Verification and Preliminary Results of the Generalized Boltzmann Fokker-Planck Method for Charged Particle Radiation Transport

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Abstract

The short mean free paths and zero/low energy transfers associated with charged particle interactions create a computationally intensive problem to model. This paper suggests an accurate and efficient moment-preserving alternative to traditional Monte Carlo transport methods. The Generalized Boltzmann Fokker-Planck Method is an approximation of the scattering cross sections used in the linear transport equation which exactly preserves a finite number of scattering moments using a discrete angle representation. Unlike condensed history, this method preserves exponentially distributed interaction sites, simplifies pre-computation and ultimately leads to simplified boundary crossing algorithms. While this method was developed using the screened Rutherford differential cross section, it has recently been updated with improved interaction physics. Transmission/reflection spectra and dose-depth profiles generated using this method has been benchmarked against both analog and condensed history calculations, and have shown an increase in computational efficiency. Moreover, this method may prove broadly applicable to any Monte Carlo simulation involving sufficiently forward-peaked probability distributions. Future work will integrate these methods into the Integrated TIGER Series (ITS) suite to analyze accuracy and performance enhancement in fully coupled photon-electron transport in realistic three dimensional (3-D) geometries.

1. Introduction

Monte Carlo simulation of energetic electron transport poses a computationally demanding problem. The Coulomb force mediates electron interactions over long ranges unlike the relatively simple discrete, binary interactions associated with neutral particle transport. Additionally, the total elastic and inelastic scattering cross sections for electrons are large, indicating short mean free paths (MFP), and the scattering differential cross section (DCS) is highly forward peaked, resulting in little to no energy transfer per scatter. Analog simulation of an electron transport requires thousands of collision events per history, most with minimal consequence. Producing statistically significant numbers of histories in complicated geometries would become prohibitively expensive in terms of runtime.

The condensed history (CH) method was developed as a practical alternative to such analog simulations.[1] While variations exist, the essence of the CH is to move the particle according to approximate spatial displacement algorithms based on infinite-medium multiple scattering angular distributions. This method has proven effective for realistic transport calculations; currently, CH is widely used in a number of production charged particle transport codes—ITS[2], EGS4[3], PENELOPE[4], MCNP[5]. However, this method is not without shortcomings. The method does not distinguish between path length and angular deflections are not distributed in accordance with any transport equation. CH boundary crossing always introduce some degree of approximation. In either case, the method must be altered to produce accurate results.

To mitigate the computational burden of analog simulation while maintaining its simplicity and without introducing the shortcomings of CH, the Generalized Boltzmann Fokker-Planck Method (GBFP) was developed. The GBFP method is a moment-preserving, modification of the analog method that creates a longer MFP and a less forward-peaked DCS by changing the scattering cross sections. These modifications begin with the transport equation itself,

$$\vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E)=\int_{4\pi}\sigma_{s,el}(\vec{r},\vec{\Omega}\cdot\vec{\Omega}',E)\psi(\vec{r},\vec{\Omega}',E)d\vec{\Omega}'+\int_0^\infty\sigma_{s,in}(\vec{r},E'\to E)\psi(\vec{r},\vec{\Omega},E')dE' - \left[\sigma_{s,el}(\vec{r},E)+\sigma_{s,in}(\vec{r},E)\right]\psi(\vec{r},\vec{\Omega},E), \quad (1)$$

where $\Psi(r, E, \Omega)$ is the angular flux of electrons at spatial location r traveling in direction $\mathbf{\Omega}(\mu, \theta)$ with energy E, $\sigma_{s,in}(r, E' \rightarrow E)$ is the differential inelastic electron

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scattering cross section, $\sigma_{s,el}(r, \Omega \cdot \Omega', E)$ is the elastic differential scattering cross section, and $[\sigma_{s,el}(r, E) + \sigma_{s,in}(r, E)]$ is the total scattering cross section. With the two scattering mechanisms separated, it is assumed that elastic scattering occurs without energy loss and inelastic scattering occurs without angular deflection, allowing for these discretizations to be addressed separately. For the ongoing discussion, we define momentum transfer moments of a DCS as,

$$\sigma_n \equiv 2\pi \int_{-1}^{1} d\mu_0 (1-\mu_0)^n \sigma_s\left(\vec{r}, \mu_0, E\right), \quad n = 1, 2, \ldots \quad (2)$$

Lewis theory[6] posits a direct correlation between preserving moments of the DCS and the accuracy of the model as measured by space-angle moments of the infinite medium solution. Unfortunately, truncated higher order Fokker-Planck expansions are asymptotic and unstable to truncation orders beyond Fokker-Planck. Higher-order moments cannot, therefore, be preserved by retaining only a finite number of terms in this expansion[7]. To constructing a transport equation that preserves low-ordered momentum-transfer moments in a stable manner, the GBFP method modifies the scattering cross sections. In practice, this can be achieved by preserving an appropriate number of momentum-transfer moments in conjunction with a strategy to construct a suitable scattering kernel. A brief discussion of the discrete and hybrid exponential scattering kernels[8–10] is presented in the following subsections.

1.1. Discrete

The discrete scattering kernel represents the approximate DCS as a superposition of discrete scattering angles as follows,

$$\tilde{\sigma}_s\left(\vec{r}, \mu_0, E\right) = \sum_{j=1}^{N} \frac{\alpha_j\left(\vec{r}, E\right)}{2\pi} \delta\left(\mu_0 - \xi_j\left(\vec{r}, E\right)\right) \quad (3)$$

The scattering amplitudes α_j and scattering cosines ξ_j are selected to preserve the first 2N momentum-transfer moments of the exact DCS. This constraint yields a nonlinear system for the α_j and ξ_j that can be solved using a robust algorithm by Sloan[11]. Despite the ease and potential accuracy of this approach, selection of a low number of discrete angles or use in an optically thin material can display ray-effects in transmitted and reflected angular distributions. In practice, these effects are rarely seen with four or more discrete angles. A scattering kernel devised to mitigate ray effects without affecting the moment-preserving feature of this approach is presented in the following subsection.

1.2. Hybrid Exponential

A completely continuous scattering kernel that preserves enough angular moments of the DCS can eliminate the ray-effects caused by discrete-angle scattering and rigorously preserve two momentum-transfer moments. The scattering kernel is composed of two parts, an exponential kernel and a screened Rutherford part, as follows,

$$\tilde{\sigma}_s\left(\vec{r}, \mu_0, E\right) = \frac{\sigma_0\left(\vec{r}, E\right)}{2\pi} \frac{2\eta(\eta+1)}{\left(1-\mu_0+2\eta^*\right)^2} + \frac{A\left(\vec{r}, E\right)}{2\beta\left(\vec{r}, E\right)} \exp\left[\frac{1-\mu_0}{2\beta\left(\vec{r}, E\right)}\right] \quad (4)$$

The modified screening parameter, η^*, is chosen to yield an appropriately long MFP and a smooth angular distribution. The parameters A and β are calculated from the residual cross section moments. Clearly, the structure of this method was motivated by the nature of the screened Rutherford DCS; however, it may remain adequately robust to model the adjusted physics.

2. Computational Methods

The GBFP methods were developed using the screened Rutherford interaction model. Screened Rutherford DCS is expressed in the compact, integrable, analytic form,

$$\sigma_{SR}\left(\mu_0\right) = \frac{C\left(E\right)}{\left(1-\mu_0+2\eta\right)^2} \quad (5)$$

where C(E) is an amplitude prescribed by the electron's energy, μ is the scattering cosine and η is a screening parameter. Furthermore, the screening parameter can be expressed as a function of energy and the atomic number of the scattering medium. The entire DCS can be expressed in a closed form with knowledge of only the energy and medium. While the screened Rutherford DCS contains the salient features of an electron scattering (i.e., large magnitude, highly forwards peaked), it excludes the spin and relativistic effects of the electron. Mott cross sections extend the screened Rutherford cross sections to include these effects. A factorization of the Mott cross section model[12] as a function of scattering cosine, μ, is given by,

$$\sigma_{Mott}\left(\mu_0\right) = \sigma_{Ruth}\left(\mu_0\right) K_{Scr}\left(\mu_0\right) K_{Rel}\left(\mu_0\right) \quad (6)$$

In this expression, the final term, $K_{rel}(\mu_0)$, represents the Mott-to-Screened Rutherford ratio. No simple expression typifies this ratio. Rather, tabulated numerical data of the Mott-to-Screened Rutherford ratio at five scattering cosines are fit with a series expansion of the form,

$$K_{Rel}(\mu_0) = \sum_{j=1}^{5} h_j \cdot (1 - \mu_0 + 2\eta)^{j-1} + \chi(E) \cdot (1 - \mu_0 + 2\eta)^{\frac{1}{2}} \qquad (7)$$

where again η is the screening parameter, χ(E) is a known function of energy and the h_j values are energy-dependent fitting parameters that make $K_{rel}(\mu_0)$ exact at all five tabulated values. A plot of this ratio for gold is shown in Figure 1 across a wide range of energies.

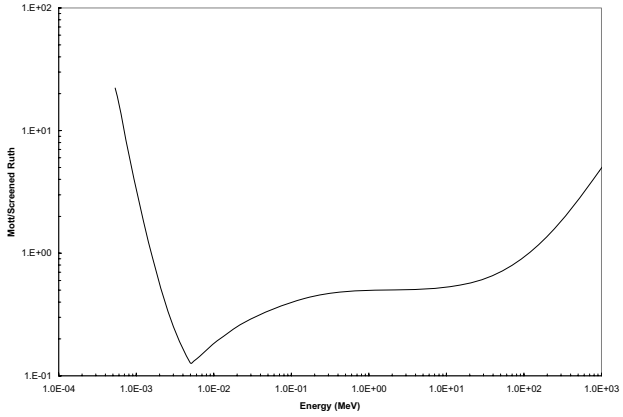

Figure 1. Ratio of Mott to Screened Rutherford Total Cross Sections versus Energy for Gold

Inserting Eq. 7 into Eq. 6 gives an analytic expression for the Mott DCS. The order of this expression did not permit direct sampling, so an analog Mott sampling algorithm was developed. The Mott DCS expression was integrated over scattering cosine to yield a cumulative distribution function (CDF). To sample the angular distribution from the Mott scattering kernel, we used the Newton-Raphson root finding method on the expression,

$$CDF(\mu_i) - \xi = 0 \qquad (8)$$

where μ_i is the current iterate of the scattering cosine and a ξ is a random number uniformly distributed on [0,1]. Momentum-transfer moments of the Mott DCS were generated numerically using the XGEN code.

To verify the versatility and accuracy of the GBFP method we used a test problem of a 1 MeV beam of electrons impinging on 0.04 cm of gold, tracked to a cutoff energy of 10 keV. Three simulations were run: discrete angles, hybrid exponential, and analog. Eight discrete angles were used (16 moments preserved). The analog results were used to benchmark the accuracy of the GBFP Method with improved physics. Dose-depth plots and transmission angular density tallies were generated in this test case using the discrete angle, hybrid exponential and analog scattering kernels after 10^7 histories.

3. Results

The analog algorithm used in this study, is roughly 6 times slower than the discrete angles scattering kernel and 2.5 times slower than the hybrid exponential scattering kernel. In the simulation, the GBFP methods show excellent agreement with the analog benchmark. As shown in Figures 2 and 3.

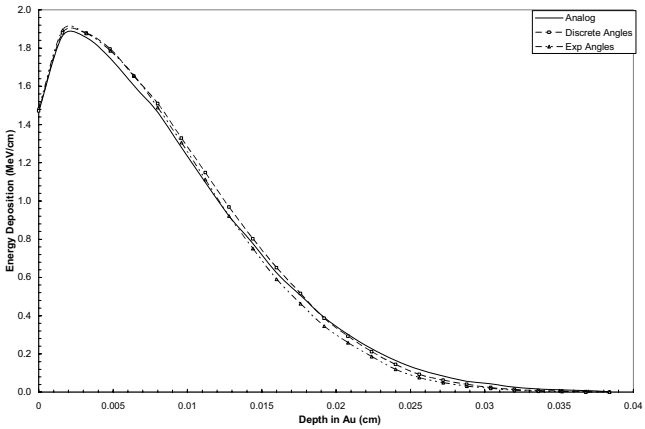

Figure 2. GBFP energy deposition profile of 1 MeV e^- in 0.04 cm Gold

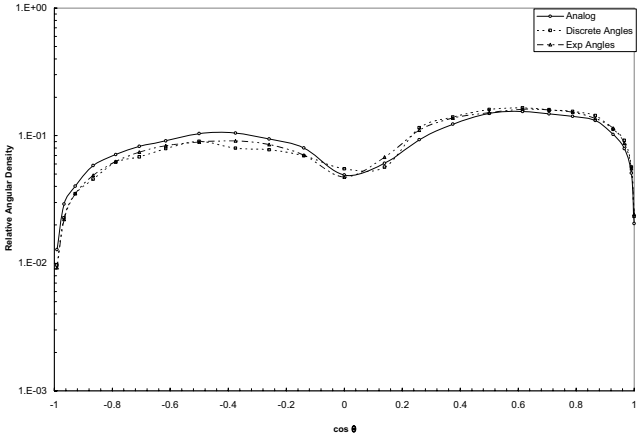

Figure 3. Transmission angular density of 1 MeV e^- on 0.004 cm Au

4. Conclusions/Future Work

This work has helped to verify the accuracy and robust nature of the GBFP method for charged particle transport. While developed using the simple screened Rutherford scattering cross section model, the method appears to depend only on the momentum-transfer moments of the DCS used, and is impervious to interaction model. A GBFP feature will be included into the electron tracking physics of future versions of the Integrated TIGER Series (ITS) suite, a coupled electron-

photon transport code capable of tracking on realistic, 3-D geometries.

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