The M_2 model for dose simulation in radiation therapy

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Abstract

The transport of photons and electrons is studied in the field of radiotherapy to compute the dose, i.e. the quantity of energy transfered to the medium by a beam of particles at each position. A kinetic model is proposed, and to decrease the computation times, it is reduced through a moment extraction. Entropy-based angular moment models of order up to two (M_1 and M_2 models) are shown to provide accurate results compared to a reference code with much lower computational costs.

keywords: photons and electrons transport, moment models, entropy-based closure

1 Introduction

Transport theory is used in radiotherapy in order to model the motion of ionizing particles through human bodies. The aim of such therapy is to deliver a maximum quantity of energy, i.e. a dose, to the tumor cells so that they are destroyed and to minimize this dose in healthy tissue. The procedure of dose deposition can be described as follows: First, beams of photons are prescribed. They ionize the medium, i.e. they transfer a part of their energy to electrons which acquire enough energy to be transported. Then those electrons also ionize the medium. During such ionization procedure, a part of the energy of the electrons is transfered to the atoms, this produces the dose.

This work is a follow up to [12, 26, 10]. The aim is to produce a numerical method for dose computation based on a physical description of those inter-

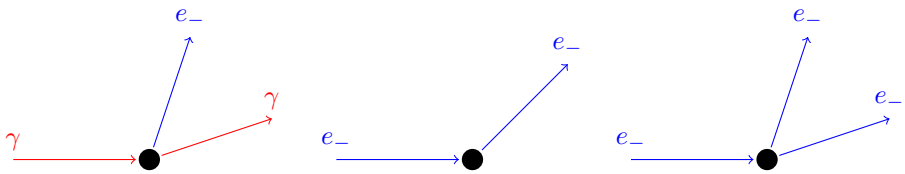

Figure 1: Schematic representation of Compton's (left), Mott's (midlle) and Møller's collisions: black balls represent atoms, red arrows are transported photons γ and blue arrows transported electrons e_-.

actions. Two main families of algorigthms are generally studied for such purpose: the statistical Monte-Carlo method ([4, 5]) and the deterministic discrete-ordinates methods ([21]). Both these approaches require high computing powers rarely available in medical centers.

Our numerical approach is deterministic and based on a kinetic model. In order to decrease the numerical cost, the kinetic model is reduced using moments extraction. This method was first studied for gas dynamics ([13, 20]) and was then applied to a large range of physics such as plasma physics ([14, 15, 22, 23]), semi-conductors ([3, 29]) or radiative transfer ([11, 19, 6]).

Through this paper, a moment model of order two, i.e. the M_2 model ([26, 15]), is shown to give satifactory results with low computational cost. In Section 2, the kinetic model and the procedure of moment extraction is described. Section 3 presents numerical comparisons between our approach and a reference Monte-Carlo code ([4, 5]). The last section is devoted to conclusions and perspectives.

2 Models

In order to compute the dose, the distributions of photons and electrons needs to be studied. First a kinetic model describing this transport is presented, then moment extraction is used.

2.1 Kinetic model

The photons travel through the medium, and they ionize it by Compton's effect ([18], see also Fig. 1). The electrons produced by those collisions are also transported. Their direction of flight and energy are altered by some other collisions (Mott's and Møller's) with atoms. Other effects on photons and electrons are neglected. Such transport of photons and electrons in radiation therapy can be

modelled by the following equations ([18, 12, 25])

$$\Omega.\nabla_x \psi_\gamma = \rho(x)\left[G_{\gamma\to\gamma}(\psi_\gamma) - \sigma_{T,\gamma}\psi_\gamma\right], \tag{1a}$$

$$\Omega.\nabla_x \psi_e = \rho(x)\left[\partial_\epsilon(S\psi_e) + G_{\gamma\to e}(\psi_\gamma) + G_{e\to e}(\psi_e) - \sigma_{T,e}\psi_e\right], \tag{1b}$$

$$G_{i\to j}(\psi_i)(x,\Omega,\epsilon) = \int_{S^2}\int_\epsilon^\infty \sigma_{i\to j}(\epsilon',\epsilon,\Omega'.\Omega)\psi_i(x,\Omega',\epsilon')d\epsilon' d\Omega'. \tag{1c}$$

The unknowns ψ_γ and ψ_e are the fluences of the photons and of the electrons. They depend on position $x \in Z$, energy $\epsilon \in [0, \epsilon_{max}]$ and direction of flight $\Omega \in S^2$. The density $\rho(x)$, the total cross sections $\sigma_{T,\gamma}(\epsilon)$ and $\sigma_{T,e}(\epsilon)$, the stopping power $S(\epsilon)$, and the different differential cross sections $\sigma_{\gamma\to\gamma}(\epsilon',\epsilon,\mu)$, $\sigma_{\gamma\to e}(\epsilon',\epsilon,\mu)$, $\sigma_{e\to e}(\epsilon',\epsilon,\mu)$ are known functions which can be found in [18, 25] and reference therein. This system is composed of two transport equations. Both equation is composed of one stationary transport term (left hand side) and one collision term (right hand side). The number of collisions is assumed to be proportionnal to the density ρ of the medium. The collision term for photons (linear Boltzmann) is composed of one gain term $G_{\gamma\to\gamma}$ and one loss term. The collision term for the electrons is composed of an energy derivative ([28, 25]), a gain term of electron due to photons $G_{\gamma\to e}$ and electrons $G_{e\to e}$ and a loss term.

The function of interest for medical physicists is the dose given by

$$D(x) = \int_0^{\epsilon_{\max}} S(\epsilon)\int_{S^2}\psi_e(x,\epsilon,\Omega)d\Omega d\epsilon.$$

The solution ψ of equation (1) depends on 3 variables of space $x \in \mathbb{R}^3$, 2 variables of direction $\Omega \in S^2$ and 1 variable of energy $\epsilon \in \mathbb{R}^+$. Solving numerically this equation is generally made by the use of Monte-Carlo algorithms (see e.g. [4, 5]) or of discrete-ordinates methods (see e.g. [21]). Both of these numerical methods typically require more numerical effort than is normally available in medical centers.

2.2 Moments models

The computational costs can be significantly reduced by working with moments ψ^i instead of fluences ψ. Let us define ψ^i, the moment of order i of ψ by

$$\psi^i = \left\langle \underbrace{\Omega\otimes\cdots\otimes\Omega}_{\text{i times}}\psi \right\rangle = \int_{S^2}\Omega\otimes\cdots\otimes\Omega\psi d\Omega.$$

Here $\otimes$ denotes the tensorial product. Extracting moments of (1) yields equations satisfied by the moments ψ^i. Moments of order 0 to 2 of (1) yield

$$\nabla_x.\psi_\gamma^1 = \rho\left[G^0_{\gamma\to\gamma}(\psi_\gamma^0) - \sigma_T\psi_\gamma^0\right], \tag{2a}$$
$$\nabla_x.\psi_\gamma^2 = \rho\left[G^1_{\gamma\to\gamma}(\psi_\gamma^1) - \sigma_T\psi_\gamma^1\right], \tag{2b}$$
$$\nabla_x.\psi_\gamma^3 = \rho\left[G^2_{\gamma\to\gamma}(\psi_\gamma^2) - \sigma_T\psi_\gamma^2\right], \tag{2c}$$
$$\nabla_x.\psi_e^1 = \rho\left[\partial_\epsilon(S\psi_e^0) + G^0_{\gamma\to e}(\psi_\gamma^0) + G^0_{e\to e}(\psi_e^0) - \sigma_{T,e}\psi_e^0\right], \tag{2d}$$
$$\nabla_x.\psi_e^2 = \rho\left[\partial_\epsilon(S\psi_e^1) + G^1_{\gamma\to e}(\psi_\gamma^1) + G^1_{e\to e}(\psi_e^1) - \sigma_{T,e}\psi_e^1\right], \tag{2e}$$
$$\nabla_x.\psi_e^3 = \rho\left[\partial_\epsilon(S\psi_e^2) + G^2_{\gamma\to e}(\psi_\gamma^2) + G^2_{e\to e}(\psi_e^2) - \sigma_{T,e}\psi_e^2\right], \tag{2f}$$

where $G^k_{i\to j}$ are given by

$$G^0_{i\to j}(\psi_i^0) = \int_\epsilon^\infty \sigma^0_{i\to j}(\epsilon',\epsilon)\psi_i^0(x,\epsilon')d\epsilon', \quad G^1_{i\to j}(\psi_i^1) = \int_\epsilon^\infty \sigma^1_{i\to j}(\epsilon',\epsilon)\psi_i^1(x,\epsilon')d\epsilon',$$
$$G^2_{i\to j}(\psi_i^2) = \int_\epsilon^\infty \frac{3\sigma^2_{i\to j} - \sigma^0_{i\to j}}{2}(\epsilon',\epsilon)\psi_i^2(x,\epsilon') + \frac{\sigma^0_{i\to j} - \sigma^2_{i\to j}}{2}(\epsilon',\epsilon)tr(\psi_i^2)(x,\epsilon')Idd\epsilon'.$$

The moments of the exact solution (ψ_γ, ψ_e) to (1) solve (2). In order to reduce computational times, one can solve (2) instead of (1). However the solution to (2) is not unique since this system has more unknowns $(\psi_\gamma^i, \psi_e^i)$ than equations. The common idea to close the system is to reconstruct some function ψ_R from the first moments ψ^i for $i \leq 2$ and then approximate ψ^3 by

$$\psi^3 \approx \langle \Omega\otimes\Omega\otimes\Omega\psi_R\rangle.$$

Applying this method here leads to writing $(\psi_e^3, \psi_\gamma^3)$ as a function of the moments $(\psi_\gamma^i, \psi_e^i)$ for $i \leq 2$, then the system (2) has as many unknowns as equations, and it has a unique solution.

The moment problem consists in finding (or chosing) one function ψ_R having the moments (ψ^0, ψ^1, ψ^2). Using a decomposition in spherical harmonics leads to writing ψ_R as a polynomial of degree 2, i.e.

$$\psi_R(\Omega) = \bar\lambda.\bar m(\Omega),$$

where $\bar m(\Omega)$ is a basis of polynomial of degree 2 and $\bar\lambda$ is the unique scalar vector of the same size such that the moments of ψ_R are (ψ^0, ψ^1, ψ^2). This closure is called the P_2 closure. This closure is very easy to compute. For our purpose, we prefer not to use the P_2 model for two reasons: first the P_2 ansatz can become negative which may produce instabilities (this problem was studied in [16, 24]). Second, radiotherapy requires the computation of the dose produced by beams of particles. Such beams are modelled by narrow Gaussians in Ω, which is badly approximated by polynomial ansatz.

Among the possible candidates for ψ_R (having the moments (ψ^0, ψ^1, ψ^2)), we chose the one that minimizes Boltzmann entropy function

$$\mathcal{H}(f) = f\log(f) - f,$$

which leads to the so-called M_2 models. The solution ψ_R to that minimization problem has the form ([7, 8, 9])

$$\psi_R(\Omega) = \exp(\bar{\lambda}.\bar{m}(\Omega)). \tag{3}$$

Chosing this ansatz, the moments system of equations has an entropy and is hyperbolic ([20]). **Remark although that other choices of entropy are available for $\mathcal{H}$ (see e.g. [19]).** Beam like distribution can be approached by this ansatz. This will also be discussed in the next section.

The coefficients of $\bar{\lambda}$ are generally determined by solving a minimization problem ([17, 2, 1])

$$\bar{\lambda} = \underset{\bar{a}}{argmin} \left\langle \exp(\bar{a}.\bar{m}(\Omega)) \right\rangle - \bar{a}.\bar{\rho}, \tag{4}$$

where $\bar{\rho}$ are the moments ψ^i associated to $\bar{m}(\Omega)$ reordered into a vector, i.e. $\bar{\rho} = \langle \bar{m}(\Omega)\psi \rangle$.

Solving such problem may also be computationally costly. As an alternative, we use the approximation proposed in [26] for the M_1 and the M_2 closure.

The M_1 equations are (2a,2b,2d,2e) where the closure ψ^2 is obtained by the previous entropy minimization method. **In that case, the ansatz** (3) **is invariant by rotation around the axis $\psi^1/|\psi^1|$, which leads to write the closure ψ^2 under the form (see [19] for the details)**

$$\psi^2 = \psi^0 \left(\frac{1-\chi}{2} Id + \frac{3\chi - 1}{2} \frac{\psi^1 \otimes \psi^1}{|\psi^1|^2} \right).$$

Here only the Eddington factor χ needs to be determined, this is one scalar function of one scalar $|\psi^1|/\psi^0$ which can easily be approximated ([26]).

In the M_2 case, the ansatz (3) **does not present such rotational invariance, and no such simple decomposition was found for the M_2 closure.** Instead, we constructed a polynomial fit such that ψ^3 is correct for some special values of (ψ^0, ψ^1, ψ^2) where ψ^3 is unique (see [26] for the details). For instance, when studying a 1D or 2D problem, the approximation of ψ^3 does not produce artificial transverse fluxes.

3 Numerical results

The kinetic (1), the M_1 (2a,2b,2d,2e) and the M_2 (2) models with the approximated closure ([26]) are compared on several test cases.

The kinetic equation is solved using upwind schemes in 1D and the probabilistic PENELOPE Monte-Carlo code ([4, 5]) in 2D. The moments equations are solved using the relaxation approach described in [27].

Both tests consist in computing the dose produced by a beam of particles inside a uniform water phantom (i.e. density ρ fixed at 1). Beams are prescribed as boundary condition

$$\psi(x = 0, y, \epsilon, \Omega) = 10^{10} \exp\left(-200(\epsilon_0 - \epsilon)^2\right) \exp\left(-1000(\Omega - e_1)^2\right). \tag{5}$$

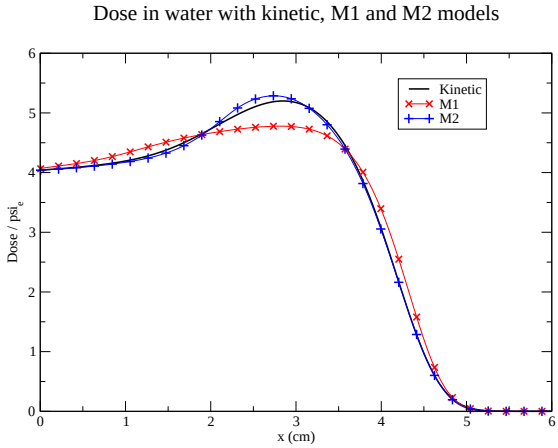

Figure 2: Normalized dose produced by a 10 MeV electron beam in a 1D water phantom using a kinetic, a M_1 and a M_2 solver with the approximated closures.

We impose a zero distribution function on the other boundary. The boundary conditions for the moment systems are defined by extracting moments from these boundary conditions.

10MeV electron beam in 1D water phantom:

The first test is a 1D computation for a 10MeV electron beam ($\psi_\gamma = 0$ and ψ_e is given by (5) with $\epsilon_0 = 10MeV$) in a 6cm long medium.

The dose normalized by

$$\int_{S^2} \int_0^{\epsilon_{max}} \psi_e d\epsilon d\Omega$$

is represented for the different models on Fig. 2 and the computation times for this test case are gathered in Table 1.

Model	Kinetic	M_1	M_2
Computation times	3 min	< 1 sec	< 1 sec

Table 1: Computation times for the 1D electron beam test with the different models

The M_N models have the right behaviour. Indeed the dose obtained with those model have the same shape as the one of the kinetic reference (slowly increasing at the entry of the medium and then falling to zero after the maximum at 3cm), although the dose obtained with the M_1 model is inaccurate. The maximum dose obtained with the M_1 model is lower than the ones with the M_2 and the kinetic models, and it drops faster after the maximum with those

two models than with the M_1 model. The slope at the entry is also inaccurate. These differences are due to an overestimation of the diffusion for the M_1 model. The results of the M_2 model follow more precisely those of the kinetic reference. As described in Table 1, solving the M_1 or M_2 equations accelerates significantly the computations compared to solving the kinetic equations.

1MeV photon beam in 2D water phantom:

The second test consists in computing the dose produced by the a 1cm long 1MeV photon beam (on the boundary $\psi_e = 0$ and ψ_γ is given by (5) with $\epsilon_0 = 1MeV$ for $y \in [3.5cm, 4.5cm]$) in a 50cm×8cm water phantom. In order to

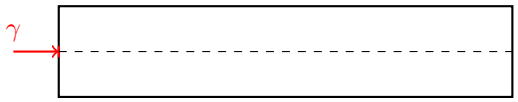

Figure 3: Configuration of the 2D photon test case

compare the results with the moment models with those of PENELOPE Monte-Carlo code, the dose is normalized by the maximum dose. This normalized dose is also called percentage dose depth (PDD).

The Fig. 4 depicts the dose along the lines at $y = 4cm$ (i.e. in the middle of the beam along its axis). The computational time for this 2D test are gathered in table 2.

Model	Kinetic	M_1	M_2
Computation times	10 h	5 min	6 min

Table 2: Computation times for the 2D photon beam test with the different models

The M_1 and the M_2 model are both very close to the reference kinetic, and the computational times are still much lower for the moments solver. The M_1 model gives much more accurate results for the photons beam case than for the electron beam case.

This difference of accuracy can be explain by the physics of the collision and the M_N approximation. The M_N ansatz (3) is accurate for single beam-like distributions (one narrow Gaussian) and in the isotropic limit (constant distribution). It is however inaccurate between those two limits. The higher the order N of the model, the better the ansatz ψ_R approximates arbitrary ψ (especially between those two limits). The advantages of the M_2 model compared to the M_1 can be seen when studying the intermediate case between the diffusion limit and the beam limit. When prescribing electron beams the electrons progressively lose energy and the fluence progressively isotropises , i.e. the continuous slowing down approximation (CSDA, [28]) can be applied to electrons cross sections (Mott and Møller's primary electron). So the M_2 model is better than the

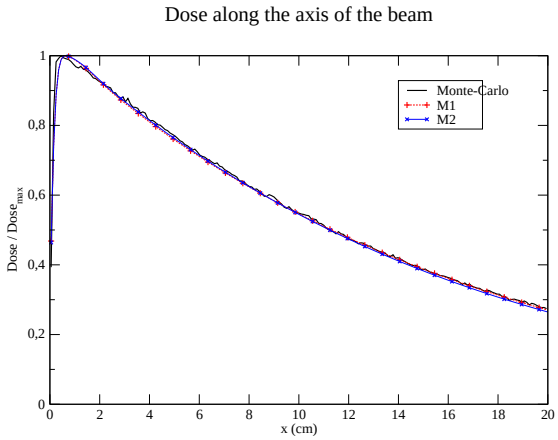

Figure 4: Normalized dose produced by a 1 MeV photon beam in a 2D water phantom along the axis of the beam (i.e. the line $y = 4cm$), using a Monte-Carlo, a M_1 and a M_2 solver with the approximated closures.

M_1 model on the electron test case. When studying photon beams of 1MeV, the photons pass quickly from a beam-like state to an isotropic state (the CSDA is invalid for those cross sections). So the difference between the M_1 and the M_2 model is smaller for the photon case.

4 Conclusion

A moment approach was presented and the moment models of order one and two were considered. Solving the moments equations (both M_1 or M_2 equations) requires lower computational times than a full kinetic solver. They were tested and compared to a full kinetic solver for two numerical test consisting of computing the dose produce by an electron beam in a 1D medium and by a photon beam in a 2D medium. These test show that the M_1 model is inaccurate when the distribution function isotropises slowly, and the M_2 model is accurate for a wider range of physical phenomena.

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