

Adjoint Monte Carlo Electron Transport in the Continuous-Slowing-Down Approximation*

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A model is developed for the Monte Carlo solution of the adjoint transport equation for primary electrons in one dimension. Energy loss is treated in the continuous-slowing-down approximation. The model also employs the condensed-history approximation required in forward Monte Carlo models for transport in extended media. It is tested extensively through numerous calculations of energy deposition and transmission coefficients in aluminum. Predictions are compared with results of the corresponding forward model. Agreement is generally very good. Small discrepancies are attributed to the use of uninterpolated tabular electron cross section data in both forward and adjoint models.

1. INTRODUCTION

Monte Carlo solution of the forward Boltzmann equation for radiation transport has reached a high level of sophistication. For most applications, the forward solution is quite satisfactory. However, for certain classes of problems—in particular, those involving highly restricted responses to highly diffuse sources—the adjoint solution has proved much more effective. Indeed the solution of such problems using conventional forward transport would have been much more difficult, if not impossible.

In recent years much effort has been directed toward development of the adjoint method. Monte Carlo codes employing the adjoint method for describing neutron, gamma, and coupled neutron/gamma transport in complex geometries are now available for general use. Unfortunately, the same cannot be said for electron transport. This is a consequence of those same unique aspects of electron transport that delayed the development of conventional forward models. The only published work on adjoint electron Monte Carlo transport is that of Jordan [1], who uses a multi-group, Green's function formalism.

We have completed the first phase of a program to provide an adjoint capability for a series of closely related continuous-energy, coupled electron/gamma Monte Carlo transport codes [2] that are routinely applied to a broad range of phenomena. This initial model describes the transport of primary electrons in one dimension using the condensed-history method [3]. Angular deflections are sampled from the multiple

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elastic scattering theory of Goudsmit and Saunderson [4], and energy loss is accounted for in the continuous-slowing-down approximation (CSDA). Section 2 presents the relevant formalism and describes the more important aspects of the Monte Carlo model. In Section 3 the adjoint model is verified through extensive comparisons with forward predictions. Section 4 summarizes the results and points out areas for future work.

2. THEORY

We begin with a general discussion of the forward-adjoint formalism as applied to the Boltzmann transport equation and proceed to a detailed description of a specific model for the Monte Carlo solution for primary-electron transport in the CSDA approximation.

2.1. *The Forward-Adjoint Formalism*

In this section we first present the forward-adjoint formalism for equations in general. Next the formalism is presented for the standard transport equation. Finally, forward and adjoint transport equations are derived for electrons under the continuous-slowing-down approximation. The unique aspects of these equations are discussed.

2.1.1. *General*

Many equations of physical interest can be expressed as

$$H\phi = q, \quad (1)$$

where H is a linear operator, q is a source function, and ϕ is the solution. Let $\langle f, g \rangle$ denote the inner product of the functions f and g :

$$\langle f, g \rangle \equiv \int_X f(\mathbf{x}) g(\mathbf{x}) d\mathbf{x}, \quad (2)$$

where

$$\begin{aligned} \mathbf{x} &\equiv (x_1, x_2, \dots, x_n), \\ d\mathbf{x} &\equiv dx_1 dx_2 \cdots dx_n, \\ X &\equiv \text{the domain of } f \text{ and } g. \end{aligned}$$

The adjoint of H is defined to be that operator, H^\dagger , which satisfies

$$\langle Hf, g \rangle = \langle f, H^\dagger g \rangle \quad (3)$$

for all $f \in D_H$, $g \in D_{H^\dagger}$, where D_H and D_{H^\dagger} denote the respective domains of H and H^\dagger . We shall not rigorously address the question of the existence and uniqueness of the adjoint operator [5]. Instead we simply state that it always exists and is unique.

However, it is not always true that $D_H = D_{H^\dagger}$. In order to illustrate this we consider three simple examples.

Let $H = d/dx$, $D_H =$ the set of all differentiable functions defined over the interval $[a, b]$. Now

$$\begin{aligned}\langle Hf, g \rangle &= \int_a^b \left[\frac{d}{dx} f(x) \right] g(x) dx, \\ &= \left|_a^b f(x) g(x) - \int_a^b f(x) \left[\frac{d}{dx} g(x) \right] dx, \right. \\ &= \left|_a^b f(x) g(x) + \langle f, -Hg \rangle.\end{aligned}\quad (4)$$

In this case, $H^\dagger = -d/dx$ and $D_{H^\dagger} =$ the set of all differentiable functions defined over the interval $[a, b]$ with $g(a) = g(b) = 0$, $g \in D_{H^\dagger}$. The domain of H^\dagger has to be restricted to ensure that the boundary term in Eq. (4) is zero. An adjoint operator does not exist such that $D_{H^\dagger} = D_H$.

Let $H = d/dx$, $D_H =$ the set of all differentiable, square-integrable functions defined over $(-\infty, +\infty)$. In this case the condition of square integrability requires that $f(\pm\infty) = 0$. Thus the boundary term in Eq. (4) is identically zero; $H^\dagger = -d/dx$, $D_{H^\dagger} = D_H$, and no restriction on D_{H^\dagger} is necessary.

Let $H = d/dx$, $D_H =$ the set of all differentiable functions as defined over the interval $[a, b]$ with $f(a) = f(b) = 0$, $f \in D_H$. As in the previous case, the domain of H is defined such that the boundary term is identically zero. However, the domain of H^\dagger can actually contain more functions than the domain of H . $H^\dagger = -d/dx$ and $D_{H^\dagger} =$ the set of all differentiable functions defined over the interval $[a, b]$. Note that in all of these examples, H^\dagger remains the same—it is only D_{H^\dagger} which changes in response to changes in D_H .

Given an arbitrary source function, q^\dagger the corresponding adjoint solution, ϕ^\dagger , satisfies

$$H^\dagger \phi^\dagger = q^\dagger. \quad (5)$$

We begin the derivation of the fundamental forward-adjoint relationship by multiplying Eq. (1) on the right with ϕ^\dagger , multiplying Eq. (5) on the left with ϕ , and subtracting the two equations:

$$H\phi\phi^\dagger - \phi H^\dagger\phi^\dagger = q\phi^\dagger - \phi q^\dagger. \quad (6)$$

Integrating over the domain of ϕ and ϕ^\dagger we get

$$\langle H\phi, \phi^\dagger \rangle - \langle \phi, H^\dagger\phi^\dagger \rangle = \langle q, \phi^\dagger \rangle - \langle \phi, q^\dagger \rangle. \quad (7)$$

The boundary conditions for ϕ are to be considered arbitrary, but once they are chosen, D_H and D_{H^\dagger} are effectively defined. It can be seen from previous examples that D_{H^\dagger} can often be smaller than the most general domain over which H^\dagger can be

defined when considered as an autonomous operator. Thus with an arbitrary source function, ϕ^\dagger , as given by Eq. (5), may not be an element of D_{H^\dagger} . Nonetheless we shall assume for the moment that it is. Under this assumption, the left side of Eq. (7) is clearly zero (by definition of the adjoint operator), and we obtain the desired result:

$$\langle \phi, q^\dagger \rangle = \langle q, \phi^\dagger \rangle. \quad (8)$$

This expression is valuable in the following way. Suppose that a function R can be found such that the quantity $\langle \phi, R \rangle$ is of interest. There are two possible ways to obtain this quantity. The forward approach is to solve the forward equation for ϕ and directly evaluate $\langle \phi, R \rangle$. The adjoint approach is to set $q^\dagger = R$, solve the adjoint equation for ϕ^\dagger , and evaluate $\langle q, \phi^\dagger \rangle$. There are two main advantages to the adjoint approach. If Monte Carlo methods are used, the variance associated with the adjoint approach can sometimes be smaller than that of the forward approach. In addition, only one adjoint calculation need be performed to obtain the quantity of interest for any number of different forward source functions.

We now wish to return our attention to the case in which ϕ^\dagger is not an element of D_{H^\dagger} . When this happens, it is usually possible to choose boundary conditions for ϕ^\dagger such that a relationship is obtained which is somewhat different from that given by Eq. (8), but is similarly useful. The exact boundary conditions used and the form of the relationships obtained are difficult to discuss in general. Instead we shall address the question in the next section specifically for the transport equation.

2.1.2. The Adjoint Boltzmann Equation

The Boltzmann transport equation can be expressed as [6]

$$(L_1 + L_2 - L_3) \phi(\mathbf{r}, \Omega, E) = q(\mathbf{r}, \Omega, E), \quad (9)$$

where

$$L_1 = \nabla \cdot \Omega,$$

$$L_2 = \sigma_T(\mathbf{r}, E),$$

$$L_3 = \int_{E'} \int_{\Omega'} d\Omega' dE' \sigma_S(\mathbf{r}, \Omega' \rightarrow \Omega, E' \rightarrow E).$$

It can easily be shown that the corresponding adjoint equation is

$$(L_1^\dagger + L_2^\dagger - L_3^\dagger) \phi^\dagger(\mathbf{r}, \Omega, E) = q^\dagger(\mathbf{r}, \Omega, E), \quad (10)$$

where

$$L_1^\dagger = -\nabla \cdot \Omega,$$

$$L_2^\dagger = \sigma_T(\mathbf{r}, E),$$

$$L_3^\dagger = \int_{E'} \int_{\Omega'} d\Omega' dE' \sigma_S(\mathbf{r}, \Omega \rightarrow \Omega', E \rightarrow E').$$

We wish to derive a forward-adjoint relationship for these equations which is applicable even when ϕ^\dagger is not an element of D_{L^\dagger} . We begin by expressing Eq. (7) in terms of L and L^\dagger :

$$\begin{aligned}
 & \int_V \int_E \int_\Omega [(\nabla \cdot \Omega \phi(\mathbf{r}, \Omega, E)) \phi^\dagger(\mathbf{r}, \Omega, E) + \phi(\mathbf{r}, \Omega, E)(\nabla \cdot \Omega \phi^\dagger(\mathbf{r}, \Omega, E))] d\Omega dE d\mathbf{r} \\
 & + \int_V \int_E \int_\Omega [\sigma_T(\mathbf{r}, E) \phi(\mathbf{r}, \Omega, E) \phi^\dagger(\mathbf{r}, \Omega, E) - \phi(\mathbf{r}, \Omega, E) \sigma_T(\mathbf{r}, E) \phi^\dagger(\mathbf{r}, \Omega, E)] d\Omega dE d\mathbf{r} \\
 & - \int_V \int_E \int_\Omega \int_{E'} \int_{\Omega'} \sigma_S(\mathbf{r}, \Omega' \cdot \Omega, E' \rightarrow E) \phi(\mathbf{r}, \Omega', E') \phi^\dagger(\mathbf{r}, \Omega, E) d\Omega' dE' d\Omega dE d\mathbf{r} \\
 & + \int_V \int_E \int_\Omega \int_{E'} \int_{\Omega'} \phi(\mathbf{r}, \Omega, E) \sigma_S(\mathbf{r}, \Omega \cdot \Omega', E \rightarrow E') \phi^\dagger(\mathbf{r}, \Omega', E') d\Omega' dE' d\Omega dE d\mathbf{r} \\
 & = \langle q, \phi^\dagger \rangle - \langle \phi, q^\dagger \rangle.
 \end{aligned} \tag{11}$$

The second integral on the left side of this equation is clearly zero. Under the assumption that the order of integration can be changed, the third and fourth integrals cancel each other. For physically meaningful calculations, this is always a valid assumption. The first integral can be expressed as a surface integral by first recognizing that the integrand can be written as $\nabla \cdot (\Omega \phi \phi^\dagger)$ and then applying the divergence theorem to obtain

$$\int_A \int_E \int_\Omega \phi(\mathbf{r}, \Omega, E) \phi^\dagger(\mathbf{r}, \Omega, E) (\Omega \cdot \mathbf{n}) d\Omega dE dA. \tag{12}$$

In infinite-medium calculations, this term is zero if q and q^\dagger go to zero at infinity. For physically meaningful problems, this is always true. Hence for infinite-medium problems we find that ϕ^\dagger is an element of D_{L^\dagger} and Eq. (11) reduces to Eq. (8). However, in finite-medium problems, the boundary (surface) term may be nonzero, and Eq. (11) reduces to

$$\langle q, \phi^\dagger \rangle - \int_A \int_E \int_\Omega \phi \phi^\dagger (\Omega \cdot \mathbf{n}) d\Omega dE dA = \langle \phi, q^\dagger \rangle. \tag{13}$$

This expression is just as useful as Eq. (8) because the adjoint boundary conditions can be chosen such that the information on the forward flux obtained from the forward boundary conditions is sufficient to evaluate the boundary term. For instance, consider a problem in slab geometry with a flux incident at the left face, vacuum boundaries at both the left and right faces, and no distributed source. Let us assume that the energy-integrated scalar flux at an interior point, $z = z_0$, is of primary interest. Clearly,

$$\int_E \int_\mu \phi(z_0, \mu, E) d\mu dE = \langle \phi, \delta(z - z_0) \rangle; \tag{14}$$

thus we set $q^\dagger = \delta(z - z_0)$. The appropriate forward boundary conditions are

$$\begin{aligned}\phi(0, \mu, E) &= \phi_0(\mu, E), & \mu > 0, \\ \phi(L, \mu, E) &= 0, & \mu < 0.\end{aligned}\tag{15}$$

In the adjoint equation, the divergence operator has a negative sign in front of it. This means that adjoint "particles" or adjunctions must be thought of as moving backward. That is to say that an adjunction directed along $\mu = 1$ travels in the negative- z direction. With vacuum boundaries and an interior source, no adjunctions should enter the slab from the vacuum regions. Keeping the backward movement of adjunctions in mind, this translates to the following conditions:

$$\begin{aligned}\phi^\dagger(0, \mu, E) &= 0, & \mu < 0, \\ \phi^\dagger(L, \mu, E) &= 0, & \mu > 0.\end{aligned}\tag{16}$$

Although these boundary conditions follow by analogy from the corresponding forward boundary conditions (after the backward movement of the adjunctions is taken into account), the true justification for these conditions is simply that Eq. (13) reduces to a useful expression. In particular, we obtain

$$\int_E \int_\mu \phi(z_0, \mu, E) d\mu dE = \int_E \int_0^1 \phi_0(\mu, E) \phi^\dagger(0, \mu, E) \mu d\mu dE.\tag{17}$$

2.1.3. The Adjoint Electron Transport Equation with Continuous Slowing Down

To an excellent approximation, the electron scattering cross section can be represented in the following form [3]:

$$\sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E) = \sigma_1(\mathbf{r}, E', \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \delta(E' - E) + \sigma_2(\mathbf{r}, E' \rightarrow E) \delta(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega} - 1),\tag{18}$$

where σ_1 represents elastic electron-nuclear scattering and σ_2 represents inelastic electron-electron scattering. Because of the special decoupled nature of this cross section, we need only deal with σ_2 in deriving a continuous-slowing-down term. The outscatter and inscatter terms corresponding to σ_2 appear in the transport equation as

$$\sigma_2(E) \phi(E) - \int_0^\infty \sigma_2(E' - E) \phi(E') dE'.\tag{19}$$

We have deleted the other variables in the notation because they play no role in this development. It is convenient to reexpress Eq. (19) as

$$\int_0^\infty [\sigma_2(E, E - Y) \phi(E) - \sigma_2(E + Y, E) \phi(E + Y)] dY.\tag{20}$$

Expanding the second term in a Taylor series, we get

$$\begin{aligned} & \sigma_2(E + Y, E) \phi(E + Y) \\ &= \sigma_2(E, E - Y) \phi(E) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\frac{\partial^n}{\partial E^n} \sigma_2(E, E - Y) \phi(E) \right] Y^n. \end{aligned} \quad (21)$$

Substituting this series into Eq. (20) gives

$$- \int_0^{\infty} \sum_{n=1}^{\infty} \frac{\partial^n}{\partial E^n} [\sigma_2(E, E - Y) \phi(E)] Y^n dY. \quad (22)$$

Assuming that the order of integration and differentiation can be reversed, we obtain

$$- \sum_{n=1}^{\infty} \frac{\partial^n}{\partial E^n} [S_n(E) \phi(E)], \quad (23)$$

where $S_n(E) = \sigma_2(E) \Delta \bar{E}^n$, $\sigma_2(E)$ = the total scattering cross section, $\Delta \bar{E}^n$ = the average value of the n th power of the energy loss per scattering event.

Truncating the series given in Eq. (23) at $n = 1$ corresponds to the continuous-slowing-down approximation. It is clear that this approximation becomes increasingly accurate as $\Delta \bar{E}$ becomes smaller. The quantity $S_1(E)$ is known as the stopping power. Note that if the stopping power is to remain constant as $\Delta \bar{E}$ is reduced, $\sigma_2(E)$ must become proportionately larger. In the limit as $\Delta \bar{E}$ becomes differential, $\sigma_2(E)$ becomes infinite and the particle scatters continuously losing a differential amount of energy at each scattering site. Of course this is precisely the physical model associated with the continuous-slowing-down approximation. Consistency between the physical and mathematical models is thus established.

We shall now derive the adjoint CSDA operator. Integrating

$$\left\langle - \frac{\partial}{\partial E} (S(E) \phi(E), \phi^*(E)) \right\rangle$$

by parts we obtain

$$\begin{aligned} & \int_{E_{\min}}^{E_{\max}} \left[- \frac{\partial}{\partial E} S(E) \phi(E) \right] \phi^*(E) dE \\ &= - \left[S(E) \phi(E) \phi^*(E) \right]_{E_{\min}}^{E_{\max}} + \int_{E_{\min}}^{E_{\max}} \phi(E) S(E) \frac{\partial}{\partial E} \phi^*(E) dE. \end{aligned} \quad (24)$$

The adjoint operator is clearly $S(E) \partial/\partial E$. If either $S(E)$, $\phi(E)$, or $\phi^*(E)$ are zero at the boundaries of the energy domain, ϕ^* will be an element of the adjoint domain. It is convenient to reexpress the adjoint operator as follows:

$$S(E) \frac{\partial}{\partial E} = - \left[\frac{d}{dE} S(E) \right] + \frac{\partial}{\partial E} S(E). \quad (25)$$

Since the first operator on the right in this equation is merely an energy dependent multiplicative factor like σ_T in Eq. (10), it is equivalent to an effective absorption cross section. The second term is equal to the forward operator with a change of sign. This means that as adjunctions traverse a medium they are absorbed at a rate proportional to $(d/dE) S(E)$ and they increase in energy at the same rate that forward particles decrease in energy.

The forward and adjoint continuous-slowing-down equations are, respectively,

$$\begin{aligned} \nabla \cdot \Omega \phi(\mathbf{r}, \Omega, E) + \sigma_1(\mathbf{r}, E) \phi(\mathbf{r}, \Omega, E) - \int_{\Omega'} \sigma_1(\mathbf{r}, E, \Omega' \cdot \Omega) \phi(\mathbf{r}, \Omega', E) d\Omega' \\ - \frac{\partial}{\partial E} [S(E) \phi(\mathbf{r}, \Omega, E)] = q(\mathbf{r}, \Omega, E), \end{aligned} \quad (26)$$

and

$$\begin{aligned} -\nabla \cdot \Omega \phi^+(\mathbf{r}, \Omega, E) + \sigma_1(\mathbf{r}, E) \phi^+(\mathbf{r}, \Omega, E) - \int_{\Omega'} \sigma_1(\mathbf{r}, E, \Omega' \cdot \Omega) \phi^+(\mathbf{r}, \Omega', E) d\Omega' \\ + \frac{d}{dE} [S(E)] \phi^+(\mathbf{r}, \Omega, E) + \frac{\partial}{\partial E} [S(E) \phi^+(\mathbf{r}, \Omega, E)] = q^+(\mathbf{r}, \Omega, E). \end{aligned} \quad (27)$$

If we follow the same procedure with these equations which led to the development of Eq. (13) for the general equations, we obtain

$$\begin{aligned} \langle q, \phi^+ \rangle - \int_A \int_E \int_{\Omega} \phi \phi^+(\Omega \cdot \mathbf{n}) d\Omega dE dA \\ + \int_V \int_{\Omega} \left[\int_{E_{\min}}^{E_{\max}} S(E) \phi(E) \phi^+(E) \right] d\Omega dV = \langle \phi, q^+ \rangle. \end{aligned} \quad (28)$$

A new boundary term appears which is highly undesirable because it requires knowledge of $\phi(E)$ throughout the spatial and angular domains. However, this term will be zero if the energies E_{\min} and E_{\max} are chosen such that $\phi(E_{\min}) = \phi(E_{\max}) = 0$. This can clearly always be done. Thus we find that Eq. (13) applies to both the standard and CSDA equations with the energy limits so chosen.

In concluding this section we would like to note that the effective absorption term for adjunctions under the continuous-slowing-down approximation can be avoided by using the Spencer-Lewis equation [7]. This equation can be derived from Eq. (26) as follows. Let E_0 be the highest source energy. The normalized residual range for a particle with $E \leq E_0$ is defined as

$$t = \left[\int_0^E S(E')^{-1} dE' \right] / \left[\int_0^{E_0} S(E')^{-1} dE' \right]. \quad (29)$$

Note that $1 \geq t \geq 0$ and that a one-to-one correspondence exists between t and E . Defining

$$\phi(E) dE = \Phi(t) dt, \quad (30)$$

Eq. (26) transforms to

$$\nabla \cdot \Omega \Phi(\mathbf{r}, \Omega, t) + \sigma_1(\mathbf{r}, t) \Phi(\mathbf{r}, \Omega, t) - \int_{\Omega'} \sigma_1(\mathbf{r}, t, \Omega' \cdot \Omega) \Phi(\mathbf{r}, \Omega', t) d\Omega' - \frac{\partial}{\partial t} \Phi(\mathbf{r}, \Omega, t) = q(\mathbf{r}, \Omega, t). \quad (31)$$

Since $(-\partial/\partial t)^+ = (\partial/\partial t)$, no absorption term is obtained. The residual range of the adjunctions is increased as they move through the system at the same rate that the residual range of the forward particles is decreased.

Because our production electron transport codes are based upon the energy variable rather than the residual-range variable, no attempt has been made to solve the Spencer-Lewis equations.

2.2. The Monte Carlo Model

Our purpose is to construct a Monte Carlo model based upon Eq. (27). Since CSDA energy loss is not a stochastic process, random sampling will only be required to describe elastic scattering. As is well known, the magnitude of the elastic scattering cross section precludes the use of a conventional Monte Carlo analog for describing electron transport through material configurations having dimensions that are significant fractions of the electron range. Unfortunately, it is just these deep penetration problems that are of most practical importance. In forward models this problem was overcome through the development of condensed-history Monte Carlo [3] in which the single-scattering analog is replaced by a random walk of macroscopic segments within which the combined effects of large numbers of collisions are described by multiple interaction theories. If it is to be of any practical value, the adjoint problem must also be solved in the context of the condensed-history approximation.

2.2.1. Forward Model

The forward model uses tabulated electron cross-section data that have been calculated for a logarithmic energy grid. Successive values in this energy grid are related by the equation

$$E_{i+1} = 2^{-1/8} E_i. \quad (32)$$

Data required for the forward solution are the random walk segment (for simplicity we omit discussion of the further subdivision of these segments as a function of atomic number),

$$D_i = \int_{E_{i+1}}^{E_i} [S(E)]^{-1} dE, \quad (33)$$

the energy loss,

$$Q_i = E_i - E_{i+1}, \quad (34)$$

and the Goudsmit-Saunderson multiple-elastic-scattering distribution [4] that is averaged over D_i according to the method of Spencer [8].

Since the Monte Carlo procedure uses only uninterpolated tabular data, according to the nearest-grid-point (NGP) method, it is optimized for electrons having initial energies that coincide with one of the grid energies. At other energies the tabular data are either too small or too large. However, the electron cross sections are only weakly dependent upon energy over the intervals defined by Eq. (32). Moreover, it is easily shown that the errors tend to compensate rather than compound during the process of slowing down.

2.2.2. Adjoint Model

Using the same cross-section data as in the forward calculation, the corresponding data required for the Monte Carlo solution of Eq. (27) are the random walk segment,

$$\hat{D}_i = \int_{E_i}^{E_{i-1}} [S(E)]^{-1} dE = D_{i-1}, \quad (35)$$

the energy loss,

$$\hat{Q}_i = E_i - E_{i-1} = -Q_{i-1}(<0), \quad (36)$$

and the multiple-elastic-scattering distribution averaged over D_{i-1} .

If there were no further differences between the forward and adjoint models, then, apart from the minus sign in Eq. (36) corresponding to upscatter, adjoint tracking would require only a shift in the energy index. However, as emphasized in Section 2.1, the absorptive term in Eq. (25) leads to the requirement for a weight correction for the segment D_i . This correction factor is given by

$$F_i = \exp \left\{ \int_0^{D_i} \frac{dS(E)}{dE} ds \right\}. \quad (37)$$

Recalling that $ds = -[S(E)]^{-1} dE$, we obtain

$$F_i = \frac{S(E_i)}{S(E_{i+1})}. \quad (38)$$

Finally, one can code pointwise tallies of the response of specific sources—i.e., let the Monte Carlo perform the inner products indicated in Eq. (13)—directly into the adjoint calculations. Results can also be obtained for other sources for which sufficiently high resolution histogrammic adjunction fluxes have been tallied. In this connection one will always be limited by the chosen energy cutoff, above which adjunction histories are terminated.

3. RESULTS

In this section the adjoint model is applied to the transport of primary electrons in aluminum. Transmission coefficients and internal energy deposition are calculated for

various sources. In order to verify different aspects of the model, results are also given for situations where either energy loss or elastic scattering is ignored. In every case results are compared with forward predictions.

3.1. Transmission Coefficients

There are many excellent references on the application of the adjoint formalism to specific problems. We have found the method of Ref. [9] especially convenient.

Consider an aluminum slab bounded by the planes $z = 0$ and $z = L$. If there is no azimuthal dependence in the source, Eq. (13) may be written as

$$\begin{aligned} & \int_E \int_\mu \phi(L) \phi^\dagger(L) \mu \, dE \, d\mu - \int_E \int_\mu \phi(0) \phi^\dagger(0) \mu \, dE \, d\mu \\ &= \int_z \int_E \int_\mu [\phi^\dagger(z) q(z) - \phi(z) q^\dagger(z)] \, dz \, dE \, d\mu. \end{aligned} \quad (39)$$

For a real surface source at the boundary $z = 0$, we wish to calculate a partial number transmission coefficient defined by

$$J(\Delta E^\dagger, \Delta \mu^\dagger) = \int_{\Delta E^\dagger} \int_{\Delta \mu^\dagger} \phi(L) \mu \, dE \, d\mu, \quad (40)$$

where ΔE^\dagger and $\Delta \mu^\dagger$ are any arbitrarily chosen energy and angular intervals. By considering only those electrons transmitted within relatively narrow ranges, ΔE^\dagger and $\Delta \mu^\dagger$, the advantage of the adjoint method over forward transport can be demonstrated. If we set

$$\begin{aligned} \phi^\dagger(L) &= 1 && \text{for } E \text{ within } \Delta E^\dagger \text{ and } \mu \text{ within } \Delta \mu^\dagger \\ &= 0 && \text{otherwise,} \end{aligned} \quad (41)$$

Eq. (40) is identical to the first term on the left-hand side of Eq. (39). Since $\phi^\dagger(0)$ vanishes for $\mu < 0$, the integrand in the second term on the left-hand side vanishes everywhere except for the ranges, ΔE and $\Delta \mu$, over which the real surface source is nonzero. Finally, since there are no internal sources in the transmission problem, $q(z) = q^\dagger(z) = 0$ for $0 < z < L$, and the right-hand side of Eq. (39) vanishes. Equation (39) then reduces to

$$\int_{\Delta E} \int_{\Delta \mu} \phi(0) \phi^\dagger(0) \mu \, dE \, d\mu = \int_{\Delta E^\dagger} \int_{\Delta \mu^\dagger} \phi(L) \mu \, dE \, d\mu. \quad (42)$$

In the Monte Carlo model it is more convenient to deal with boundary currents. Thus defining $\psi = \phi\mu$, we obtain

$$N \int_{\Delta E} \int_{\Delta \mu} \frac{\psi(0) \psi^\dagger(0)}{\mu} \, dE \, d\mu = N^\dagger J(\Delta E^\dagger, \Delta \mu^\dagger), \quad (43)$$

where we have introduced the normalization constants N and N^+ . If $J(\Delta E^\dagger, \Delta\mu^\dagger)$ and $\psi^\dagger(0)$ are normalized to one incident electron and one incident adjunction, respectively, as they are in the Monte Carlo calculations, then

$$N = \left\{ \int_{\Delta E} \int_{\Delta\mu} \psi(0) dE d\mu \right\}^{-1} \quad (44)$$

and

$$N^+ = \left\{ \int_{\Delta E^\dagger} \int_{\Delta\mu^\dagger} \psi^\dagger(L) dE d\mu \right\}^{-1}. \quad (45)$$

Using Eq. (40), $J(\Delta E^\dagger, \Delta\mu^\dagger)$ is obtained from a forward calculation. The same transmission coefficient is then obtained from an adjoint calculation using Eq. (43). The left-hand side of Eq. (43) can be tallied (pointwise) in the adjoint calculation for an arbitrary number of real surface sources. In the following examples, results from the two methods are compared.

3.1.1. Energy Loss Only

As a first example we consider the transmission problem in the absence of angular scattering. Results obtained from this nonstochastic transport calculation constitute a definitive check on the logic and numerical accuracy of the adjoint model. A normally incident step function source of electrons between 0.95 and 1.0 MeV was transmitted through 0.4691 g/cm² of aluminum. As a result of the dispersion caused by the energy-dependent stopping power, a substantial number of electrons were transmitted within the energy bins, 0.15–0.20 and 0.20–0.25 MeV. A comparison of the forward and adjoint results is shown in Table I.

The standard results were obtained, as in conventional forward calculations, by using uninterpolated tabulated cross-section data (NGP method). In the high-energy bin, disagreement is less than 1 %, while it is about 4 % in the low-energy bin. In an attempt to understand this discrepancy, calculations were repeated for the low-energy bin using quadratic interpolation to obtain cross-section data at the instantaneous electron energy. These results are labeled “differential” in Table I. The differential results are in excellent agreement. However, interpolation doubled the running time.

TABLE I

Partial Transmission Coefficients without Elastic Scattering for a Normally Incident Source Current with Energies Distributed Uniformly between 0.95 and 1.0 MeV

ΔE^\dagger (MeV)	Method	Number per source electron	
		Forward	Adjoint
$0.20 \leq E \leq 0.25$	NGP	0.720	0.715
$0.15 \leq E \leq 0.20$	NGP	0.280	0.291
$0.15 \leq E \leq 0.20$	Differential	0.286	0.284

It is important to note that the inaccuracy caused by the NGP approximation is almost as bad in the forward calculation as it is in the adjoint. In the expectation that the stochastic effects introduced by elastic scattering would tend to wash out discrepancies due to the NGP approximation, interpolation was not employed in the remainder of this work.

3.1.2. *Angular Scattering Only*

Next, we ignore inelastic scattering (energy loss) so as to isolate any effects due only to angular scattering. Since the weight correction is due entirely to the approximate (CSDA) treatment of inelastic processes, it is unnecessary in these calculations. On the other hand, transport is now stochastic, so that we must be concerned with statistical accuracy. To the extent that the condensed-history, Goodsmi-Saunderson [4] treatment correctly describes the self-adjoint elastic scattering, we expect that the same multiple-elastic-scattering distributions should be used for electrons and adjunc-tions of the same energy.

We consider two source currents at $z = 0$, both with energies distributed uniformly between 0.35 and 1.0 MeV. The angular distribution of the first source current is proportional to μ with $0 \leq \mu \leq 1$ (2π -cosine). The angular distribution of the second source current is isotropically distributed between 40° and 45° (polar angles, θ). For each source the adjoint model was used to calculate the transmission currents within polar angle intervals $0^\circ \leq \theta \leq 5^\circ$ and $40^\circ \leq \theta \leq 45^\circ$ for an aluminum slab of thickness 0.1350 g/cm^2 . From Eq. (41) it is seen that the adjoint surface source $\psi^+(L)$ is proportional to μ , i.e., cosine law within the appropriate limits. For the cosine-law source current the left-hand side of Eq. (43) is tallied as the sum of the adjunc-tion weights at $z = 0$. For the isotropic source current, the left-hand side of Eq. (43) is tallied as the sum of the adjunc-tion weights divided by μ ($40^\circ = \theta = 45^\circ$), again at $z = 0$.

The results of the forward and adjoint calculations are compared in Table II for comparable statistical uncertainties. Agreement is excellent in all four cases. The run-time ratios (forward time divided by the adjoint time) clearly demonstrate that the more diffuse the source and the more restricted the response (smaller the solid angle), the more efficient is the adjoint method. This ratio is approximately equal to the ratio of the numbers of histories in the two calculations.

3.1.3. *Both Energy Loss and Angular Scattering*

In this section we consider the combined effects of CSDA energy loss and angular scattering upon the adjoint predictions of the partial transmission coefficients. Results are obtained for two source-current densities and six partial transmission coefficients (responses). The first source is identical with the cosine-law source of the previous subsection and is broadly distributed in both energy and angle. The second source is highly restricted in both energy and angle—isotropic over the polar angle interval between 40° and 45° , and uniform in energy between 0.95 and 1.0 MeV. The six partial transmission currents are identified in Table III by the appropriate intervals ΔE^+ and $\Delta\mu^+$. They also range from highly restricted partial currents to the total transmission

TABLE II
Partial Transmission Currents without Energy Loss

Source current distributions			Number per source electron ^a		Run-time ratio	
Energy step (MeV)	Angle	ΔE^+ (MeV)	$\Delta\mu^+$	Forward		
$0.35 \leq E \leq 1.0$	2π -cosine	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 5^\circ$	$5.684 \times 10^{-3} (2.61)$	$5.748 \times 10^{-3} (2.18)$	1200.
$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$ isotropic	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 5^\circ$	$5.896 \times 10^{-3} (2.65)$	$5.784 \times 10^{-3} (2.08)$	15.
$0.35 \leq E \leq 1.0$	2π -cosine	$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$	$5.575 \times 10^{-3} (1.05)$	$5.629 \times 10^{-3} (0.86)$	34.
$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$ isotropic	$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$	$5.889 \times 10^{-3} (0.67)$	$5.876 \times 10^{-3} (0.71)$	1.4

^a The numbers in parentheses are the estimated 1σ statistical uncertainties expressed as percentages of the given quantities.

TABLE III

Partial Transmission Currents with Both Elastic Scattering and Energy Loss for a Source Current with Energies Distributed Uniformly between 0.35 and 1.0 MeV, and with an Angular Distribution Proportional to the Cosine of the Angle of Incidence with Respect to the Inward Normal

Partial transmission current (response) number	ΔE^\dagger (MeV)	$\Delta\mu^\dagger$	Number per source electron ^a		Run-time ratio
			Forward	Adjoint	
1	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 90^\circ$	1.184×10^{-1} (1.32)	1.213×10^{-1} (1.30)	2.0
2	$0.35 \leq E \leq 0.40$	$0^\circ \leq \theta \leq 90^\circ$	2.049×10^{-2} (1.15)	2.087×10^{-2} (1.72)	62
3	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 5^\circ$	1.338×10^{-3} (1.44)	1.446×10^{-3} (1.76)	730
4	$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$	1.070×10^{-2} (1.05)	1.088×10^{-2} (0.94)	16
5	$0.35 \leq E \leq 0.40$	$0^\circ \leq \theta \leq 5^\circ$	1.945×10^{-4} (4.01)	2.029×10^{-4} (2.46)	2400
6	$0.35 \leq E \leq 0.40$	$40^\circ \leq \theta \leq 45^\circ$	1.833×10^{-3} (1.32)	1.893×10^{-3} (1.06)	380

^a The numbers in parentheses are the estimated 1σ statistical uncertainties expressed as percentages of the given quantities.

above the problem cutoff of 0.35 MeV. The areal density of the aluminum slab is 0.1890 g/cm^2 .

Results for the cosine-law source are given in Table III. In four of the six cases the adjoint and forward results agree within the estimated one-sigma statistical uncertainties. An attempt was made to adjust the number of histories so that the statistical uncertainties for a given response would be comparable. The run-time ratios are for the actual calculations; however, they may be approximately normalized to equal statistical errors by multiplying by the square of the ratio of the given statistical errors. For example, the run-time ratio for response 5 would then increase to about 6400. The forward calculation for this response required 4×10^6 histories, while the adjoint calculation required only 1500. In responses 3 and 5, the small solid angles strongly favor the adjoint model.

Corresponding results for the restricted source are given in Table IV. In five of the six cases the adjoint and forward results agree within the estimated 1σ statistical uncertainties. The run-time ratios indicate a clear preference for the adjoint method only in the two cases involving the smallest solid angle, Nos. 3 and 5. A highly restricted source and a highly distributed response favor the forward method.

In 10 of the 12 cases given in Tables III and IV the adjoint result is greater than the corresponding forward value. Furthermore, in 3 of these 10 the difference is greater than twice the sum of the estimated 1σ uncertainties. This suggests the possibility that the NGP approximation still (see also Table I) leads to significant inaccuracy, even in the presence of stochastic processes. The error, if it exists, is small and its confirmation using interpolation of cross-section data as in the no-scattering case would be expensive. To do so it would now be necessary to also interpolate the Goudsmit-Saunderson

TABLE IV

Partial Transmission Currents with Both Elastic Scattering and Energy Loss for a Source Current with Energies Distributed Uniformly between 0.95 and 1.0 MeV, and with Angles Distributed Isotropically over the Solid Angle Bounded by Polar Angles of 40 and 45°

Partial transmission current (response) number	ΔE^+ (MeV)	$\Delta\mu^+$	Number per source electron ^a		Run-time ratio
			Forward	Adjoint	
1	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 90^\circ$	4.643×10^{-1} (1.71)	4.594×10^{-1} (2.44)	.021
2	$0.35 \leq E \leq 0.40$	$0^\circ \leq \theta \leq 90^\circ$	2.634×10^{-2} (2.04)	2.674×10^{-2} (2.78)	.28
3	$0.35 \leq E \leq 1.0$	$0^\circ \leq \theta \leq 5^\circ$	5.142×10^{-3} (2.02)	5.586×10^{-3} (1.72)	6.0
4	$0.35 \leq E \leq 1.0$	$40^\circ \leq \theta \leq 45^\circ$	4.217×10^{-2} (2.72)	4.313×10^{-2} (2.70)	.30
5	$0.35 \leq E \leq 0.40$	$0^\circ \leq \theta \leq 5^\circ$	2.158×10^{-4} (2.27)	2.081×10^{-4} (3.07)	5.0
6	$0.35 \leq E \leq 0.40$	$40^\circ \leq \theta \leq 45^\circ$	2.338×10^{-3} (2.14)	2.403×10^{-3} (2.00)	1.1

^a The numbers in parentheses are the estimated one-sigma statistical uncertainties expressed as percentages of the given quantities.

data and to run enough histories to unambiguously ensure that statistical uncertainties do not mask the NGP error.

3.2. Energy Deposition

We now apply the adjoint model to the calculation of energy deposition at some internal depth, z' , due to electrons incident at $z = 0$. Returning to Eq. (39), there is no internal source so that $q(z) = 0$. The internal adjoint source must be of the form $q^+(z) = \delta(z - z') Q^+$, where at this point Q^+ could be some arbitrary function of energy and angle. Since $\phi(L) = 0$ for $\mu > 0$ and $\phi^+(L) = 0$ for $\mu < 0$, the first term on the left-hand side of Eq. (39) vanishes, so that we are left with

$$\int_E \int_\mu \phi(0) \phi^+(0) \mu dE d\mu = \int_E \int_\mu \phi(z') Q^+ dE d\mu. \quad (46)$$

We now define the restricted differential electron energy deposition as

$$D_R(z') = \int_{E \geq E_{\text{cut}}} \int_{\text{all } \mu} \phi(z') S(E) dE d\mu, \quad (47)$$

where we have ignored deposition due to the electron flux below some cutoff energy E_{cut} . This is identical to the right-hand side of Eq. (46), if we choose

$$\begin{aligned} Q^+ &= S(E) & \text{for } E \geq E_{\text{cut}} \\ &= 0 & \text{otherwise.} \end{aligned} \quad (48)$$

Again, since $\phi^+(0)$ vanishes for $\mu < 0$, the integrand on the left side of Eq. (46) vanishes everywhere except within the ranges, ΔE and $\Delta\mu$, over which the real surface source is nonzero. Introducing the normalization constants, N and N^+ , Eq. (46) becomes

$$N \int_{\Delta E} \int_{\Delta\mu} \frac{\psi(0) \psi^+(0)}{\mu} dE d\mu \equiv N^+ D_R(z'). \quad (49)$$

The constant N is given by Eq. (44), while N^+ is given by

$$\begin{aligned} N^+ &= \left\{ \int_0^L \int_{E_{\text{cut}}}^{\infty} \int_{-1}^1 q^+(z') dz' dE d\mu \right\}^{-1} \\ &= \left\{ 2 \int_{E_{\text{cut}}}^{\infty} S(E) dE \right\}^{-1}. \end{aligned} \quad (50)$$

Using Eq. (47), $D_R(z')$ is obtained from a forward calculation. It is then obtained from an adjoint calculation using Eq. (49). The left-hand side of Eq. (49) can be tallied (pointwise) in the adjoint calculation for an arbitrary number of sources. In the following examples, results from the two methods are compared.

The forward result is obtained as follows. When a random-walk segment crosses the plane $z = z'$, linear interpolation is employed to determine the energy at z' . This energy is then used in a quadratic interpolation on stopping-power data. The interpolated stopping power divided by the absolute value of the cosine of the polar angle is then tallied.

In an adjoint calculation, the adjunction histories are initiated at $z = z'$ with directions sampled from a 4π isotropic angular distribution. Initial energies of the adjunctions are sampled from the cumulative probability distribution,

$$P(E) = \left\{ \int_{E_L}^{E_U} S(E) dE \right\}^{-1} \int_{E_L}^E S(E) dE. \quad (51)$$

Conservatively, E_U should be at least as large as the highest source electron energy under consideration. However, it is only necessary that the interval $E_L \leq E \leq E_U$ span the range of electron energies over which $\phi(z')$ in Eq. (47) is nonzero. Consequently, in special cases (see Section 3.2.1) one may also get by with E_L greater than E_{cut} .

3.2.1. Energy Loss Only

In order to verify the logic and numerical accuracy, we consider first the case of no elastic scattering, so that statistical uncertainties are eliminated. Electrons with initial energies distributed uniformly between 0.95 and 1.0 MeV are normally incident upon an aluminum slab with an areal density of 0.4691 g/cm². We are interested in the deposition at a depth equal to 95% of this thickness by all electrons with energies above a cutoff value of 0.01 MeV. From the forward calculation the minimum and

maximum energies of electrons depositing at this depth were found to be 0.22891 and 0.29527 MeV, respectively. The adjoint source spectrum must span this interval.

Results are shown in Table V. The first two adjoint calculations agree with the equivalent forward results to less than 1 %. The agreement here verifies the accuracy of the coding and demonstrates the value of any knowledge of the ranges of variables (in this case, energy) involved in the response. The last adjoint result shows the importance of the weight correction. The ratio of the deposition obtained with the weight correction to that obtained without it is very nearly equal to the ratio of the stopping power at the mean energy of the real source to that at the mean energy of the adjoint source.

TABLE V

Adjoint Results for Energy Deposition without Elastic Scattering, for
Comparison with a Forward Value of 1.957 MeV-cm²/g-electron

E_L (MeV)	E_U (MeV)	Energy deposition (MeV-cm ² /g-electron)
0.2	0.3	1.972
0.2289	0.2953	1.961
0.2289	0.2953	2.581 ^a

^a No weight correction.

3.2.2. Deposition with Scattering and Energy Loss

We now introduce elastic angular scattering into the calculation of energy deposition. Results are obtained for an aluminum slab with a total thickness of 0.1899 g/cm², at a depth corresponding to 45 % of this thickness for two external source currents: one with a cosine-law angular distribution and a uniform energy spectrum between 0.35 and 1.0 MeV, and the other having the same energy distribution, but distributed isotropically over the solid angle between polar angles of 40 and 45°. The cutoff energy in Eq. (47) was again set at 0.01 MeV.

Results from the forward and adjoint models are compared in Table VI. Agreement is excellent. These differential data are also in excellent agreement with the values obtained from the standard 10-zone histogrammic profile of the forward model, indicating that contributions to the deposition by electrons with energies below 0.01 MeV are negligible.

The purpose of these calculations was simply to demonstrate the validity of the adjoint model. However, the runtime ratios in Table VI show that the adjoint method is not necessarily preferred for deposition in one dimension. This is because energy deposition in *one dimension* involves nonzero response over a broad range of variables in Eq. (47). For other types of one-dimensional responses, the adjoint method can be preferable. Moreover, in multidimensional neutron and gamma transport codes, the adjoint method has proved to be an extremely powerful approach for predicting the response of point, or small-volume, detectors.

TABLE VI

Energy Deposition with Both Elastic Scattering and Energy Loss

Source current distribution		Energy deposition ^a (MeV-cm ² /g-electron)		Run-time ratio
Energy step (MeV)	Angle	Forward	Adjoint	
0.35 < E < 1.0	2 π -cosine	2.808 (1.98)	2.785 (1.75)	1.1
0.35 < E < 1.0	40° < θ < 45° isotropic	2.936 (1.70)	2.954 (2.00)	0.19

^a The numbers in parentheses are the estimated 1 σ statistical uncertainties expressed as percentages of the given quantities.

4. CONCLUSIONS

We have developed an adjoint formalism for primary electron transport using the condensed-history Monte Carlo method. Energy loss and deposition are accounted for in the CSDA approximation, while multiple elastic scattering is described by the theory of Goudsmit and Saunderson. The one-dimensional model has been tested extensively for aluminum slabs through various calculations of energy deposition and electron transmission.

In all cases, predictions have been compared with those obtained from a corresponding forward model. In general, agreement is very good. Results obtained without elastic scattering (nonstochastic) indicate some inaccuracy due to the NGP approximation. However, the observed discrepancies are about as large in the forward calculations as they are in the adjoint. Moreover, in most cases, these small discrepancies are masked by statistical uncertainties when angular scattering is included. As expected, for a single source and a single response, computational speed favors the adjoint (forward) method for a highly distributed (restricted) source and a highly restricted (distributed) response.

This work represents the completion of the first phase of a long-range effort to develop a multidimensional, coupled electron/photon adjoint capability. In order to achieve this goal, the following tasks must still be accomplished.

(a) Multimaterial, multidimensional capability. This work appears to be straightforward, requiring a relatively minor effort.

(b) Replacement of CSDA with collisional straggling. An adjoint formulation of Landau-type straggling will probably be one of the more difficult tasks.

(c) Adjoint photon transport. Adjoint photon models already exist; however, combining these techniques with the electron transport will require a major effort.

(d) Secondary production and electron/gamma coupling. Although the cross sections employed in forward models appear to be adequate, much effort will be needed to construct the adjoint distribution functions and the attendant sampling procedures.

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