An Iterative Method for Transport Equations in Radiotherapy

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Summary. Treatment with high energy ionizing radiation is one of the main methods in modern cancer therapy that is in clinical use. During the last decades, two main approaches to dose calculation were used, Monte Carlo simulations and semi-empirical models based on Fermi–Eyges theory. A third way 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. In this work, we study a full discretization of the transport equation, whose solution is supposed to serve as a benchmark for simplified methods. The computational challenge is that scattering is forward-peaked, which makes a fine resolution and thus a very large linear system of equations necessary. Traditional methods like source iteration are inefficient or fail in this case. Therefore we propose a new method which combines an incomplete factorization of the scattering matrix and several iterative steps to obtain a fast and accurate solution. Numerical examples are given.

1 Introduction

The history of external beam radiation therapy starts with a remarkable anecdote: Literally two weeks after their discovery, X-rays were already used for cancer therapy. Röntgen discovered X-rays on December 28, 1895. Emil Grubbe, an undergraduate student at a medical school in Chicago, heard of Röntgen's work and obtained a vacuum discharge tube. He started experiments with the new rays, by producing X-ray images of himself. Obvious for us today, he started to suffer from radiation dermatitis. He realized the harmful effect of X-rays on tissue and on January 12, 1896, at the suggestion of one of his colleagues, he used his experimental setup to treat previously untreatable carcinoma. In February of 1896, he founded the first radiation therapy facility in Chicago.

Besides surgery and chemotherapy, the use of ionizing radiation is one of the main tools in the therapy of cancer today. According to WHO data, in the year 2007, there were about 11.3 million new cancer cases. More than half

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of the patients that are treated receive radiation therapy at one point during their treatment.

There are many challenges facing an applied mathematician in this field. One is optimal treatment planning which aims at ensuring that enough energy is deposited in cancer cells so that they are destroyed, while at the same time healthy tissue around the cancer cells should be harmed as little as possible and some regions at risk should receive almost no radiation at all. In this work, we focus on a different aspect, namely methods for dose calculation.

Most dose calculation algorithms in clinical use rely on the Fermi–Eyges theory of radiation. In recent work [6], it has been shown that these can produce errors of up to 12% near inhomogeneities. In this work, we consider dose calculation using a Boltzmann transport equation. 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 [2]. Electron and combined photon and electron radiation were recently studied in [5,7–9]. For a review on neutral particle codes that have been applied to the dose calculation problem we refer the reader to [4].

Here we study a full discretization of the transport equation, whose solution is supposed to serve as a benchmark for simplified methods. The computational challenge is that scattering is forward-peaked, which makes a fine resolution in energy and angle and thus a very large linear system of equations necessary. Traditional methods like source iteration are inefficient or fail in this case. Therefore we propose a simple iterative method which combines an incomplete factorization of the scattering matrix and several iterative steps to obtain a fast and accurate solution.

2 The Radiative Transfer Equation

The transport of particles that undergo inelastic scattering in a medium can be described by a Boltzmann transport equation

$$\begin{aligned}\mu\partial_x\psi(x,\epsilon,\mu) = \rho(x)\int_0^\infty\int_{-1}^1 s(x,\epsilon',\epsilon,\mu',\mu)\psi(x,\epsilon',\mu')d\mu' d\epsilon' \\ - \rho(x)\int_0^\infty\int_{-1}^1 s(x,\epsilon',\epsilon,\mu',\mu)\psi(x,\epsilon,\mu)d\mu' d\epsilon' + q(x,\epsilon,\mu)\end{aligned} \tag{1}$$

Here, ψ can be thought of being the number of particles at $x \in \mathbb{R}^3$ with energy ϵ, and direction $\mu \in [-1,1]$. To simplify the following presentation, we have written the radiative transfer equation in slab geometry (one-dimensional in both space and direction). However, our method can be easily extended and we show a two-dimensional (in both space and angle) result in the end. Scattering

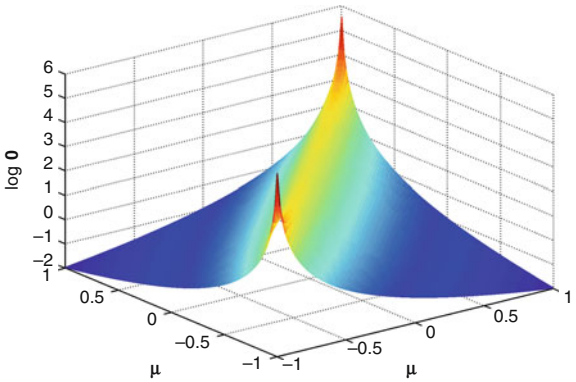

Fig. 1. Model Henyey–Greenstein scattering kernel ($g = 0.8$) as a function of μ and μ'

is determined by the density ρ of the medium and by the scattering kernel s, which can be seen as the probability that a particle with initial energy ϵ' and initial direction μ' has energy ϵ and direction μ after the scattering event. A model kernel is shown in Fig. 1. Note that the scale is logarithmic, which means that small angle changes are very likely. In order to resolve these small angle changes by a direct discretization, a large number of angles is necessary. As is well known and as we will again demonstrate later, traditional source iteration methods are inefficient for large scattering coefficients. Thus we propose a new iterative scheme. We should note that there exist several approximate methods to treat forward-peaked scattering (cf. [3]). These, however, introduce an additional approximation error. Our purpose here is to show that the equations can be solved by a direct method whose error can be controlled by the discretization only.

3 An Iterative Scheme

We discretize the unknown ψ in all variables. Let the index i denote direction, j energy, l space and n time, i.e.

$$\psi^n_{i,j,l} \sim \psi(t_n, x_l, \epsilon_j, \mu_i).$$

Here we have introduced an artificial time which we use as relaxation. Consider an implicit discretization in time, an upwind discretization in space and some discretization in energy and angle (e.g. finite differences or finite volume):

$$\frac{\psi^{n+1}_{i,j,l} - \psi^{n}_{i,j,l}}{\Delta t} + \mu_i^+ \frac{\psi^{n+1}_{i,j,l} - \psi^{n+1}_{i,j,l-1}}{\Delta x} + \mu_i^- \frac{\psi^{n+1}_{i,j,l+1} - \psi^{n+1}_{i,j,l}}{\Delta x}$$
$$= \rho_l \left(\sum_{i',j'} \sigma_{i,i',j,j'} \psi^{n+1}_{i',j',l} - \sum_{i',j'} \sigma_{i,i',j,j'} \psi^{n+1}_{i,j,l} \right).$$

We have neglected the source q and defined $\mu^+ = \max(\mu, 0)$, $\mu^- = \min(\mu, 0)$. Write this as

$$\left(\frac{1}{\Delta t} + \frac{|\mu_i|}{\Delta x} + \sum_{i',j'} \rho_l \sigma_{i,i',j,j'} \right) \psi^{n+1}_{i,j,l} - \sum_{i',j'} \rho_l \sigma_{i,i',j,j'}$$
$$= \frac{1}{\Delta t} \psi^{n}_{i,j,l} + \frac{\mu_i^+}{\Delta x} \psi^{n+1}_{i,j,l-1} - \frac{\mu_i^-}{\Delta x} \psi^{n+1}_{i,j,l+1}.$$

The left hand side is a matrix-vector multiplication in the i, j variables, the first term being a diagonal part. If we arrange the i, j in a suitable way into a vector ψ^n_l, we can write this as

$$M_l \psi^{n+1}_l = \frac{1}{\Delta t} \psi^{n}_{i,j,l} + \frac{\mu_i^+}{\Delta x} \psi^{n+1}_{i,j,l-1} - \frac{\mu_i^-}{\Delta x} \psi^{n+1}_{i,j,l+1}.$$

The symmetric matrix M_l is strongly diagonal-dominant but it is not sufficient to consider only its diagonal in an iterative scheme. The key idea is to factorize it as

$$M_l = A_l + B_l,$$

B_l containing the diagonal and a to be specified number of sub-/super-diagonals, and A_l containing the remainder. We want to invert the B_l part of M_l, thus we write

$$B_l \psi^{n+1}_l = \frac{1}{\Delta t} \psi^{n}_l + \frac{\mu_i^+}{\Delta x} \psi^{n+1}_{l-1} - \frac{\mu_i^-}{\Delta x} \psi^{n+1}_{l+1} - A_l \psi^{n+1}_l.$$

This is an implicit equation for ψ^{n+1}, which we solve iteratively by sweeping in the l variable. Let l run from 0 to $l_{\max}$, i.e. from left to right. The new iterate $\psi^{n+1,k+1}_l$ is given by

$$B_l \psi^{n+1,k+1}_l = \frac{1}{\Delta t} \psi^{n}_l + \frac{\mu_i^+}{\Delta x} \psi^{n+1,k+1}_{l-1} - \frac{\mu_i^-}{\Delta x} \psi^{n+1,k}_{l+1} - A_l \psi^{n+1,k}_l$$

and if we sweep from right to left

$$B_l \psi^{n+1,k+1}_l = \frac{1}{\Delta t} \psi^{n}_l + \frac{\mu_i^+}{\Delta x} \psi^{n+1,k}_{l-1} - \frac{\mu_i^-}{\Delta x} \psi^{n+1,k+1}_{l+1} - A_l \psi^{n+1,k}_l.$$

For $k \to \infty$ this gives us ψ^{n+1}. It only remains to iterate over the time index $n \to \infty$.

Table 1. Number of iterations as a function of time relaxation parameter

Relaxation Δt	10^1	10^2	10^3	10^4	10^5	10^6	10^7
Iterations	605	78	19	10	9	9	8

Table 2. Number of iterations for 64 directions and different matrix decompositions

Diagonals	0	1	2	4	8	12	14	16	32
Iterations	124	108	93	67	31	14	11	9	8

4 Numerical Results

First we study the convergence of our method. To that end we vary the relaxation time Δt and, more importantly, study the influence of the matrix decomposition. As a test case we choose an example from the medical physics literature [1]. It consists of a layered medium with depth 120 mm, consisting of three layers of 40 mm each, out of which the first and third are optically thick and the second is optically thin. It was sufficient to take 64 directions for the angle discretization. Table 1 shows the number of external iterations as a function of the time relaxation parameter, which should be chosen to be greater than 10^4. Table 2 shows how the performance of the algorithm depending on the matrix decomposition. The traditional source iteration method corresponds to the case of taking zero diagonals. We observe a significant decline in external iterations of more than one order of magnitude when we take several diagonals into matrix B_l. Of course the computational effort increases with the number of diagonals, since a larger linear system has to be solved. However, this increase is set off by the decrease in external iterations. Thus taking 16 diagonals (a quarter of the matrix dimension) is a sensible choice here.

We conclude with a test case in a two-dimensional quadratic domain which contains a void-like layer, shown in gray in Fig. 2. The physical parameters are detailed in [1]. An isotropic source of particles is placed on the left boundary. The propagation into the medium, as well as the void-like layer are equally well resolved in the numerical solution. The simulation used 64 directions and ran for about 10 min on 32 processors.

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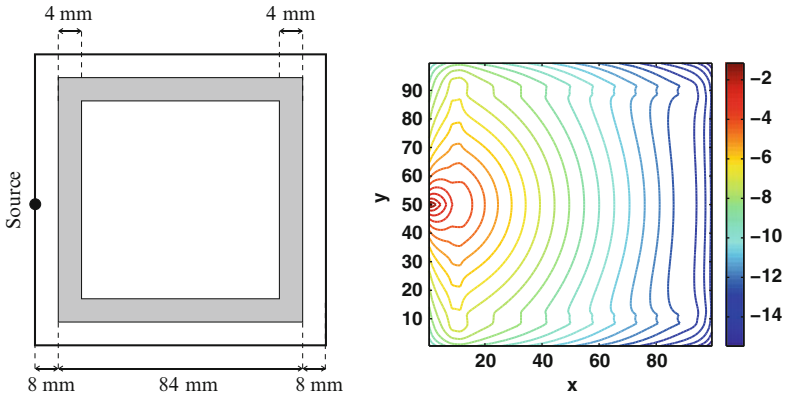

Fig. 2. Medium with void-like layer (*left*) and corresponding particle flux (*right*)

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