^\infty dE' \, \Sigma_e(E' \to E)\psi(s,E') - \int_0^\infty dE E^n \, \Sigma_e(E)\psi(s,E) \\ &= \int_0^\infty dE' \psi(s,E') \int_0^\infty dE \, E^n \Sigma_e(E' \to E) - \int_0^\infty dE E^n \, \Sigma_e(E)\psi(s,E) \\ &= \int_0^\infty dE \psi(s,E) \int_0^\infty dE' \, E'^n \Sigma_e(E \to E') - \int_0^\infty dE E^n \, \Sigma_e(E)\psi(s,E), \end{aligned} \tag{6}$$

where in the last step the E and E' variables have been switched. Next, the total cross section $\Sigma_e(E)$ is expressed in terms of the differential cross section as:

$$\Sigma_e(E) = \int_0^\infty dE' \, \Sigma_e(E \to E'). \tag{7}$$

Substituting Eq.(7) in Eq.(6) and combining the inscatter and outscatter terms then yields:

$$\frac{dI_n(s)}{ds} = -\int_0^\infty dE\psi(s,E) \int_0^\infty dE' \, \left(E^n - E'^n\right) \Sigma_e(E \to E'). \tag{8}$$

Note that for $n = 0$ the right hand side of Eq.(8) vanishes which indicates that $I_0(s)$ must be a constant and equal to its value at $s = 0$, i.e., $I_0(s) = I_0(0)$. Equations (2) and (5) then yield $I_0(0) = 1$ and hence $I_0(s) = 1, \; s \geq 0$. This is just an expression of conservation of particles in the absence of absorption. Proceeding, it is convenient to rewrite the integral over E' in terms of the energy transfer variable $Q = E - E'$. To this end, E'^n is first expressed as a binomial expansion:

$$E'^n = (E - Q)^n = \sum_{m=0}^{n} (-1)^m \begin{pmatrix} n \\ m \end{pmatrix} Q^m \, E^{n-m}, \tag{9}$$

and this result is then used to write:

$$E^n - E'^n = -\sum_{m=1}^{n} (-1)^m \begin{pmatrix} n \\ m \end{pmatrix} Q^m \, E^{n-m}. \tag{10}$$

Note that the $m = 0$ term vanishes. Substituting Eq.(10) in Eq.(8) and also introducing the energy transfer cross section $\Sigma_e(E, Q)$ defined in Eq.(3), the equation for the energy-flux moments becomes:

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n} (-1)^m \begin{pmatrix} n \\ m \end{pmatrix} \int_0^\infty dE \, E^{n-m}\psi(s,E) \int_0^\infty dQ \, Q^m \, \Sigma_e(E,Q), \tag{11}$$

or, more compactly,

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \int_0^\infty dE \, E^{n-m} Q_m(E) \, \psi(s,E), \quad n = 1, 2 \cdots \,, \tag{12}$$

where

$$c_{nm} = (-1)^m \left(\begin{array}{c} n \\ m \end{array} \right) \ , \tag{13}$$

and we have introduced the energy-loss moments $Q_m(E)$ defined previously in Eq.(4). The initial conditions on the I_n are obtained using Eqs.(2) and (5) to get:

$$I_n(0) = E_0^n, \quad n = 0, 1, \cdots \ . \tag{14}$$

Although the energy-loss moments appear explicitly, Eq.(12) has no practical value. This is because the unknown flux $\psi(s, E)$ is explicitly present so that Eq.(12) is not a closed equation for the energy-flux moments. Nevertheless, this result unambiguously shows that there is an implicit relationship between the two types of moments. In order to proceed, let us first state our goal more precisely. Consider a second transport problem that differs from the above analog transport problem in only one respect - the differential energy transfer cross section, and hence in the energy-loss moments. Using hatted variables to denote the quantities associated with this second problem, it immediately follows that the equation for the energy-loss moments are given by:

$$\frac{d\hat{I}_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \int_0^\infty dE \, E^{n-m} \hat{Q}_m(E) \, \hat{\psi}(s, E), \quad n = 1, 2 \cdots \ , \tag{15}$$

with initial conditions:

$$\hat{I}_n(0) = E_0^n, \quad n = 0, 1, \cdots \ , \tag{16}$$

and where the energy-loss moments for this problem, $\hat{Q}_m(E)$, are defined by:

$$\hat{Q}_n(E) = \int_0^\infty dQ \, Q^n \, \hat{\Sigma}_e(E, Q) \quad n = 1, 2, \cdots \ , \tag{17}$$

$\hat{\Sigma}_e(E, Q)$ being the appropriate differential energy transfer cross section. Now, let the second problem represent a moment-preserving approximation to the analog problem, i.e., a pseudo-transport problem. In other words, the differential energy transfer cross sections are not identical but they have identical energy-loss moments up to some fixed but finite order:

$$\hat{Q}_n(E) = Q_n(E), \quad n = 1, 2, \cdots N \ . \tag{18}$$

Our goal then is to provide a concrete answer to the following question: does the equivalence of a finite number of energy-loss moments between the analog and pseudo-transport problems imply a corresponding equivalence of energy-flux moments $\hat{I}_n$ and I_n? Based on the respective equations for the energy-flux moments, namely, Eqs.(12) and (15), the answer is no. Since the fluxes $\psi(s, E)$ and $\hat{\psi}(s, E)$ will differ regardless of any finite number of energy-loss moments preserved, it follows that the moments $\hat{I}_n$ and I_n can never be identical for any order $n > 1$. One can speculate that the differences between $\hat{I}_n$ and I_n might decrease with increasing numbers of moments preserved, but it is clear that a moment-preserving theory of the Lewis type does not exist for straggling in the general setting considered above. The issue then becomes whether moment equivalence can be realized under a suitable constraint that does not diminish the value of the ultimate result.

Let us consider Eq.(18) to hold for a fixed energy E^* in the allowable range $0 < E^* \leq E_0$, that is:

$$\hat{Q}_n(E^*) = Q_n(E^*), \quad n = 1, 2, \cdots N. \tag{19}$$

Let us now assume that $\{Q_n(E), n = 1 \cdots N\}$ do not differ from their corresponding values at $E = E^*$ over this energy range. From Eq.(19) the same will then be true for the moments $\hat{Q}_n(E)$. Therefore, we can write:

$$Q_n(E) = Q_n(E^*), \quad \hat{Q}_n(E) = \hat{Q}_n(E^*), \quad 0 < E, E^* \leq E_0, \quad n = 1, 2, \cdots N. \tag{20}$$

We reiterate that the energy-loss moments for $n > N$ are not restricted in any way and in particular they can be different for the two problems. Using the above in Eqs.(12) and (15), we note that the Q_n and $\hat{Q}_n$ terms can be taken out of the respective integrals and the latter can immediately be expressed as energy-flux moments for the analog and pseudo-transport problems. In this way, we get :

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} Q_m(E^*)\, I_{n-m}(s); \quad I_n(0) = E_0^n, \quad n = 1, 2, \cdots \tag{21}$$

and:

$$\frac{d\hat{I}_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \hat{Q}_m(E^*)\, \hat{I}_{n-m}(s); \quad \hat{I}_n(0) = E_0^n, \quad n = 1, 2, \cdots \tag{22}$$

with $I_0(s) = 1 = \hat{I}_0(s)$. We observe that Eqs.(21) and (22) are linear system of closed moment equations for $I_n(s)$ and $\hat{I}_n(s)$ which can be solved sequentially for $n \geq 1$. More importantly, for $1 \leq n \leq N$ when $\hat{Q}_n(E^*) = Q_n(E^*)$, the equations and initial conditions are identical so that the solutions must also be identical. That is:

$$\hat{I}_n(x) = I_n(x), \quad n = 0, 1, \cdots N. \tag{23}$$

We conclude that if the differential energy transfer cross section corresponding to the pseudo-transport problem has the same energy-loss moments as the true or analog differential energy transfer cross section through order N, *and* if these energy-loss moments do not vary over the allowable energy range, then the two transport problems will have identical energy-flux moments through order N. This will be true for thin layers or steps where the mean energy-loss is small, and E^* would then be equated to the initial energy E_0. But these are precisely the conditions of validity of the Landau/Vavilov theory. Therefore our moment-equivalence result, which is the central result of this work, is true for any moment-preserving model within the constraints of Landau/Vavilov straggling theory.

4. Conclusions

We have shown that the numerically observed accuracy of moment-preserving approximations of Landau/Vavilov energy straggling theory results from the concomitant preservation of moments of the energy spectrum or flux. Specifically, the number of energy-flux moments preserved exactly is equal to the number of energy-loss moments of the differential cross section exactly preserved by the approximate straggling model.

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