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High performance modelling of the transport of energetic particles for photon radiotherapy

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ABSTRACT

This work consists of the validation of a new Grid Based Boltzmann Solver (GBBS) conceived for the description of the transport and energy deposition by energetic particles for radiotherapy purposes. The entropic closure and a compact mathematical formulation allow our code (M1) to calculate the delivered dose with an accuracy comparable to the Monte-Carlo (MC) codes with a computational time that is reduced to the order of few minutes without any special processing power requirement. A validation protocol with heterogeneity inserts has been defined for different photon sources. The comparison with the MC calculated depth-dose curves and transverse profiles of the beam at different depths shows an excellent accuracy of the M1 model.

1. Introduction

External radiotherapy is one of the major cancer treatments that targets the tumor volume while keeping the radiation dose to healthy tissues as low as possible. The dose needs to be computed rapidly and accurately by simulating the particle transport and the energy deposition. This is achieved through specific software, the Treatment Planning System (TPS), based on efficient particle transport algorithms.

In principle, an exact dose calculation for the photon and electron beam can be performed by solving the linear Boltzmann transport equation (LBTE). This equation describes the transport of a system of particles. The cross sections determine the particles' (electron and photons) interactions with the surrounding media. The Monte Carlo (MC) method, often used as a benchmark, is among the different methods devised to solve the LBTE [1–3]. This technique consists of stochastic integration of the LBTE requiring low memory. However, a large number of stochastic events are necessary to reduce the statistical noise to an acceptable level. Consequently, the MC method can be very time consuming if it is not optimized using parallelization, variance reduction techniques or hardware improvements. In the last few decades, alternative methods, so called kernel models, have been proposed. Based on the Fermi-Eyges theory of radiative transport, they could be more efficient but regrettably fail in complicated settings where density gradients are present [4–6].

A third approach implies a deterministic solution of LBTE. The first commercially available deterministic algorithm, called Acuros® XB,[1] was introduced by Varian Medical Systems. This algorithm has proven to be an accurate method for dose calculation [7–9]. In order to solve the particle transport, Acuros® XB discretizes the LBTE in space, energy and in directions. Energy and spatial discretizations are performed using the multi-group method and adaptive meshing refinement (AMR), respectively. For the angular discretization, Acuros® XB uses the discrete ordinates technique. In order to reduce the number of directions, an angular quadrature is used. In the steady-state LBTE, this represents a 6D phase space that has to be calculated and stored. This approach, compared to BEAMnrc/DOSXYZnrc calculations, shows an agreement within ±2%/2 mm even in heterogeneous phantoms [9].

Here, we present a new method for solving the LBTE. This deterministic algorithm, called M1, is based on a multi-group energy approach combined with a specific angular momentum closure [10–12]. For each energy group, the equations for two angular moments (one scalar and one vector) are closed with an algebraic relation derived from the entropy maximization principle. The first model, describing the electron transport [12], is extended to

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photons and using an appropriate cross section library greatly improves the accuracy of calculations. Furthermore, we present numerical validation tests based on different stress cases which highlight the features of our method.

2. Materials and methods

2.1. M1 model

The M1 model was first derived in [10] for simulations of the radiation transport in plasmas and then adapted for the relativistic electron transport in [11]. In this section, we briefly revise the principal elements of the proposed algorithm. The dose calculation is based on the deterministic solution of the LBTE. The full distribution function depends on six variables (three space variables, two direction variables and one energy variable) and it includes two type of particles: the electrons and photons. The system of two coupled transport equations reads:

$$\Omega \cdot \nabla \cdot \psi^i + \sigma_t^i \psi^i = \sum_{p=[i,j]} \int d\epsilon \int_{S^2} d\Omega \sigma^{p,i}(\epsilon \to \epsilon\prime, \Omega \to \Omega\prime)\psi^i(r,\epsilon,\Omega) \tag{1}$$

where i,j are the species of particles, r is the position vector, ϵ the particle energy, Ω the flight direction, ψ is the particle angular flux, σ_t the total cross section for each species and $\sigma(r,\epsilon,\Omega)$ the differential cross section.

The common technique for discretizing the phase space variables in the LBTE is the discrete-ordinates method [13]. In this approach, the transport equation has to hold for a finite number of angles. To ensure the convergence to the analytic solution, the number of angles has to be sufficiently large otherwise, a detrimental numerical "ray-effect" arises that produces oscillations in the solution. Sophisticated computational techniques are required to mitigate it [14].

In contrast, our method is based on a reduced number of moment equations. Such an approach allows reducing the number of degrees of freedom, while keeping a good accuracy of calculations. The moments are defined as integrals over the unit sphere in the phase space of the flux functions ψ^i. As those moments depend on fewer variables (r,ϵ) than the fluences (r,ϵ,Ω), their computation requires less numerical effort. The first three angular moments of the distribution function are:

$$\psi_0^i(r,\epsilon) = \int_{S^2} \psi^i(r,\epsilon,\Omega)\, d\Omega,$$
$$\psi_1^i(r,\epsilon) = \int_{S^2} \Omega \cdot \psi^i(r,\epsilon,\Omega)\, d\Omega,$$
$$\psi_2^i(r,\epsilon) = \int_{S^2} (\Omega \otimes \Omega)\psi^i(r,\epsilon,\Omega)\, d\Omega,$$

where ψ_0 is a scalar, ψ_1 is a vector and ψ_2 is a tensor. The kinetic equations for the first two moments are:

$$\sigma_t^i(\epsilon\prime)\psi_0^i(r,\epsilon\prime) + \nabla \cdot \psi_1^i(r,\epsilon\prime) = \sum_{p=[i,j]} \int \sigma_0^{p,i}(\epsilon \to \epsilon\prime)\psi_0^i(r,\epsilon) d\epsilon,$$
$$\sigma_t^i(\epsilon\prime)\psi_1^i(r,\epsilon\prime) + \nabla \cdot \psi_2^i(r,\epsilon\prime) = \sum_{p=[i,j]} \int \sigma_1^{p,i}(\epsilon \to \epsilon\prime)\psi_1^i(r,\epsilon) d\epsilon.$$

The originality of our approach comes from the use of the entropy maximization principle (Boltzmann's H-theorem) to close this system of two pairs of equations for ψ_0^i and ψ_1^i containing three variables. The higher moment ψ_2^i is expressed as a function of ψ_0^i and ψ_1^i. The underlying distribution function ψ_{ME}^i that maximizes the entropy under the constraint of the two first moments definition has the form:

$$\psi_{ME}^i = a_0 e^{-\Omega \cdot a_1} \tag{2}$$

where a_0 and a_1 are the Lagrange multipliers, $a_0 \geqslant 0$ is a scalar, and $a_1 \in \mathbb{R}^3$ is a vector. This is a Maxwell–Boltzmann-type distribution function where a_0 and a_1 are related to the angular moments as follows:

$$\psi_0^i = 4\pi a_0 \frac{\sinh(|a_1|)}{|a_1|},$$
$$\psi_1^i = 4\pi a_0 \frac{\sinh(|a_1|)(|a_1|\coth(|a_1|) - 1)}{|a_1|^2} a_1.$$

The combination of these two equations leads to the definition of the anisotropy factor:

$$|\alpha| = \frac{|\psi_1^i|}{\psi_0^i} = \frac{1 - |a_1|\coth(|a_1|)}{|a_1|}. \tag{3}$$

The tensor ψ_2^i is explicitly related to the lower moments through the Eddington factor χ according to the following equation:

$$\psi_2^i = \psi_0^i \left(\frac{1-\chi(\alpha)}{2} \mathrm{I} + \frac{3\chi(\alpha) - 1}{2} \frac{\psi_1^i}{|\psi_1^i|} \otimes \frac{\psi_1^i}{|\psi_1^i|} \right). \tag{4}$$

The Eddington factor is related to the anisotropy factor by the following interpolation relation:

$$\chi = \frac{1}{3}(1 + \alpha^2 + \alpha^4). \tag{5}$$

The M1 model is able to treat various regimes of non-equilibrium, from the mono directional pencil beam case ($\alpha = 1$) to the isotropic case ($\alpha = 0$). M1 is the first member of this hierarchy allowing the treatment of most of clinically relevant configurations. Since the moments method is an approximation of the LBTE solution, for a better precision, one can consider the next member in the hierarchy, M2 [15], to get closer to the exact solution.

The M1 model, as described above, has been validated for medical applications limited to the electron transport in [12]. In the present paper, the system of coupled equations for the electrons and photons is analyzed. The accuracy of calculations is greatly improved by using the multigroup cross sections implemented by CEPXS software [16]. Consequently, a consistent and complete physical model, valid in the energy range from 1 keV to 100 MeV, is implemented and used as a numerical code allowing considering various clinical applications.

2.2. Numerical parameters of the M1 transport model

In the contrast to the discrete-ordinates method, the M1 model only requires a discretization in energy and space. In the present study, the energy range has been set between 1 keV and 10 MeV. The energy variable has been discretized into 50 energy groups both for electrons and photons. Spatial discretization was performed using the finite volume scheme based on the HLL approximate Riemann solver [17]. In the performed simulations a uniform orthogonal spatial discretization has been used with a cubic mesh of 1 mm^3.

2.3. Parameters of the MC reference simulations

The dose depositions calculated by the M1 model were compared to the MC simulations performed with the code PENELOPE-2014 [18]. This code simulates coupled electron-photon transport in the energy range from 100 eV to 1 GeV. In order to have the same initial conditions in the two codes, a phase-space input file has been generated for each particle source. In addition, each simulation have been

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