A deterministic partial differential equation model for dose calculation in electron radiotherapy

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Abstract
High-energy ionizing radiation is a prominent modality for the treatment of many cancers. The approaches to electron dose calculation can be categorized into semi-empirical models (e.g. Fermi–Eyges, convolution-superposition) and probabilistic methods (e.g. Monte Carlo). A third approach to dose calculation has only recently attracted attention in the medical physics community. This approach is based on the deterministic kinetic equations of radiative transfer. We derive a macroscopic partial differential equation model for electron transport in tissue. This model involves an angular closure in the phase space. It is exact for the free streaming and the isotropic regime. We solve it numerically by a newly developed HLLC scheme based on Berthon et al. (2007 J. Sci. Comput. 31 347–89) that exactly preserves the key properties of the analytical solution on the discrete level. We discuss several test cases taken from the medical physics literature. A test case with an academic Henyey–Greenstein scattering kernel is considered. We compare our model to a benchmark discrete ordinate solution. A simplified model of electron interactions with tissue is employed to compute the dose of an electron beam in a water phantom, and a case of irradiation of the vertebral column. Here our model is compared to the PENELOPE Monte Carlo code. In the academic example, the fluences computed with the new model and a benchmark result differ by less than 1%. The depths at half maximum differ by less than 0.6%. In the two comparisons with Monte Carlo, our model gives qualitatively reasonable dose distributions. Due to the crude interaction model, these so far do not have the accuracy needed in clinical practice. However, the new model has a computational cost that is less than one-tenth of the cost of a Monte Carlo simulation. In addition, simulations can be set up in a similar way as a Monte Carlo simulation. If more detailed effects such as coupled electron–photon transport, bremsstrahlung, Compton scattering and the production of $\delta$ electrons are added to our model, the computation time will only slightly increase. Its margin of error, on the
other hand, will decrease and should be within a few per cent of the actual dose. Therefore, the new model has the potential to become useful for dose calculations in clinical practice.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Together with surgery and chemotherapy, the use of ionizing radiation is one of the main tools in cancer therapy. The aim of radiation treatment is to treat the tumour while minimizing the dose to normal tissue as much as possible. Furthermore, some regions at risk should receive a dose below a certain threshold.

Most electron dose calculation algorithms in clinical use rely on the Fermi–Eyges theory of radiation which does not include large-angle scattering. As a consequence of the small-angle scattering assumption, Fermi–Eyges theory equates path length and penetration depth. Therefore, models based on Fermi–Eyges theory can in principle only describe layered heterogeneities (Hensel et al 2006). By this reasoning, Krieger and Sauer (2005) explain that in one of their experiments, the pencil beam method produces a relative error of up to 12% in the dose in a heterogeneous phantom. This work, on the other hand, starts with a Boltzmann transport model for the radiation which in principle accurately describes all physical interactions.

Until recently, dose calculation using a Boltzmann transport equation has not attracted much attention in the medical physics community. This access is based on deterministic transport equations of radiative transfer. Similar to Monte Carlo simulations it relies on a rigorous model of the physical interactions in human tissue that can in principle be solved exactly. Monte Carlo simulations are widely used, but it has been argued that a grid-based Boltzmann solution should have the same computational complexity (Börgers 1998). Electron and combined photon and electron radiations were studied in the context of inverse therapy planning, cf Tervo et al (1999), Tervo and Kolmonen (2002) and most recently Tervo et al (2008). A consistent model of combined photon and electron radiation was developed (Hensel et al 2006) that includes the most important physical interactions. Furthermore, several neutral particle codes have been applied to the dose calculation problem, see Gifford et al (2006) for a review and most recently Vassiliev et al (2009), (2010).

In this paper, we wish to present a macroscopic approximation to the mesoscopic transport equation. After the problem formulation we derive the approximation of the macroscopic model. This approximation consists of a system of nonlinear hyperbolic partial differential equations, whose properties we briefly discuss. Due to the possibility of shock solutions, hyperbolic PDEs have to be solved with great care. We therefore introduce a scheme which is adapted to the problem at hand. We apply our model to several test cases. The case of a void-like layer is taken from Aydin et al (2002). We then compute the dose of an electron beam in a water phantom, before we consider a case of irradiation of the vertebral column, similar to Treutwein and Bogner (2007). Results are compared either to a highly resolved benchmark solution (in the academic test case) or to results from the PENELOPE Monte Carlo code.

2. Methods and materials

2.1. A deterministic model for dose calculation

A ray of high-energy electrons that interacts with human tissue is subject to elastic scattering processes and inelastic ones. It is these latter processes that lead to energy deposition in the tissue.
To formulate a transport equation for electrons we study their fluence \( \psi \) in phase space. The following quantities will be used:

- \( r \) position vector, unit: length,
- \( \epsilon \) particle energy, unit: energy,
- \( \Omega \) fluence in phase space, unit: \( \text{length}^{-2} \cdot \text{energy}^{-1} \cdot \text{time}^{-1} \),
- \( \rho_{\text{in}} \), \( \rho_{\text{el}} \) densities of inelastic and elastic scattering centres respectively, unit: \( \text{length}^{-3} \),
- \( \sigma_{\text{in}} \) differential cross section for inelastic scattering, unit: \( \text{length}^2 \cdot \text{energy}^{-1} \),
- \( \sigma_{\text{el}} \) differential cross section for elastic scattering, unit: \( \text{length}^2 \),
- \( \sigma_{\text{in}}^{\text{tot}} = \int_{S^2} \sigma_{\text{in}} \, d\Omega \) total cross section for inelastic scattering, unit: \( \text{length}^2 \),
- \( \sigma_{\text{el}}^{\text{tot}} = \int_{S^2} \sigma_{\text{el}} \, d\Omega \) total cross section for elastic scattering, unit: \( \text{length}^2 \),
- \( S \) stopping power, unit: \( \text{energy} \cdot \text{length}^{-3} \),
- \( D \) dose, unit: \( \text{energy} \cdot \text{mass}^{-1} \).

The term fluence means that

\[ \psi(r, \epsilon, \Omega) \cos \Theta \, dA \, d\Omega \, d\epsilon \]

can be interpreted as the number of electrons at position \( r \) that move in time \( dt \) through the area \( dA \) into the element of solid angle \( d\Omega \) around \( \Omega \) with an energy in the interval \((\epsilon, \epsilon + d\epsilon)\). The angle between direction \( \Omega \) and the outer normal of \( dA \) is denoted by \( \Theta \).

A more detailed description of this quantity and graphical interpretations can be found in textbooks on transport theory, e.g. Modest (1993), Mihalas and Weibel-Mihalas (1999), Davison (1958). The transport equation can generally be formulated as

\[
\Omega \cdot \nabla \psi(r, \epsilon, \Omega) = \rho_{\text{in}}(r) \int_0^\infty \int_{S^2} \sigma_{\text{in}}(\epsilon', \epsilon, \Omega') \psi(r, \epsilon', \Omega') \, d\Omega' \, d\epsilon' \\
+ \rho_{\text{el}}(r) \int_{S^2} \sigma_{\text{el}}(r, \epsilon, \Omega') \psi(r, \epsilon, \Omega') \, d\Omega' \\
- \rho_{\text{in}}(r) \sigma_{\text{in}}^{\text{tot}}(\epsilon) \psi(r, \epsilon, \Omega) - \rho_{\text{el}}(r) \sigma_{\text{el}}^{\text{tot}}(r, \epsilon) \psi(r, \epsilon, \Omega).
\]

Explicit formulae for the cross sections that we used in this model can be found in section 2.3. They are based on the model developed in Hensel et al (2006). The energy integration is performed over \((\epsilon, \infty)\) since the electrons lose energy in every scattering event.

Besides the transport equation we need an equation for the absorbed dose. It was derived in Hensel et al (2006) as an asymptotic limit of a model with a finite lower energy bound \( \epsilon_s > 0 \). The formula is exact if we choose the lower energy limit \( \epsilon_s = 0 \), as we do here:

\[
D(r) = \frac{T}{\rho(r)} \int_0^\infty S(r, \epsilon') \psi^{(0)}(r, \epsilon') \, d\epsilon' 
\]

with

\[
\psi^{(0)}(r, \epsilon) := \int_{S^2} \psi(r, \epsilon, \Omega') \, d\Omega'.
\]

\( T \) being the duration of the irradiation of the patient and \( \rho \) the mass density of the irradiated tissue. If all quantities are calculated in SI units, (2) leads to SI units \( \text{J} \cdot \text{kg}^{-1} \) or Gy (Gy) for the dose.

\( S \) is the stopping power related to the inelastic cross section. It is defined as

\[
S(r, \epsilon) = \rho_{\text{in}}(r) \int_0^\epsilon \epsilon' \sigma_{\text{in}}(\epsilon, \epsilon') \, d\epsilon'.
\]

In SI units, \( S \) is given in \( \text{J} \cdot \text{m}^{-1} \).

Finally, let us note that this mathematical framework is not restricted to electrons. Indeed, any particle that interacts with a medium can be described by an equation of the form (1).
albeit with different scattering coefficients. In Hensel et al. (2006), a similar equation has been used to describe photon transport in tissue. Although we restrict ourselves to electron transport here, we expect that the methods can be generalized to other particles as well.

2.2. Continuous slowing-down approximation

Electron transport in tissue has very distinctive properties. The soft collision differential scattering cross sections have a pronounced maximum for small-scattering angles and small energy loss. This allows for a simplification of the scattering terms in the Boltzmann equation. The Fokker–Planck equation is the result of an asymptotic analysis for both small energy loss and small deflections. It has been rigorously derived in Pomraning (1992) and has been applied to the above Boltzmann model in Hensel et al. (2006). However, some electrons will also experience hard collisions with large changes in direction and energy losses which have to be described by Boltzmann integral terms. Thus, we only use an asymptotic analysis to describe energy loss, called continuous slowing-down approximation. This approximation has a greater domain of validity than the Fokker–Planck approximation. The Boltzmann equation in continuous slowing-down approximation (BCSD) is (Larsen 1997)

$$\Omega \cdot \nabla \psi(r, \epsilon, \Omega) = \rho_{\text{in}}(r) \int_{S^2} \sigma_{\text{CSD}}(\epsilon, \Omega', \Omega) \psi(r, \epsilon, \Omega') d\Omega'$$

$$+ \rho_{\text{el}}(r) \int_{S^2} \sigma_{\text{el}}(r, \epsilon, \Omega') \psi(r, \epsilon, \Omega') d\Omega' - \rho_{\text{in}}(r) \sigma_{\text{tot}}(\epsilon) \psi(r, \epsilon, \Omega)$$

$$- \rho_{\text{el}}(r) \sigma_{\text{el}}(r, \epsilon) \psi(r, \epsilon, \Omega) + \frac{\partial}{\partial \epsilon} (S(r, \epsilon) \psi(r, \epsilon, \Omega)), \quad (4)$$

where

$$\sigma_{\text{CSD}}(\epsilon, \mu) = \int_{0}^{\infty} \sigma_{\text{in}}(\epsilon, \epsilon', \mu) d\epsilon'$$

is the energy-integrated inelastic scattering cross section. Note that in this model δ rays are not transported.

A truncation in the energy space is introduced, which does not allow particles with arbitrary high energy:

$$\lim_{\epsilon \to \infty} \psi(r, \epsilon, \Omega) = 0. \quad (5)$$

In the numerical simulations, we use a sufficiently large cutoff energy. Furthermore, we prescribe the ingoing radiation at the spatial boundary,

$$\psi(r, \epsilon, \Omega) = \psi_b(r, \epsilon, \Omega) \quad \text{for} \quad n \cdot \Omega < 0, \quad (6)$$

where $n$ is the unit outward normal vector.

2.3. Modelling of scattering cross sections

2.3.1. Henyey–Greenstein scattering theory. The detailed interactions of electrons with atoms give rise to complicated explicit formulae for the scattering coefficients. Because of this, many studies use the simplified Henyey–Greenstein scattering kernel for elastic scattering (Aydin et al. 2002):

$$\sigma_{\text{HG}}(\mu) = \frac{1 - g^2}{4\pi(1 + g^2 - 2g\mu)^{3/2}}. \quad (7)$$

The parameter $g$, which can depend on $r$, is the average cosine of the scattering angle and is a measure for the anisotropy of the scattering. The case where $g \neq 0$ matches an anisotropic scattering configuration.
2.3.2. Mott and Møller scattering. A more realistic model for elastic and inelastic scattering of electrons in tissue has been developed in Hensel et al (2006). This model introduces material parameters (namely densities $\rho_e$ and $\rho_c$, ionization energy $\epsilon_B$ and effective atomic charge $Z$). The energy integration for inelastic scattering is cut off at $\epsilon_B$.

The model uses the Mott scattering formula for elastic scattering of an electron by an ion (Mott and Massey 1965, Lehmann 1977):

$$\sigma_{\text{Mott}}(r, \epsilon, \Omega' \cdot \Omega) = \frac{Z^2(r)e^2(1 + \epsilon)^2}{4(\epsilon(\epsilon + 2))^2(1 + 2\eta(r, \epsilon) - \cos \vartheta)^2},$$

with $\vartheta = \arccos(\Omega' \cdot \Omega)$, and $\epsilon$ is the outcoming electron energy in $m_e c^2$ units. Here, $\alpha \approx 1/137$ is the fine structure constant, $Z$ is the atomic number of the irradiated medium, $r_e$ is the classical electron radius. $Z$ depends on $r$ to account for heterogeneous media. To avoid an otherwise occurring singularity at $\vartheta = 0$ a screening parameter

$$\eta(r, \epsilon) = \frac{\pi^2 \alpha^2 Z^2}{r} \frac{1 + 2}{\epsilon(\epsilon + 2)}$$

can be introduced (Zerby and Keller 1967) that models the screening effect of the electrons of the atomic shell, denoted by $a$.

The inelastic scattering process is Møller scattering, where an electron impinges an atom that releases itself an additional electron

$$e^- + a \rightarrow a^+ + 2 e^-.$$

For this process, the electrons can be considered indistinguishable. The electron which has the higher energy after the collision is called the primary electron; the other electron is called the secondary electron. Due to kinematical reasons of the scattering processes the range of solid angles in Møller scattering is restricted. After the collision, the angle between the directions of the electrons is at most $\pi/2$. For an angle in $[0, \pi/4]$, the electron with energy $\epsilon$ is the primary electron; for an angle in $[\pi/4, \pi/2]$, it is the secondary electron. Therefore, the Møller cross section can be written as

$$\sigma_M = \delta_M \chi_{\{0 < \Omega' \cdot \Omega < \pi/2\}} + \delta_M \delta \chi_{\{\pi/2 < \Omega' \cdot \Omega < 1\}},$$

where $\chi$ denotes the characteristic function of a set,

$$\delta_M(\epsilon', \epsilon, \Omega' \cdot \Omega) = \sigma_M(\epsilon', \epsilon) \delta_M(\mu, \mu_p) \frac{1}{2\pi}, \quad \mu = \Omega' \cdot \Omega,$$

is the Møller differential cross section of primary electrons and

$$\delta_M(\epsilon', \epsilon, \Omega' \cdot \Omega) = \sigma_M(\epsilon', \epsilon) \delta_M(\mu, \mu_p) \frac{1}{2\pi}, \quad \mu = \Omega' \cdot \Omega,$$

is the Møller differential cross section of secondary electrons. Here,

$$\sigma_M(\epsilon', \epsilon) = \frac{2\pi r_e^2}{\epsilon'(\epsilon' + 2)} \left[ \frac{1}{\epsilon'^2} + \frac{1}{(\epsilon' - \epsilon)^2} + \frac{1}{(\epsilon' + 1)^2} - \frac{2e' + 1}{(\epsilon' + 1)^2e'(\epsilon' - \epsilon)} \right],$$

and

$$\delta_M(\mu_e, \mu_p) = \delta \left( \mu_e - \sqrt{\frac{\epsilon' + 2}{\epsilon' + 2}} \right), \quad \text{for} \quad \epsilon > \frac{(\epsilon' - \epsilon_B)}{2},$$

$$\delta_M(\mu_e, \mu_p) = \delta \left( \mu_e - \sqrt{\frac{\epsilon' + 2}{\epsilon' + 2}} \right), \quad \epsilon < \frac{(\epsilon' - \epsilon_B)}{2}. \quad (8)$$

In the simulations the model parameters $\rho_{el}$, $\rho_m$, $\epsilon_B$ and $Z$ are fitted to tabulated values taken from the database of the PENELOPE Monte Carlo code (Salvat et al 2008).
2.4. Partial differential equation model

We attempted to reduce the computational cost of solving system (1) by assuming a minimum entropy principle for the angle distribution of particles. This principle has been first proposed by Jaynes (1957) as a method to select the most likely state of a thermodynamical system having only incomplete information. It has subsequently been developed in Minerbo (1978), Levermore (1984), Anile et al. (1991), Dubroca and Feugeas (1999) and Dubroca et al. (2010), among others, and has become the main concept of rational extended thermodynamics (Müller and Ruggeri 1993). A full account and an exhaustive list of references on the historical development can be found in Hauck et al. (2008).

We define the first three moments in angle:

\[
\psi^0(r, \epsilon) = \int_{S^2} \psi(r, \epsilon, \Omega) d\Omega, \tag{10}
\]

\[
\psi^1(r, \epsilon) = \int_{S^2} \Omega \psi(r, \epsilon, \Omega) d\Omega, \tag{11}
\]

\[
\psi^2(r, \epsilon) = \int_{S^2} (\Omega \otimes \Omega) \psi(r, \epsilon, \Omega) d\Omega, \tag{12}
\]

where we note that \(\psi^0\) is a scalar, \(\psi^1\) is a vector and \(\psi^2\) is a tensor.

If we integrate the system (4) over \(\Omega\), we can derive the following equations:

\[
\nabla_x \psi^1 = \frac{\partial}{\partial \epsilon} (S \psi^0), \tag{13}
\]

\[
\nabla_x \psi^2 = -(TM + TMott) \psi^1 + \frac{\partial}{\partial \epsilon} (S \psi^1). \tag{14}
\]

We have introduced the transport coefficients

\[
T_{in}(r, \epsilon) = \pi \rho_{in}(r) \int_{\epsilon_{min}}^{(\epsilon - \epsilon_{B})/2} \int_{-1}^{1} (1 - \mu) \sigma_{in}(\epsilon, \epsilon', \mu) d\mu d\epsilon', \tag{15}
\]

\[
T_{el}(r, \epsilon) = \pi \rho_{el}(r) \int_{-1}^{1} (1 - \mu) \sigma_{el}(\epsilon, \mu) d\mu. \tag{16}
\]

These coefficients and the stopping power can be computed for both Henyey–Greenstein and Mott/Möller scattering. Explicit expressions can be found in Hensel et al. (2006), Frank et al. (2007).

The remaining problem is the computation of moment \(\psi^2\) as a function of \(\psi^0\) and \(\psi^1\). The minimum entropy \(M^1\) closure for electrons (Brunner and Holloway 2001) can be derived in the following way. To close the system we determine a distribution function \(\psi_{ME}\) that minimizes the entropy of the electrons,

\[
H^*_R(\psi) = - \int_{S^2} \psi \log \psi d\Omega, \tag{17}
\]

under the constraint that it reproduces the lower order moments,

\[
\int_{S^2} \psi_{ME} d\Omega = \psi^0 \quad \text{and} \quad \int_{S^2} \Omega \psi_{ME} d\Omega = \psi^1. \tag{18}
\]

By using this entropy, we have implicitly assumed that the electrons obey classical Maxwell–Boltzmann statistics. This is justified, since quantum effects can be neglected here.
Analogous to the calculations in Levermore (1984) we can show that the entropy minimizer has the following form:

$$\psi_{\text{ME}} = a_0 \exp\left(-\Omega \cdot a_1\right),$$

(19)

where $a_0$ is a non-negative scalar, and $a_1$ is a three-component real-valued vector. This is a Maxwell–Boltzmann-type distribution and $a_0, a_1$ are the (scaled) Lagrange multipliers enforcing the constraints. An important parameter is the anisotropy parameter $\alpha$,

$$\alpha = \frac{\psi^{(1)}}{\psi^{(0)}},$$

whose norm is by construction less than or equal to 1. If we compute the different moments of the distribution function given by (19), we obtain

$$\psi^{(0)} = 4\pi a_0 \frac{\sinh(|a_1|)}{|a_1|}, \quad \psi^{(1)} = 4\pi a_0 \frac{\sinh(|a_1|)(1 - |a_1| \coth(|a_1|))}{|a_1|^3} a_1.$$

(20)

In fact, these relations can be combined to give

$$\alpha = \frac{1 - |a_1| \coth(|a_1|)}{|a_1|^2} a_1,$$

(21)

or by taking the modulus

$$|\alpha| = \frac{|a_1| \coth(|a_1|) - 1}{|a_1|}.$$

(22)

Relation (22) cannot be inverted explicitly by hand. This means that we cannot express $|a_1|$ as a function of $\alpha$ in a closed form. However, this relation determines a unique solution which can in principle be computed. If we assume that we know $a_1$, $\psi^{(2)}$ can be computed as

$$\psi^{(2)} = \psi^{(0)} \left( \frac{1 - \chi(\alpha)}{2} I + \frac{3\chi(\alpha) - 1}{2} \alpha \otimes \alpha \right),$$

(23)

where

$$\chi = \frac{|a_1|^2 - 2|a_1| \coth(|a_1|) + 2}{|a_1|^2}.$$

(24)

For its efficient numerical evaluation, the Eddington factor has to be approximated. Several possibilities exist.

- One could solve the closure relation (22) for $|a_1|$ e.g. by a Newton iteration in each step during the simulation.
- One could precompute a table that gives the Eddington factor $\chi$ as a function of $\alpha$.
- One could approximate $\chi(\alpha)$ by a suitable special function.

The second approach has been followed in Frank et al (2007). It is advantageous only if the space in which we interpolate is low dimensional. For more moments, this approach becomes more expensive, and the first approach appears to be more advantageous.

In some cases, an ansatz for $\chi$ can provide a good approximation. This is the approach we are following here. The Eddington factor $\chi$ can be approximated by a very simple rational function,

$$\chi(\alpha) \approx \frac{a_6 \alpha^6 + a_4 \alpha^4 + a_2 \alpha^2 + a_0}{\alpha^4 + b_2 \alpha^2 + b_0}.$$
This approximation is very accurate (the difference with the exact curve is about $10^{-15}$). The coefficients are given by

$$
a_0 = 0.762\,066\,949\,972\,264, \quad b_0 = 2.286\,200\,849\,916\,777,
\quad a_2 = 0.219\,172\,080\,193\,380, \quad b_2 = -2.107\,582\,089\,698\,400,
\quad a_4 = -0.259\,725\,400\,168\,378,
\quad a_6 = 0.457\,105\,130\,221\,120.
$$

The Eddington factor $\chi$ is shown in figure 1. Furthermore, we show the system eigenvalues in two dimensions. These eigenvalues show the speed at which a signal is propagated (normalized by the speed of light). In the isotropic regime (anisotropy parameter zero), they coincide with the P1 eigenvalues. On the other hand, in the case of free-streaming ($|\alpha| = 1$), they coincide and have an absolute value 1. Thus, the system (13), (14), (23) is hyperbolic and the speed of propagation is limited by 1. Moreover, the system is hyperbolic symmetrizable (Dubroca and Feugeas 1999). Analytical results have been obtained in Goudon and Coulombel (2006), Frank and Pinnau (2007). Since the reconstruction (19) of the kinetic distribution $\psi$ is always positive, it can be expected that the system (13), (14), (23) must admit a positive solution $\psi^{(0)}$ and a limited flux $||\alpha|| < 1$. To our knowledge, however, there exists no proof of this fact. In the absence of sources or boundaries, the total number of particles, momentum and energy are conserved. In addition, the minimum entropy system recovers the equilibrium diffusion regime as a relaxation limit for large absorption coefficients (Coulombel et al 2005).

In a two- or three-dimensional geometry, we have in addition (Berthon et al 2007): let $n$ be the unit normal vector to an interface; then the system exhibits two acoustic waves, with velocities $\lambda_L(n)$ and $\lambda_R(n)$, supplemented by a contact wave with velocity $\beta(n)$. The quantity $\beta \cdot n$ satisfies the inequality $\lambda_L(n) \leq \beta(n) \cdot n \leq \lambda_R(n)$. The Riemann invariants associated with the contact wave are $\{\beta, \Pi\}$. They are defined by the relations

$$
\psi_1 = (\Pi + \psi_0)\beta, \\
\psi_2 = (\psi_0 + \Pi)\beta \otimes \beta + \Pi I d.
$$

Figure 1. Eddington factor $\chi$ and system eigenvalues versus anisotropy parameter $|\alpha|$. (a) Eddington factor. (b) Eigenvalues.
2.4.1. Numerical method. The system (13), (14), (23) is a hyperbolic system of partial differential equations. There are many ways to numerically solve such a system. We have followed the approach outlined in Berthon et al (2007), and constructed a scheme that (among other properties) guarantees the positivity of the dose.

We adopt a pseudo-time technique. This means that a time dependence is added to the equations, and the equations are solved until a steady state is reached. We write the system in the form

\[
\frac{\partial}{\partial t} U + \text{div}_x [\mathcal{F}(U)] = -T U + \frac{\partial}{\partial \epsilon} U ,
\]

where

\[
\mathcal{F} = \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} \quad \text{and} \quad T = \begin{pmatrix} 0 & 0 \\ (T_{in} + T_{el}) & 0 \end{pmatrix}.
\]

We call \(\mathcal{F}\) the mathematical flux. The construction of the finite-volume scheme starts with a simple Harten–Lax–van Leer (HLL) scheme (Harten et al 1983) for the discretization of \(\mathcal{F}\). Since we also have to resolve the contact discontinuity in 2D and 3D, which effectively occurs at the lateral edges of a beam, this scheme has to be augmented to become an HLLC (Batten et al 1997) scheme. ‘C’ stands for contact discontinuity. This yields a scheme which is only first-order consistent. To speed up the convergence, we used a MUSCL (monotone upstream-centred schemes for conservation laws) (van Leer 1979) technique to obtain a second-order accurate scheme.

2.5. Setup

2.5.1. \(M_1\) model. As a Monte Carlo code, our model requires cross section data. Once this is given (either as the Heney–Greenstein formula, or Mott/Møller scattering), the stopping power and the transport coefficients can be computed. This can be done in a preprocessing step and does not have to be repeated. For Mott/Møller scattering, to obtain a good fit with the tabulated scattering data, we have fixed our model parameters for water as \(\epsilon_B = 16.0\) eV, \(Z = 9.40, \rho_{el} = 0.256 \times 10^{23} \text{ g cm}^{-3}, \rho_{in} = 6.21 \times 10^{23} \text{ g cm}^{-3}\). These parameters are directly inserted into the model (4), and subsequent derived models issued from (4).

The densities can be given as Hounsfield values in a voxelized geometry. To model the incoming beams, we have taken a very narrow Gaussian in energy, and a \(\delta\) pulse in angle:

\[
\psi_b = \psi_0 \exp(-200(\epsilon - \epsilon_{beam})^2)\delta(\mu - 1).
\]

Other energy spectra are possible. From these, the angular moments \(\psi^{(0)}\) and \(\psi^{(1)}\) have to be computed, which are used in the code.

2.5.2. Monte Carlo code and CT data. As a comparison to our method, we use the state-of-the-art Monte Carlo code PENELOPE (Salvat et al 2008). This code has been extensively validated against experimental results. PENELOPE was set up in a pseudo-2D setting with a large beam size perpendicular to the plane in which the beam propagated. We have used penEasy2009 in a voxelized geometry with standard simulation parameters. The energy cutoff for the initial source energy was set to 15 MeV. Electrons and positrons are assumed to be absorbed when their energy becomes less than 150 keV. For photons, this value was set to 15 keV. The critical angle \(\theta_c\) and critical energy \(W_c\) that separate hard events and soft events were set in the following way: for inelastic collisions, we set \(W_c = 150\) keV, for bremsstrahlung emission \(W_c = 15\) keV. The average angular deflection between consecutive hard elastic events \(C_1 = 0.1\) and the maximum average fractional energy loss between consecutive hard elastic
events \( C_2 = 0.1 \) uniquely determine \( \theta_c \). The maximum allowed step length for electrons and positrons is set to infinity: \( D_{\text{SMAX}} = 10^{35} \) cm. No variance reduction method was used.

2.6. Test cases

2.6.1. Academic test case. Our first test case, taken from Aydin et al (2002), is a two-dimensional quadratic domain which contains a void-like layer, shown in grey in figure 2(a). We consider only elastic scattering. This is an academic test case, which uses the Henyey–Greenstein scattering kernel. In Aydin et al (2002), it has been presented in context with photon transport. However, the setup may also serve as a test case for the electron transport equation.

We take \( \sigma_t = 0.5 \) mm\(^{-1} \) and \( \sigma_a = 0.005 \) mm\(^{-1} \) inside the square, and \( \sigma_t = 0.01 \) mm\(^{-1} \) and \( \sigma_a = 0.0001 \) mm\(^{-1} \) in the void-like ring. In both regions, \( g = 0 \). An isotropic source of particles is placed on the left boundary.
2.6.2. Electrons on water phantom. As a first test case that includes energy loss, we consider a 10 MeV electron beam impinging onto a slab of water. In figure 3 we compare the results computed with our code to the dose computed by PENELOPE.

2.6.3. Vertebral column. We took a two-dimensional slice from three-dimensional CT data. We apply our model to a case from the literature, a case of an irradiation of the vertebral column (Treutwein and Bogner 2007). The vertebral column is irradiated with a 15 MeV electron beam of width 8 cm. In each of the voxels, the material is described by its Hounsfield grey value $G(x, y)$. The grey values can be translated into physical parameters as follows:

$$\rho(x, y) = \left( \frac{G(x, y)}{1000} + 1 \right) \rho_w.$$ 

This means that the densities $\rho_{el}$ and $\rho_{in}$ for water are multiplied by a specified factor.

3. Results

3.1. Academic test case

In a 2D contour plot (figure 2), the fluxes $\psi^{(0)}$ from the discrete ordinate method and from the minimum entropy method are virtually indistinguishable. The propagation into the medium, as well as the void-like layer, is equally well resolved. A difference between the models only becomes apparent in a logarithmic plot of a cut through the centre of the square at $y = 50$ mm. Figure 2 shows the particle flux along this line. This is a logarithmic plot, so small differences are amplified. The depths at half maximum are 1.79 mm for $M_1$ and 1.80 mm for MC, which is a small difference. The difference between the fluences is at most 1%.

3.2. Electrons on water phantom

In order to compare the different models, both depth–dose curves in figure 3 have been normalized to dose maximum 1. The depth at half maximum $R_{50}$ for the $M_1$ model is
Figure 4. Isodose curves for the electron beam on the vertebral column. Normalized by \( D_{\text{max}} \), they are shown as 5% red, 10% orange, 25% yellow, 50% light blue, 70% dark blue, 80% violet. (a) Monte Carlo solution. (b) Minimum entropy solution.

4.21 g cm\(^{-2}\), and for MC it is 4.63 g cm\(^{-2}\). The reference depths are 2.43 g cm\(^{-2}\) for \( M_1 \) and 2.68 g cm\(^{-2}\) for MC. Thus, there is roughly a 10% difference between the penetration depth computed with the \( M_1 \) model and the Monte Carlo result. In addition, there is a major difference near the boundary, where the \( M_1 \) model overestimates the dose by about 15%. Because the above academic test case has shown good agreement between the \( M_1 \) result and a benchmark code, this difference can only be due to an oversimplified physical model. Indeed,
several effects have not been taken into account so far. These include Bremsstrahlung and the creation of $\delta$ electrons. For a detailed discussion of the underlying physical model we refer the reader to Hensel et al (2006). However, we believe that this result can serve as a proof of the concept of a PDE-based modelling of dose computation.

3.3. Vertebral column

This test case is similar to the one in Treutwein and Bogner (2007). The PENELOPE calculation took roughly 15 h; the $M_1$ computation took about 50 min. The statistical uncertainty of the MC calculation with 200 million particles is about 1.2%. The dose distributions computed with $M_1$ and with PENELOPE are shown in figure 4. Qualitatively, the isodose curves for the regions with lower dose agree reasonably well. Again, there appears to be a larger deviation near the boundary, which can be inferred from the difference in the 80% isodose curves. Figure 5 shows the differences between the two dose distributions. The biggest differences occur at the beam’s lateral edges. There, the beam width slightly differs. In most regions, the differences are below 2% (yellow isodose curves). Overall, 90.3% of the voxels are within 3% or 3 mm distance-to-agreement. This is of course not sufficient to be relevant in practice yet. The reason for the difference lies in an oversimplified model of the physical interactions.

4. Conclusions

We have developed a very simple and computationally inexpensive PDE model for electron dose calculation. From a mathematical perspective, this model has several desirable properties. In academic test cases, where we assume simple formulae for the differential cross sections, it agrees very well with benchmark results.

To show the method’s potential, a simplified model of electron interactions with tissue was employed to compute the dose of an electron beam in a water phantom, and a case of
irradiation of the vertebral column. The model can be set up in the same fashion as a Monte Carlo simulation is set up.

We observed qualitatively good agreement with dose distributions computed with PENELOPE. Quantitatively, however, there are still non-negligible differences. The model we have used, however, is very simple, and if properly augmented it will increase in accuracy while still maintaining its computational advantage.

The results show that if our model is developed further, it may serve as an alternative to existing dose computation methods.

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References

Anile A M, Pennisi S and Sammartino M 1991 A thermodynamical approach to Eddington factors J. Math. Phys. 32 544–50

Aydin E D, Oliveira C R E and Goddard A J H 2002 A comparison between transport and diffusion calculations using finite element-spherical harmonics radiation transport method Med. Phys. 29 2013–23

Batten P, Clarke N, Lambert C and Causon D M 1997 On the choice of wavespeeds for the HLLC Riemann solver SIAM J. Sci. Comput. 18 1553–70

Berthon C, Charrier P and Dubroca B 2007 An HLLC scheme to solve the $M_1$ model of radiative transfer in two space dimensions J. Sci. Comput. 31 347–89

Börgers C 1998 Complexity of Monte Carlo and deterministic dose-calculation methods Phys. Med. Biol. 43 517–28

Brunner T A and Holloway J P 2001 One-dimensional Riemann solvers and the maximum entropy closure J. Quant. Spectrosc. Radiat. Transfer 69 543–66

Coulombel J-F, Golse F and Goudon T 2005 Diffusion approximation and entropy-based moment closure for kinetic equations Asymptotic Anal. 45 1–39

Davison B 1958 Neutron Transport Theory (Oxford: Oxford University Press)

Dubroca B and Feugeas J L 1999 Entropic moment closure hierarchy for the radiative transfer equation C. R. Acad. Sci., Paris I 329 915–20

Dubroca B, Feugeas J L and Frank M 2010 Angular moment model for the Fokker-Planck equation Eur. Phys. J. D to be published

Frank M, Hensel H and Klar A 2007 A fast and accurate moment method for dose calculation in electron radiotherapy SIAM J. Appl. Math. 67 582–603

Frank M and Pinnau R 2007 Existence, uniqueness and bounds for the half moment minimum entropy approximation to radiative heat transfer Appl. Math. Lett. 20 189–93

Gifford K A, Horton J L Jr, Waringe T A, Failla G and Mourtada F 2006 Comparison of a finite-element multigroup discrete-ordinates code with Monte Carlo for radiotherapy calculations Phys. Med. Biol. 51 2253–65

Goudon T and Coulombel J-F 2006 Entropy-based moment closure for kinetic equations: Riemann problem and invariant regions J. Hyperbolic Differ. Equ. 3 649–72

Harten A, Lax P D and van Leer B 1983 On upstream differencing and Godunov-type schemes for hyperbolic conservation laws SIAM Rev. 25 35–61

Hauck C D, Levermore C D and Tits A L 2008 Convex duality in entropy-based moment closures: characterizing degenerate densities SIAM J. Control Optim. 47 1977–2015

Hensel H, Iza-Teran R and Siedow N 2006 Deterministic model for dose calculation in photon radiotherapy Phys. Med. Biol. 51 675–93

Jaynes E T 1957 Information theory and statistical mechanics Phys. Rev. 106 620–30

Krieger T and Sauer O A 2005 Monte Carlo-versus pencil-beam-/collapsed-cone-dose calculation in a heterogeneous multi-layer phantom Phys. Med. Biol. 50 859–68
Larsen E W, Miftn M M, Frass B A and Bruinvis I A D 1997 Electron dose calculations using the method of moments Med. Phys. 24 111–25
Lehmann C 1977 Interaction of Radiation with Solids and Elementary Defect Production (Amsterdam: North-Holland)
Levermore C D 1984 Relating Eddington factors to flux limiters J. Quant. Spectrosc. Radiat. Transfer 31 149–60
Mihalas D and Weibel-Mihalas B 1999 Foundations of Radiation Hydrodynamics (New York: Dover)
Minerbo G N 1978 Maximum entropy Eddington factors J. Quant. Spectrosc. Radiat. Transfer 20 541–5
Modest M F 1993 Radiative Heat Transfer 2nd edn (New York: Academic)
Mott N F and Massey H S W 1965 The Theory of Atomic Collisions (Oxford: Clarendon)
Müller I and Ruggeri T 1993 Rational Extended Thermodynamics 2nd edn (New York: Springer)
Pomraning G C 1992 The Fokker–Planck operator as an asymptotic limit Math. Models Methods Appl. Sci. 2 21–36
Salvat F, Fernandez-Varea J M and Sempau J 2008 PENELLOPE-2008, A Code System for Monte Carlo Simulation of Electron and Photon Transport (Issy-les-Moulineaux: OECD Nuclear Energy Agency)
Tervo J and Kolmonen P 2002 Inverse radiotherapy treatment planning model applying Boltzmann-transport equation Math. Models Methods Appl. Sci. 12 109–41
Tervo J, Kolmonen P, Vauhkonen M, Heikkinen L M and Kaipio J P 1999 A finite-element model of electron transport in radiation therapy and related inverse problem Inverse Problems 15 1345–61
Tervo J, Vauhkonen M and Bonan E 2008 Optimal control model for radiation therapy inverse planning applying the Boltzmann transport equation Linear Algebra Appl. 428 1230–49
Treutwein M and Bogner L 2007 Elektronenfelder in der klinischen Anwendung Strahlenther. Onkol. 183 454–8
van Leer B 1979 Towards the ultimate conservative difference scheme V: a second-order sequel to Godunov’s method J. Comput. Phys. 32 101–36
Vassiliev O N et al 2009 Feasibility of a multigroup deterministic solution method for 3d radiotherapy dose calculations Int. J. Radiat. Oncol. Biol. Phys. 72 220–7
Vassiliev O N et al 2010 Validation of a new grid-based Boltzmann equation solver for dose calculation in radiotherapy with photon beams Phys. Med. Biol. 55 581–98
Zerby C D and Keller F L 1967 Electron transport theory, calculations and experiments Nucl. Sci. Eng. 27 190–218