A Generalized Boltzmann Fokker-Planck Electron Transport Method

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We present a transport-based method for electrons that incorporates the correct transport mechanics and is computationally efficient for implementation in single event Monte Carlo codes. The method yields accurate dose profiles across a broad range of energies in heterogeneous media and presents a viable alternative to the established condensed history method. Our approach is mathematically rigorous, building on higher order Fokker-Planck and Boltzmann Fokker-Planck representations of the scattering process, and we accordingly refer to it as a Generalized Boltzmann Fokker-Planck (GBFP) approach. We postulate the existence of single collision scattering distributions (differential cross sections) and impose the constraint that the first few momentum transfer moments be identical to corresponding analog values. Details of specific moment-preserving strategies are described. Results are presented for dose in heterogeneous media due to a pencil beam of monoenergetic electrons. The computational efficiency of our GBFP formulations are contrasted against two different condensed history implementations.

Introduction

The condensed history method (Berger, 1963) has long been used for electron transport calculations, and the theoretical basis of the method has been extensively evaluated (Larsen, 1992; Kawrakow and Bielajew, 1998). Condensed history has proven to be an effective approach for modeling realistic transport problems. However, it is known to have some deficiencies, such as inaccuracy near material boundaries and not distinguishing between pathlength and displacement. Several "fixes" have been implemented but the fact remains that the algorithm is often fundamentally altered in order to circumvent the inherent shortcomings. In recent years several methods have been proposed as alternatives to the condensed history technique (Tolar and Larsen, 2001; Pomraning, 1996; Prinja and Pomraning, 2001; Leakeas and Larsen, 2001). A common feature of these methods is that an approximate transport problem is solved,

characterized by a longer mean free path and a less forward peaked differential cross section than analog values. These approximate schemes differ in the strategies employed to construct model cross sections but a hallmark of all approaches is that accuracy can be systematically increased by retaining increasingly more accurate physics; indeed several of these methods limit to analog accuracy. Moreover, the correct transport mechanics is naturally accommodated with the use of an explicitly linear transport (Markovian) formulation as the physical and mathematical basis of the approach. In particular, with Poisson collision statistics, the new algorithms handle material and vacuum interfaces naturally. That is, no alteration of the tracking algorithm is necessary for boundary crossings. All of these features combine to make computationally efficient single event Monte Carlo simulation feasible for charged particles in general and electron transport in particular.

Theoretical analysis shows that sensitivity of the transport process to elastic scattering is well captured by angular moments of the underlying differential cross section, specifically the generalized momentum transfer moments. It is well known, for instance, that if scattering is sufficiently forward peaked the Boltzmann scattering operator can be approximated by the angular diffusion or Fokker-Planck (FP) operator with the diffusion coefficient given by the transport cross section, which is just the first momentum transfer moment. Moreover, it has been shown that large scattering-angle effects can be incorporated using higher order Fokker Planck expansions and this essentially amounts to an expansion in higher order momentum transfer moments. However, truncated higher order FP expansions are not mathematically stable and the challenge is to construct equivalent Boltzmann collision operators that possess the same generalized FP expansion up to a finite order as the analog case. This can be achieved in practice by preserving an appropriate number of momentum transfer moments in conjunction with a strategy to construct a suitable scattering kernel. Here we demonstrate a number of such strategies which prove computationally efficient and accurate for energetic electron transport. Our approach builds on higher order Fokker-Planck and Boltzmann Fokker-Planck representations of the scattering process, and we accordingly refer to it as a Generalized Boltzmann Fokker-Planck (GBFP) approach.

Various strategies are presented in the next section and their numerical implementation for a heterogeneous medium are later demonstrated. The accuracy of the methods is assessed using analog benchmark calculations. We present a comparison of computational efficiencies of the GBFP methods and condensed history methods. We do not consider inelastic scattering in this paper and use the continuous slowing down (CSD) approximation to simplify the comparison of our GBFP and condensed history angular scattering algorithms. The GBFP approach to inelastic scattering has been considered elsewhere (Prinja and Harding, 2003; Franke and Prinja, 2005) and is independent of the elastic scattering approximation.

GBFP Angular Scattering Models

The angular flux $\Psi(\boldsymbol{r},E,\boldsymbol{\Omega})$ of electrons at spatial location $\boldsymbol{r}(x,y,z)$ traveling in direction $\boldsymbol{\Omega}(\mu,\theta)$ with energy E satisfies the following transport equation,

(1)

where $\sigma_s(\mathbf{r},E)$ is the total electron scattering cross section, $\sigma_s(\mathbf{r},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}',E)$ is the differential scattering cross section and $S(\mathbf{r},E)$ the material stopping power. The true differential cross section (DCS) for electron scattering is highly peaked about $\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'\equiv\mu_0=1$ while the corresponding total scattering cross section is large. As a consequence, this analog problem is computationally very expensive when implemented in single event Monte Carlo. For the following discussion, we define momentum transfer moments of the elastic DCS as

(2)

The essence of our method is to replace the analog DCS by an approximate DCS, such that the associated momentum transfer moments are identical to the exact moments for n = 1, 2, …N, where N is arbitrary but finite. All higher moments, as well as σ_0, are approximated in terms of these N moments. By not rigorously preserving all momentum transfer moments we are modeling a scattering process with a longer mean free path (mfp) than the actual mfp and a less peaked angular-scattering distribution. On the other hand, *strictly* preserving a number of low-order moments should ensure some measure of accuracy. This approach is motivated in part by Lewis theory (Lewis, 1950), which demonstrates 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, and in part by the effectiveness of moment-preservation in Generalized Fokker-Planck expansions (Pomraning, 1996; Prinja and Pomraning, 2001; Leakeas and Larsen, 2001).

We have implemented this method with several forms of the approximate DCS: purely discrete scattering angles (Franke and Prinja, 2002a), a discrete scattering angle hybridized with a smooth screened Rutherford kernel (Franke and Prinja, 2002b), and an exponential scattering distribution hybridized with a smooth screened Rutherford kernel (Prinja and Franke, 2004). We briefly describe each of these scattering kernels in the following subsections.

Discrete

Perhaps the simplest approach, conceptually and practically, is to represent the approximate DCS as a superposition of discrete scattering angles, as follows:

(3)

The scattering amplitudes α_n and scattering cosines ξ_n are then constrained to yield the exact first 2N momentum transfer moments as given by Eq. (2). This condition yields a nonlinear algebraic system for the α_n and ξ_n that can be solved using a robust algorithm by Sloan (1983). Discrete angle representations were first introduced in neutral particle transport in the MORSE code (Straker et al., 1970) and the idea was subsequently extended by Sloan (1983) and Morel et al. (1996) for peaked scattering. This approach,

while easy to implement and potentially very accurate, displays ray-effects in transmitted and reflected angular distributions when few discrete angles are used and when the material is optically thin. The next two sections describe methods devised to mitigate ray-effects without affecting the moment-preserving feature of this approach.

Hybrid Discrete

Ray-effect mitigation in the discrete scattering-angle formalism can be realized by the superposition of a continuous in angle, or smooth, component that has a long associated mean free path, is not forward peaked, and is easy to sample from. Furthermore, by requiring the large scattering angle shape and amplitude of this smooth component to be close to the corresponding analog cross section, the higher angular moments will be accurately captured. For the screened Rutherford DCS this decomposition into discrete and smooth components can be effected as follows:

(4)

The first term is just the screened Rutherford scattering kernel (Evans, 1976) but with η^* chosen to yield a long mfp and hence a smooth angular distribution. The second term is the discrete scattering-angle model discussed in the previous section. The choice of η^* is somewhat arbitrary, providing that it is larger than the analog value. A larger value of η^* produces a greater speed-up but is more approximate. The strategy we have adopted is to select this parameter to give a smooth component mean free path that is related to the step size in condensed history methods. Once η^* is thus chosen, the discrete scattering cosines and amplitudes are calculated by preserving the residual cross section moments. Numerical testing has shown that ray-effects with just one discrete component are greatly reduced with the addition of a continuous component.

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. We have shown using a Generalized Fermi expansion (Prinja and Franke, 2004) that a kernel based on exponentials can rigorously preserve angular moments while remaining robust. Our specific numerical implementation has included a single exponential, which exactly preserves the first two momentum transfer moments, and an exponential kernel hybridized with the smoothed Rutherford part to capture both forward-peaked and large-angle scattering components. The latter decomposition can be expressed as:

(5)

As with the hybrid discrete kernel, 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.

Computational Methods

The computational results presented here are obtained with restricted physics both for simplicity of implementation and to isolate the effects of the angular scattering algorithms being tested. Thus, no secondary photons or electrons are simulated, a continuous-slowing-down (CSD) approximation is used in all calculations, and analog angular scattering is modeled using the screened Rutherford scattering model (Evans, 1976). The energy dependence of the simulation is accomplished by defining physical parameters on an energy grid. These parameters are generated by the XGEN cross section generating code (Halbleib et al., 1992).

The method we label as "ITS-like" condensed history applies the multiple-scattering angular deflection of the particle at the end of each step, i.e. the end of the pathlength for which the angular deflection has been precomputed. The algorithm differs from the implementation in the ITS codes in that: our angular distribution is based only on screened Rutherford scattering and ignores inelastic scattering angular deflection; we sample from the precomputed angular deflection distribution nearest in energy to the particle energy when the angular deflection is applied; and we have implemented a simpler (and less accurate) material boundary crossing algorithm. These modifications simplify the implementation and provide a consistent basis for comparison with the analog calculations and GBFP methods. The same simplifications apply to the "Random Hinge" condensed history algorithm. It differs from the ITS-like algorithm only in that the angular deflection of the particle is applied at a uniformly sampled random position within each step.

There are many intricate algorithms that have been proposed to cope with the boundary crossing problem in condensed history methods [see Jensen (1988), for example]. We have implemented an admittedly simple boundary crossing algorithm. When a material interface is encountered in GBFP or analog transport, the sampled distance-to-collision is scaled by the ratio of the total cross sections in the two materials, such that the distance is preserved as measured in mean free paths. This is the correct transport treatment. When a material interface is encountered in condensed history, we preserve the fractional step-size remaining between the two materials. This is an approximation for the condensed history algorithms.

Results

To test the methods described in this paper and to compare their efficiencies against condensed history methods, two problems have been simulated. Both consist of a pencil beam normally incident on a block of material with a second material, with a higher atomic number (Z) and higher density, inserted through half of the block, such that the material interface is aligned with the incident beam. In the first case, illustrated in Fig. 1(a), we simulated 10 MeV electrons incident on a block of water with a slab of cortical bone included. In the second case, illustrated in Fig. 1(b), we simulated 200 keV electrons incident on a block of silicon with a slab of gold included.

Figure 1. The problem geometries for (a) a high-energy beam on low-Z materials and (b) a low-energy beam on higher-Z materials.

The dose distributions for the two problems were calculated with each of the approximate scattering kernels and with the analog scattering kernel. The dose was integrated through the block in the X dimension (such that the effect of the material interfaces can be observed). The dose distributions for the analog benchmark calculations are shown in Fig. 2. The energy deposition in these plots is shown in keV per gram per source electron. The normalization by density accounts for the lowered deposition values in the gold region of Fig. 2(b). The difference in density between water and bone is not large enough to produce such a visible discontinuity in Fig. 2(a).

(a) (b)

Figure 2. Benchmark dose distributions in keV/g calculated with analog elastic scattering for (a) a high-energy beam on low-Z materials and (b) a low-energy beam on higher-Z materials.

Efficiency

A suite of calculations was performed with each of the approximate scattering kernels by varying a parameter that affects the mean distance between interactions. For the condensed history methods, the step length was varied. For the hybrid discrete and hybrid exponential kernels, the mean free path of the smooth screened Rutherford component was varied. For the discrete scattering-angle kernel, the number of discrete angles was varied (unlike the other kernels, this does not vary continuously). Shorter mean distances between interactions produce increased computational expense of the calculations and are expected to increase the accuracy. For each of these approximate calculations, the distribution of the error in the dose was calculated relative to the analog calculation. Here, we examine the efficiency of the methods by evaluating the accuracy of the method versus the computational expense.

For the geometries discussed in the previous section and illustrated in Fig. 1, the error versus runtime is displayed in Fig. 3. While the results shown are informative, we offer two points of caution. We have chosen to measure error as an L_2-norm of the relative error over the entire problem geometry. Other measures of error are possible, which could

emphasize different aspects of the solution or give different weightings to the errors. Also, the runtime comparisons presented here should be considered approximate. Undoubtedly, some algorithmic improvements could be made to accelerate each of the implementations, and runtime variations would be experienced with different compilers or computer architectures.

(a) (b)

Figure 3. The L_2-norm of the relative error of approximate methods versus computation time for (a) a high-energy beam on low-Z materials and (b) a low-energy beam on higher-Z materials.

In assessing error and runtime there are factors that we have attempted to remove. To obtain detailed dose results, particles were tracked through a Cartesian tally grid, and this tracking was the dominant fraction of runtime for the faster calculations. In a production implementation of the methods, it would not be necessary to track particles on the refined grid on which dose is being tallied. Therefore, the runtimes presented are for calculations that omit the detailed tally grid. Instead runtimes are based on identical calculations with minimal geometry boundaries for defining the problem. In assessing the error of the methods there is statistical uncertainty in both the analog benchmark and approximate results. This statistical uncertainty is the dominant factor in the relative difference between the two dose distributions for the more accurate calculations. Using two independent analog benchmark calculations, we have estimated the contribution of statistical uncertainty to the calculation of the L_2-norm of the relative difference and subtracted it from all results. For the high-energy, low-Z problem, this statistical uncertainty factor was $1.434\times10^{-2} \pm 4.2\times10^{-4}$. For the low-energy, high-Z problem, this statistical uncertainty factor was $6.52\times10^{-3} \pm 7.3\times10^{-4}$.

The important sources of error can be discerned by studying the individual error distributions. These results are too numerous to include here, but we offer a few samples and some general observations that can be made. In Fig. 4, we show the relative difference between approximate and benchmark results for the high-energy, low-Z problem. (We define the relative difference as one minus the ratio of the approximate result to the analog benchmark result.) The four results shown are for four different methods, with each approximate calculation requiring about 2000 seconds.

Figure 4. Relative error in approximate methods with comparable runtimes for the high-energy, low-Z problem using (a) hybrid discrete GBFP, (b) hybrid exponential GBFP, (c) random hinge condensed history, and (d) ITS-like condensed history.

We observe that in all of the methods there are significant errors at the bottom of the

block as the beam initially penetrates the material and disperses. This source of error is smallest for the random hinge and greatest for the ITS-like algorithm, with the errors in the GBFP methods falling in between for comparable runtimes. In all cases, these errors are due to overestimation of the uncollided flux, manifested as overestimation of the dose by the approximate method along the central axis of the beam and underestimation of the dose at the periphery of the beam.

In Fig. 5, we show the relative difference between approximate and benchmark results for the low-energy, high-Z problem. The four results shown are for four different methods, with each approximate calculation requiring about 20000 seconds. In this second problem, with weakly anisotropic scattering, similar errors due to overestimation of the uncollided flux were observable in all methods. However, the error for the condensed history results was dominated by error in the gold region of the problem. It is not clear whether this is due to difficulty modeling the weak anisotropy of scattering in the gold, due to the error introduced by the material interface, or due to a combination of the two effects.

Figure 5. Relative error in approximate methods with comparable runtimes for the low-energy, high-Z problem using (a) hybrid discrete GBFP, (b) hybrid exponential GBFP, (c) random hinge condensed history, and (d) ITS-like condensed history.

By the measures presented here, the random hinge and hybrid discrete kernels generally look most appealing, and the ITS-like method generally looks least appealing. However, no single kernel performs best in all circumstances.

Conclusions

The GBFP methods offer computational efficiency comparable to the widely-used random hinge condensed history method. The weaknesses of condensed history methods include approximation near material interfaces and, for the ITS-like algorithm, underestimation of reflected electrons. Unlike condensed history methods, the GBFP methods remain accurate and retain algorithmic simplicity in the presence of material interfaces. The weakness of the GBFP methods is overestimation of the uncollided (and few-collided) flux at shallow depths. Just as strategies have been developed to compensate for the weaknesses of condensed history methods, strategies may be developed to mitigate this weakness of the GBFP methods. The contrasting strengths and weaknesses of the two electron transport strategies may make one or the other more appropriate for a given class of problems. The accuracy and efficiency of the GBFP method makes it a viable alternative to condensed history methods.

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