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Innovative Electron Transport Methods in EGS5

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Abstract

The initial formulation of a Monte Carlo scheme for the transport of high-energy ($>\approx 100$ keV) electrons was established by Berger in 1963. Calling his method the "condensed history theory", Berger combined the theoretical results of the previous generation of research into developing approximate solutions of the Boltzmann transport equation with numerical algorithms for exploiting the power of computers to permit iterative, piece-wise solution of the transport equation in a computationally intensive but much less approximate fashion. The methods devised by Berger, with comparatively little modification, provide the foundation of all present day Monte Carlo electron transport simulation algorithms. Only in the last 15 years, beginning with the development and publication of the PRESTA algorithm, has there been a significant revisitation of the problem of simulating electron transport within the condensed history framework. Research in this area is ongoing, highly active, and far from complete. It presents an enormous challenge, demanding derivation of new analytical transport solutions based on underlying fundamental interaction mechanisms, intuitive insight in the development of computer algorithms, and state of the art computer science skills in order to permit deployment of these techniques in an efficient manner. The EGS5 project, a modern ground-up rewrite of the EGS4 code, is now in the design phase. EGS5 will take modern photon and electron transport algorithms and deploy them in an easy-to-maintain, modern computer language—ANSI-standard C++. Moreover, the well-known difficulties of applying EGS4 to practical geometries (geometry code development, tally routine design) should be made easier and more intuitive through the use of a visual user interface being designed by Quantum Research, Inc., work that is presented elsewhere in this conference. This report commences with a historical review of electron transport models culminating with the proposal of a new, previously unpublished algorithm, for the EGS5 project.

1 Introduction

Berger's founding paper[1], *Monte Carlo Calculation of the penetration and diffusion of fast charged particles,* ushered in the modern era of electron transport in Monte Carlo applications. The principle difficulty in applying the Monte Carlo method to electron transport lies in the fact that electrons interact frequently until their kinetic energy is exhausted. A relativistic electron may have 10^4–10^5 elastic interactions and 10^5–10^6 inelastic interactions before falling to an energy so low that it stops ionizing or exciting atoms individually or collectively in the material through which it is being transported. Clearly, it was not feasible to model all of these interactions in an analog Monte Carlo code in the early 1960's, the era when Berger issued his famous report[1]. To overcome this difficulty, Berger devised the "condensed history theory" (CHT). The CHT gathers together many elastic and

[1]Analog calculations are feasible today only in 1D geometries and are used, primarily, to study the physics of multiple interactions. Analog calculations are not feasible for many applications requiring 3D geometries or applications that may require millions or billions of primary source particles.

inelastic interactions into "virtual" interactions, permitting efficiency gains of up to 3 or 4 orders of magnitude.

The computational speed-up achieved with Berger's CHT is impressive, but comes at a cost. The electron transport becomes approximate! Consider, for example, an electron initially positioned at the origin, $\vec{x} = \vec{0}$, directed along the $\vec{z}$-axis with some initial energy E_0. This electron is to be moved a total prescribed pathlength of some distance, say, t. For the moment, the method we adopt to choose t is not pertinent to the discussion[2]. Let us now ask, after the electron is transported a distance t, where will its path terminate? The only thing we can say with absolute certainty is that its path will terminate at some position $\vec{x}$, such that $\vec{x} \leq t$. The direction of the electron will be (Θ, Φ)'s selected from an elastic multiple scattering theory and the electron will have a lower energy, E, determined from an inelastic multiple scattering theory. The final position of these electrons should look something like the depiction in figure 1. Because of the energy dependence of the differential scattering cross

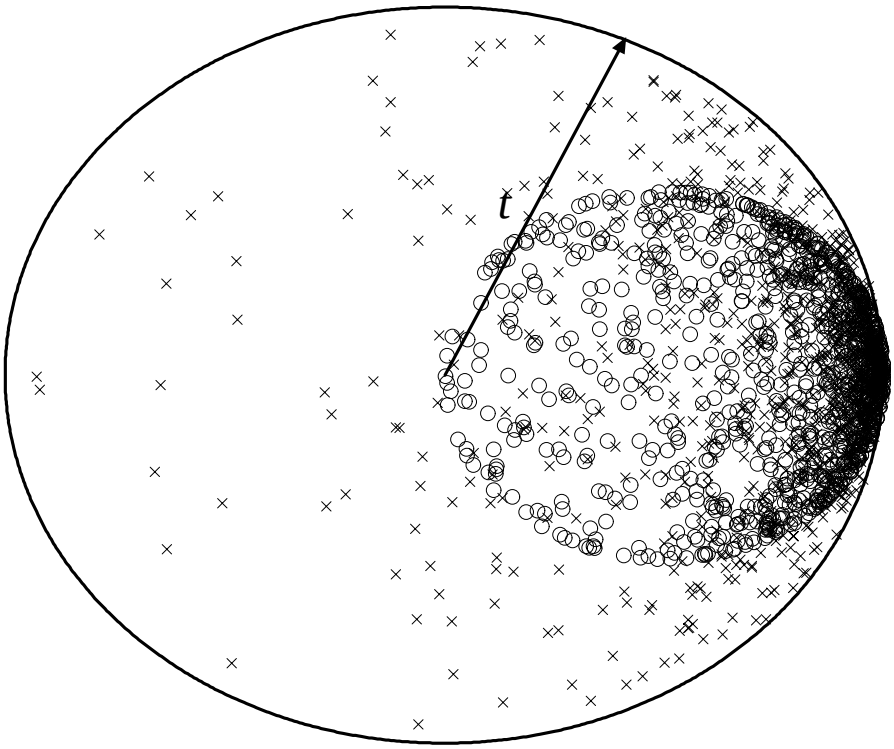

Figure 1: The termination points of 1000 electrons starting at the origin, $\vec{x} = \vec{0}$, directed along the $\vec{z}$-axis, and transported a total pathlength t.

section, the distribution that one observes depends on the energy of the electron. At high energies where the elastic scattering is forward directed, there is a strong clustering of the endpoints in the forward direction with a few electrons scattered widely and even fewer that terminate in the reverse hemisphere. At lower energies where the scattering becomes more isotropic, the sphere gets populated more uniformly.

[2]The distance t is usually chosen to satisfy a number of constraints: 1) t is the distance to a discrete event, like a Møller or bremsstrahlung interaction, 2) t is small enough so that the energy of the electron over the pathlength is approximately constant, 3) t is small enough so that the determination of the scattering angle is accurate.

2 Transport Mechanics

Given an elastic scattering cross section of arbitrary form and ignoring energy losses along the transport step, the directions of the electrons after a pathlength t is known exactly from the multiple scattering theory of Goudsmit and Saunderson[2, 3] or Lewis's adaptation[4], assuming that the electron loses energy continuously (an approximation in itself that only applies at high energies). Other successful multiple scattering theories make assumptions which are rigorously applicable only for small angles, for specific forms of the elastic cross section, or for a restricted range of t[5, 6, 7, 8, 9, 10, 11]. While the direction is well characterized, the ending position is not. Indeed, there is very little theoretical development along these lines and that which exists is not accurate enough for general-purpose Monte Carlo. Therefore, we must "invent" a scheme to give a recipe for where to place the electron at the end of the step and how to deduct energy losses. These schemes have come to be known as "transport mechanics".

Although transport theory solutions derived from the Boltzmann equation directly have not been successful in predicting the coupled space-angle-energy distributions, they do provide expressions for the moments of spatial distributions and the couplings of moments between space and angle which may be evaluated easily, independent of the form of the scattering cross sections employed. This development, attributed to Lewis[4], may be employed to evaluate a mechanics scheme once it is devised. In addition, Larsen has developed an analysis[12] that predicts the convergence rate of a mechanics scheme compared to the solution obtained by analog (event-by-event) simulation. The dependence of Monte Carlo tallies on electron step-size is known as "step-size dependence" and is a function of the nature of the tally, the mechanics scheme employed and the treatment of electron transport in the vicinity of interfaces where the interaction cross sections or densities change[13, 14]. It should be mentioned that Larsen convergence requires that the multiple elastic scattering scheme be robust (exhibit no numerical or physical artifacts) as the pathlength is reduced to zero. This limit is problematic for both the original implementations of Goudsmit-Saunderson theory[2, 3] and Moliére theory[5, 6], although the difficulties with both these theories have now been treated successfully[10, 11].

2.1 ETRAN, ITS, MCNP

Berger[1] recommended the following scheme for determining the position of the endpoint of a transport step:

$$\begin{aligned} x + iy &= \frac{t}{2}\left(\sin\Theta e^{i\Phi} + k\sqrt{\frac{\langle\cos^2\Theta\rangle}{6}}\right) \\ z &= \frac{t}{2}(1+\cos\Theta) \end{aligned} \tag{1}$$

where $\Re(k)$ and $\Im(k)$ are two independent random numbers selected according to a Gaussian distribution with zero mean and unit variance. This scheme (and those that follow) assume that the electron starts off at the origin and is initially directed along the $\vec{z}$-axis. We generalize to other starting positions and orientations through 3D translation and rotation.

However, the above scheme has not been implemented in ETRAN[15, 16]. Instead, the simple and practical scheme $\vec{x} = t\hat{z}$ is employed. That is, the electron is placed on the sphere along the line of its initial direction and is then deflected according to the theory of Goudsmit and Saunderson[2, 3]. The energy is considered constant along the pathlength and an energy loss mechanism, the theory of Blunck and Leisegang[17], an adaptation of Landau theory[18], is applied. The ITS Monte Carlo code[19, 20, 21] and the MCNP Monte Carlo code[22, 23, 24] use the same mechanics scheme as ETRAN.

2.2 EGS4, PRESTA

The EGS4 Monte Carlo code[25, 26, 27] employed a small variation on the ETRAN theme. The EGS4 mechanics is expressed as $\vec{x} = f(t, Z, E)t\hat{z}$ where the function $f(t, Z, E)$ is called a pathlength or detour correction. The idea behind this scheme comes from the recognition that the forward penetration distance z must be shorter than t. An approximate theory based upon the developments of Yang's[28] adaptation of Fermi-Eyges theory[29] is employed. It has subsequently been shown that the amount of correction applied by this method over-predicts by a factor of about two[30], one of the motivating reasons for the development of the Parameter Reduced Electron-Step Transport Algorithm (PRESTA)[30, 14].

PRESTA's mechanics scheme can be summarized as:

$$\begin{aligned} x + iy &= \frac{t}{2} \sin\Theta e^{i\Phi} \\ z &= tf'(t, Z, E) \ , \end{aligned} \tag{2}$$

which introduces a more robust detour correction, $f'(t, Z, E)$, and a lateral transport that is correlated to the angle, as suggested by Berger[1].

2.3 PENELOPE

Primarily intended to address the problems of low-energy electron transport (1 keV $< E <$ 100 keV) but suitable for applications up to 1 GeV, the PENELOPE (PENetration and Energy LOss of Positrons and Electrons) code[31, 32, 33] is a relatively new arrival on the $e^{\pm}\gamma$ Monte Carlo scene. PENELOPE's mechanics can be expressed as:

$$\begin{aligned} x + iy &= tr \sin\Theta e^{i\Phi} \\ z &= t[(1 - r) + r\cos\Theta(t)] \end{aligned} \tag{3}$$

where r is a random number sampled uniformly on $[0, 1]$. This mechanics is also known as the "random hinge" because it can be visualized as a hinge (deflection) placed randomly along the track. For very low computational cost, indeed fewer calculation than the Berger 1963 or PRESTA mechanics, the random hinge fills in the entire transport sphere realistically and demonstrates superior performance with respect to the Lewis moments[34]. The PENELOPE mechanics also is the only method which has the property $\langle\vec{x}(\Theta = \pi)\rangle = \vec{0}$, a property that can be derived from a Lewis-like moments analysis but without integrating over the scattering angle[35].

2.4 PRESTA-II, EGSnrc

It takes a great deal of computational effort to improve upon the PENELOPE mechanics. The PRESTA-II mechanics[36, 37, 38] now incorporated into the latest National Research Council release of EGS4 called EGSnrc[39] has adopted the following scheme:

$$\begin{aligned} x &= t\left[\left(\frac{1}{3} + \delta\right)\sin\theta_1\cos\phi_1 + \left(\frac{1}{3} - \delta\right)\sin\theta_2(\cos\phi_1\cos\phi_2 - \cos\theta_1\sin\phi_1\sin\phi_2) + \frac{1}{6}\sin\Theta\cos\Phi\right] \\ y &= t\left[\left(\frac{1}{3} + \delta\right)\sin\theta_1\sin\phi_1 + \left(\frac{1}{3} - \delta\right)\sin\theta_2(\sin\phi_1\cos\phi_2 + \cos\theta_1\cos\phi_1\sin\phi_2) + \frac{1}{6}\sin\Theta\sin\Phi\right] \\ z &= t\left[\frac{1}{6} + \left(\frac{1}{3} + \delta\right)\cos\theta_1 + \left(\frac{1}{3} - \delta\right)\cos\theta_2 + \frac{1}{6}\cos\Theta\right] \ , \end{aligned} \tag{4}$$

where the final direction implied by (Θ, Φ) corresponding to a pathlength t is formed from the vectorial sum of two $t/2$ scatterings (both from the original forward direction), (θ_1, ϕ_1) and (θ_2, ϕ_2). The factor δ is chosen[34] to make the spatial-angular moments conform closely to the predictions of Lewis[4]. Note that this technique requires two samples of the multiple scattering angular distribution and two rotations. Additionally, the EGSnrc implementation randomizes the fixed 1/3, 1/6 step fractions

according to a recipe that can be found in the reference[39]. PENELOPE's random hinge iterated twice appears to perform as well, although a moments analysis of a two-step random hinge has not been undertaken.

The PRESTA-II mechanics adds an important new physical feature. The final direction implied by (Θ, Φ) and the final direction with respect to the starting point $\vec{x}/|\vec{x}|$ are now decoupled, as physically they should be. (They are strongly correlated but not rigidly coupled.)

2.5 An extension to PENELOPE's mechanics

The PRESTA-II mechanics removes the rigid coupling between the direction and position vector, but requires two samplings of the multiple scattering angle, which is typically the most computationally costly part of the transport algorithm. Moreover, the five moments $\langle z \rangle$, $\langle x \sin\Theta \cos\Phi + y \sin\Theta \sin\Phi \rangle$, $\langle z \cos\Theta \rangle$, $\langle x^2 + y^2 \rangle$, and $\langle z^2 \rangle$ can not all be perfectly preserved by the PRESTA-II/EGSnrc scheme. A new mechanics scheme has been found[40] which does have all these features and requires only one sampling of the multiple scattering angle. This scheme takes the form:

$$\begin{aligned} x + iy &= t[fr \sin\Theta e^{\Phi_1} + \sigma \cos\Theta e^{\Phi_2}] \\ z &= t[k(1-r) + c + (kr + d)\cos\Theta] \ , \end{aligned} \tag{5}$$

where the five constants f, σ, k, c, d can be fixed so as to reproduce the above five moments exactly. This improvement in moment compliance is obtained with only a single sampling of the multiple-scattering angle, although there are two azimuthal angle samplings (which are relatively inexpensive). However, in initial tests of this extension to PENELOPE's mechanics, there appears to be no advantage to using the extension over a double sampling of PENELOPE's simpler scheme, either from the standpoint of computational efficiency or compliance with higher order moments.

2.6 EGS5 mechanics

Given that the simpler PENELOPE mechanics, when sampled twice appears to be more useful either the PRESTA-II/EGSnrc or extended PENELOPE mechanics, we have decided to adopt the PENELOPE mechanics with a new extension which accounts for energy changes to first order in an elegant way. The algorithm is best expressed in the followed pseudo-code:

1) SAMPLE two uniformly distributed random numbers, r_1 and r_2.

2) IF $r_1 < r_2$ **THEN:**

1. Transport the electron in the forward direction a distance $r_1 t$ assuming that the energy is constant $E = E_0$, the energy at the beginning of the step.
2. Deduct energy according to some energy loss model as if it had gone the complete step. The electron now has energy $E = E_0 - \Delta(E_0, t)$. Note that the energy loss model depends on the energy of the electron at that point.
3. Transport the electron in the forward direction a distance $(r_2 - r_1)t$ assuming that the energy is constant at the revised energy.
4. Deflect the particle by sampling from the multiple scattering angular distribution assuming that it has gone the full step t at the revised energy $E = E_0 - \Delta(E_0, t)$.
5. Transport the electron in the new direction a distance $(1 - r_2)t$ assuming that the energy is constant at the revised energy.

3) ELSE:

1. Transport the electron in the forward direction a distance $r_2 t$ assuming that the energy is constant $E = E_0$, the energy at the beginning of the step.

2. Deflect the particle by sampling from the multiple scattering angular distribution assuming that it has gone the full step t at the starting energy $E = E_0$.
3. Transport the electron in the forward direction a distance $(r_1 - r_2)t$ assuming that the energy is constant at the starting energy.
4. Deduct energy according to some energy loss model as if it had gone the complete step. The electron now has energy $E = E_0 - \Delta(E_0, t)$.
5. Transport the electron in the new direction a distance $(1 - r_1)t$ assuming that the energy is constant at the revised energy.

Note that the energy-loss processes can occur on either side (in a time-wise fashion) of the direction change and that the energy employed in the selection of the angle is, on average, the mean energy of the step. This gives the correct first-order correction for energy loss in the deflection process.

2.6.1 Accounting for discrete interactions

Conventionally, as in the EGS4 code, an initial distance to a discrete interaction is determined and then broken up into multiple scattering sub-steps, using some mechanics scheme. A drawback to this approach is that the cross sections employed to sample the distance to a discrete interaction depends on the energy of the particle, which changes during the course of transporting the particle according to a given mechanics scheme.

In the revised EGS5 model, we permit discrete interactions to occur *within* the multiple scattering step. If we consider the transport segments to occur without energy change (energy change is effected at the energy "hinge points" only) and resample the distance to discrete interaction after each change in energy, we can account for the variation in the cross sections with respect to energy along the path. Note that when an interaction occurs, energy is deducted, daughter particles are created and directions may change. These are allowed to occur in accordance with the laws of physics. One simply has to resample the distance to the next interaction point and transport the remaining distance the the next real or virtual event.

2.6.2 Transport across interfaces

The most accurate way to cross interfaces is to choose a step-size that guarantees that the transport step does not cross the interface, reducing the electron step-size to such a degree that the multiple-interaction condensed history physics "evaporates" and the electron is permitted to cross the interface in analog mode without approximation[41]. This technique, while perfectly accurate, is computationally very costly. Therefore, we seek a technique that is approximate, yet sufficiently accurate for most applications, and faster, with the increase in speed coming about by allowing electrons to drift across interfaces during the sub-step segments.

Since the step-size is no longer constrained by geometry, we consider several constraints on the electron step-size. The first, measured in terms of the first elastic scattering transport moment (which is proportional to the average amount of deflection), controls the accuracy of the geometrical development of the electron track. The second, measured in terms of the first inelastic scattering transport moment (which is proportional to the average amount of energy loss), controls the accuracy of the energy-loss modeling along the electron track. Superimposed upon this is the discrete interaction physics.

Assume that the elastic scattering constraint is expressed as a distance T_{elastic} such that a prescribed average amount of scattering has occurred and that the inelastic scattering constraint is defined by a distance $T_{\text{inelastic}}$ such that a prescribed average amount of energy loss has occurred. The algorithm takes the following form:

1. Determine the distance to a cumulative elastic scattering event, $t_{\text{elastic}} = r_1 T_{\text{elastic}}$, where r_1 is a uniformly sampled random number between 0 and 1. Note that the algorithm is sufficiently general to allow for other prescriptions for choosing this distance.

2. Determine the distance to a cumulative inelastic scattering event, $t_{\text{inelastic}} = r_2 T_{\text{inelastic}}$, where r_2 is another uniformly sampled random number between 0 and 1.

3. Determine the distance to a discrete scattering event, $t_{\text{discrete}} = -\Sigma^{-1} \ln(r_3)$, where r_3 is another uniformly sampled random number between 0 and 1 and Σ is the macroscopic cross section in units of cm^{-1}.

4. Determine the distance, t_{geom}, the distance along the particle's current direction to an interface.

5. Determine the minimum of the 4 distances: t_{geom}, t_{elastic}, $t_{\text{inelastic}}$, and t_{discrete}. Subtract this distance from all 4.

6. Transport the electron this distance along its current direction of motion.

7. If $t_{\text{geom}} = 0$:

   (a) Rescale the distances t_{elastic} and $t_{\text{inelastic}}$, and resample t_{discrete} accounting for the new interaction physics, if the medium on the other side of the interface is different.

8. Else if $t_{\text{elastic}} = 0$:

   (a) Sample the interaction using the parameters of the current medium and deflect the electron.
   (b) Calculate the new t_{elastic}, $t_{\text{elastic}} = (T_{\text{elastic}} - t_{\text{elastic}}) + r_4 T_{\text{elastic}}$, where r_4 is another uniformly sampled random number between 0 and 1.

9. Else if $t_{\text{inelastic}} = 0$:

   (a) Sample the interaction using the parameters of the current medium and deduct energy from the electron.
   (b) Calculate the new $t_{\text{inelastic}}$, $t_{\text{inelastic}} = (T_{\text{inelastic}} - t_{\text{inelastic}}) + r_4 T_{\text{inelastic}}$, where r_4 is another uniformly sampled random number between 0 and 1.

10. Else if $t_{\text{discrete}} = 0$:

    (a) Sample the interaction using the parameters of the current medium. Create daughter particles, deflect the parent particle and deduct the energy of the daughter particles from it, as appropriate.
    (b) Calculate the new t_{discrete}, $t_{\text{discrete}} = -\Sigma^{-1} \ln(r_4)$, where r_4 is another uniformly sampled random number between 0 and 1.

11. Go to step 4 unless the electron's energy has fallen below the transport threshold.

Note that this scheme has characterized 4 types of interaction, interface intercept, discrete interaction, energy loss due to cumulative events, and direction change due to cumulative events. It places all these "interactions" on a more-or-less equal footing and deals with each separately. Uniformly randomizing the position at which energy loss due to cumulative events occurs effectively samples the average energy for the elastic and discrete events, the correct prescription to first order. Note also that we interpret any event that can cause any change in the phase space of the particles in the problem to have equal status. This would allow us to introduce many forms of variance reduction as a new class of event, and facilitate the introduction of variance reduction techniques.

If we treat the above algorithm in an infinite medium, $t_{\text{geom}} = \infty$ we note that it collapses to the algorithm described previously. Similarly, it is easy to avoid any species of interaction by setting its interaction distance to infinity. Note that this algorithm can be used to model analog transport, which is accomplished by setting $t_{\text{inelastic}} = t_{\text{elastic}} = 0$. Therefore, this algorithm can be applied to photon transport as well. Indeed, as far as the algorithm is concerned, an electron is transported in a similar fashion to a photon except that an electron has two extra interaction channels.

3 Conclusions

Transport mechanics algorithms have been reviewed. Based upon recent developments in EGS4/ PRESTA-II, EGSnrc and extensions to the PENELOPE code, an efficient algorithm which takes into account energy losses and provides realistic spatial-angular correlations has been described. Future work will demonstrate the step-size stability of this algorithm under a variety of conditions.

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