Numerical Solution of a Degenerate Parabolic Equation from Boltzmann-Fokker-Planck Equation. Application to Radiotherapy

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Abstract

The number of photons and electrons are needed for the dose calculation of radiotherapy of cancer treatment. The number of photons are calculated employing the Boltzmann Transport equation (BTE) by direct calculation. But it is very difficult to solve directly the BTE for electrons as the mean free path of electrons is much smaller than the mean free path of photons. Thus, alternatively, one can solve the Fokker- Planck equation instead of BTE, which is an approximation of the BTE based on the fact that the scattering process for electrons are very forward-peaked. In this paper, we propose a new numerical scheme for a degenerate parabolic partial differential equation using finite difference method of final value problem.

Keywords: Electron, Photon, Radiotherapy, forward-peaked, degenerate parabolic partial differential equation.

1 Introduction

Modern technology is considered by many to be one of the significant forces that drive the next major treatment revolution of the current century. In the present time, the high energy photon radiotherapy is very much useful for cancer treatment. For this reason it is most important to calculate the expected dose distribution, before starting the treatment of the patient, i.e. the distribution of absorbed radiative energy in the patient, has to be calculated. The major part for a treatment plan is the perfect dose calculation before beginning the treatment that should effect the real treatment as far as possible. When the dose of radiotherapy in the tumour tissue is not very low then it can be expected a curative effect. But when the dose is so high then the many healthy tissue surrounding the tumour will be destroyed or they will not be able to protect or avoid the undesirable side effect from the high dose.

We can find the exact dose calculation for photon and electron radiation. By well known physical principles of interaction of radiation with human tissue, the transport of energy into the patient's body can be modelled and calculated by an appropriate Monte Carlo (MC) algorithm [1]. If we work carefully then the results will be exact of the dose distribution in arbitrary geometries and nowadays highly developed MC codes for dose calculations are available but the computational time is very high in this case.

So, day by day in clinical use of this process is going to be unattractive.

The alternative approach to circumvent the drawback of the MC codes called kernel models [2] offers a reliable and fast alternative for most types of radiation treatment. The pencil beam models are probably most in use and these models are based on the Fermi-Eyges theory of radiative transfer [4] & [5]. The first introduce was for pure electron radiation [6] and later generalized to photon radiation [7] & [8], too. Although the result was good but the pencil beam models fail in complicated setting like air cavities or other inhomogeneities. This failure is based on the underlying Fermi-Eyges theory that assume, that multiple scattering only leads to small changes in the direction of the radiation. Because the theory was originally developed for astrophysical problems but it fails in human tissue by multiple scattering can lead to large angle changes even if every single scattering event in forward peaked. As a consequence of the small angle scattering the Fermi-Eyges theory that equals path length and depth of

the radiations particles approximately [5]. Because of this depth dependence of the physical parameters pencil-beam models can only account for layered heterogeneities that have to be approximated by a rescaling of the kernels [6].

In the last few years, it is seen that the deterministic Boltzmann equation of radiative transfer which the third access to dose calculation, which is based on the physical interactions of radiation in tissue. A mathematical model can be developed that allows in principle an exact dose calculation like as MC models. The resent studies for pure electron radiation were mostly done by Borgers and Larsen [10]. Electron and combined photon and electron radiation were studied by Tervo et al [11], Tervo and Kolmonen [12] in the context of inverse therapy planning and by Zhengming et al [13] who restricted their model to one dimensional slab geometry.

To the best knowledge of the authors, the solution of degenerate parabolic equation has not been analyzed numerically. The present study is focused only the numerical solution of degenerate parabolic equation employing Finite Difference Method. This degenerate equation has been taken from the Fokker-Planck approximation of the Boltzmann Transport equation for electrons.

2 The Fokker-Planck Equation

To find the exact dose calculation we need the number of electron which is found from the solution of the Fokker-Planck equation which is the approximation of the Boltzmann transport equation for electrons. In addition, the degenerate parabolic equation that is the important part of the Fokker-Planck approximation is presented here.

The Fokker-Planck equation is [3]

$$\Omega_{\mathsf{e}} \cdot \nabla \psi_{\mathsf{e}}(\mathbf{r}, \Omega_{\mathsf{e}}, \epsilon_{\mathsf{e}}) - [T_{\mathrm{Mott}}(\mathbf{r}, \epsilon_{\mathsf{e}}) + T_{\mathrm{M}}(\mathbf{r}, \epsilon_{\mathsf{e}})]L\psi_{\mathsf{e}} - \frac{\partial}{\partial \epsilon_{\mathsf{e}}} [S_{\mathrm{M}}(\mathbf{r}, \epsilon_{\mathsf{e}})\psi_{\mathsf{e}}] = Q(\mathbf{r}, \Omega_{\mathsf{e}}, \epsilon_{\mathsf{e}}), \qquad (1)$$

where L is the Laplace operator on the sphere which is given by

$$L = \frac{\partial}{\partial \mu_{\mathsf{e}}} (1 - \mu_{\mathsf{e}}^2) \frac{\partial}{\partial \mu_{\mathsf{e}}} + \frac{1}{1 - \mu_{\mathsf{e}}^2} \frac{\partial^2}{\partial \varphi_{\mathsf{e}}^2}, \qquad \mu_{\mathsf{e}} = \cos \vartheta_{\mathsf{e}}. \tag{2}$$

where;
$$0 \le \vartheta_{\mathsf{e}} \le \pi$$
. (3)

where, Q is the Compton source term.

$$Q(\mathbf{r}, \Omega_{\mathsf{e}}, \epsilon_{\mathsf{e}}) = \rho_{\mathsf{e}}(\mathbf{r}) \int_{0}^{\infty} \int_{S_{1/2}^{2}} \tilde{\sigma}_{C,\mathsf{e}}(\epsilon_{\gamma}', \epsilon_{\mathsf{e}}, \Omega_{\gamma}' \cdot \Omega_{\mathsf{e}}) \psi_{\gamma}(\mathbf{r}, \Omega_{\gamma}', \epsilon_{\gamma}') \,\mathrm{d}\Omega_{\gamma}' \,\mathrm{d}\epsilon_{\gamma}'$$
$$= \rho_{\mathsf{e}}(\mathbf{r}) \int_{S_{1/2}^{2}} \int_{0}^{\infty} \tilde{\sigma}_{C,\mathsf{e}}(\epsilon_{\gamma}', \epsilon_{\mathsf{e}}, \Omega_{\gamma}' \cdot \Omega_{\mathsf{e}}) \psi_{\gamma}(\mathbf{r}, \Omega_{\gamma}', \epsilon_{\gamma}') \,\mathrm{d}\epsilon_{\gamma}' \,\mathrm{d}\Omega_{\gamma}'. \tag{4}$$

Where the coefficient T_M , T_{Mott} and S_M are defined and evaluated in the appendix. This three coefficient are defined by atomic cores and the scattering cross section and the densities of the electrons. $\tilde{\sigma}_{C,e}(\epsilon'_{\gamma}, \epsilon_{e}, \Omega'_{\gamma} \cdot \Omega_{e})$ is the differential cross section for Compton scattering of electrons that is defined in the appendix. In addition, ϵ_{e} represents the energy of electrons, ϵ'_{γ} stands for the energy of incoming photon, Ω'_{γ} is the incoming direction of photon and Ω_{e} indicates the direction of electron.

3 The Degenerate parabolic partial differential equation

In this part, some notation for the Fokker-Planck equation (1) are used and discussed. A numerical scheme based on finite differences for this equation is presented here. We have tested the numerical scheme for an exact test. If we consider

$$\mu_{e} = \cos(\text{zenith angle}) = x; \ \varphi_{e} = \text{polar angle} = y; \ \lambda = z, \ \text{energy} = \epsilon_{e} = t \ \psi_{e} = u,$$

$$T_{\text{Mott}} + T_{\text{M}} = \text{constant} = T \text{ and } \frac{\partial S_{\text{M}}}{\partial \epsilon_{e}} = \text{constant} = B$$
(5)

then equation (1) becomes

$$\frac{\partial u}{\partial z} - T \left[\frac{\partial}{\partial x} (1 - x^2) \frac{\partial}{\partial x} + \frac{1}{1 - x^2} \frac{\partial^2}{\partial y^2} \right] u - S_{\rm M} \frac{\partial u}{\partial t} - Bu = Q \tag{6}$$

where $-1 \le x \le 1$, $0 \le y < 2\pi$, $0 \le z \le \lambda$.

To solve the equation (6), it is needed to select an appropriate method. For choosing the method, we take and solve some partial differential equations which are related to the equation (6). One of them is the following.

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left[(1 - x^2) \frac{\partial u}{\partial x} \right] = M(t, x), \tag{7}$$

where $x \in [-1, 1]$ and $t \in [0, T]$ (say). This equation is similar to the heat equation. We know the heat equation

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left[k(x) \frac{\partial u}{\partial x} \right] = M(t, x), \tag{8}$$

where the k(x) > 0 is heat conductivity. Our equation contains '+' sign in front of $\frac{\partial}{\partial x}$ instead of the '-' sign of the heat equation.

It is well known that for solving the heat equation an initial condition is needed. What we need now is a final condition due to the fact that we have a '+' sign in front of $\frac{\partial}{\partial x}$ instead of '-' sign.

Thus we consider the following final condition associated with the partial differential equation (7):

$$u(T,x) = u_T(x). \tag{9}$$

Let, on the other hand,

$$a(x) = (1 - x^2) \ge 0$$
 (since $-1 \le x \le 1$). (10)

4 Numerical Scheme

In this section, our numerical scheme is discussed in details. We look for a difference scheme of order one in t and order two in x. Regarding the x discretization, note that at the boundary of [-1, 1], the central difference formula cannot be used for the first order derivative with respect to x. So at -1, the forward difference formula for the first order derivative with respect to x is employed, while at 1, the backward difference formula for the first order derivative with respect to x is used (see [19], page

207). For the interior nodes of [-1, 1], that is to say, for the nodes belonging to the open interval (-1, 1), the appropriate central difference formula has been used.

Let n_x be the number of nodes in [-1, 1] and n_t - 1 be the number of "time" steps covering [0, T]. The following notations are considered

$$x_i = -1 + (i-1)h$$
, where $i = 1, ..., n_x$ and $\Delta x = h = \frac{2}{n_x - 1}$,
 $t_j = (j-1)k$, where $j = 1, ..., n_t$ and $\Delta t = k = \frac{T}{n_t - 1}$. (11)

For i = 1

The numerical scheme of (7)

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{-3a(x_i)\frac{\partial}{\partial x}u(t_j, x_i) + 4a(x_{i+1})\frac{\partial}{\partial x}u(t_j, x_{i+1}) - a(x_{i+2})\frac{\partial}{\partial x}u(t_j, x_{i+2})}{-2h} + M(t_j, x_i).$$
(12)

Despite having explicit appearance, this is an implicit approximation because we are solving a final value problem. We use the following notations.

$$u(t_j, x_i) \approx U_i^j, \ a(x_i) = a_i, \text{ and } M(t_j, x_i) = M_i^j.$$
 (13)

Note that here

$$a(x_i) = a(x_1) = a_1 = a(-1) = 0.$$
 (14)

Therefore we get from (12)

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{-1}{2h} \left[4a_{i+1} \frac{u(t_j, x_{i+2}) - u(t_j, x_i)}{2h} - a_{i+2} \frac{u(t_j, x_{i+3}) - u(t_j, x_{i+1})}{2h} \right] + M(t_j, x_i), \tag{15}$$

which suggests the following numerical scheme.

$$\frac{U_i^{j+1} - U_i^j}{k} = \frac{-1}{2h} \left[4a_{i+1} \frac{U_{i+2}^j - U_i^j}{2h} - a_{i+2} \frac{U_{i+3}^j - U_{i+1}^j}{2h} \right] + M_i^j, \quad (16)$$

$$\Leftrightarrow \left(\frac{a_{i+1}}{-h^2} - \frac{1}{k}\right) U_i^j = \frac{a_{i+1}}{-h^2} U_{i+2}^j + \frac{a_{i+2}}{4h^2} \left(U_{i+3}^j - U_{i+1}^j\right) - \frac{1}{k} U_i^{j+1} + M_i^j.$$
(17)

For i = 2

The numerical scheme of (7) is

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{a_{i+1} \frac{\partial}{\partial x} u(t_j, x_{i+1}) - a_{i-1} \frac{\partial}{\partial x} u(t_j, x_{i-1})}{-2h} + M_i^j.$$
(18)

Note that

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$$a_{i-1} = a_1 = a(x_1) = a(-1) = 0.$$
 (19)

Then we get from equation (18)

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{-1}{2h} \left[a_{i+1} \left(\frac{u(t_j, x_{i+2}) - u(t_j, x_i)}{2h} \right) \right] + M_i^j$$

$$\Rightarrow \frac{U_i^{j+1} - U_i^j}{k} = \frac{1}{-2h} \left[a_{i+1} \left(\frac{U_{i+2}^j - U_i^j}{2h} \right) \right] + M_i^j$$

$$\Leftrightarrow \left(\frac{a_{i+1}}{-4h^2} - \frac{1}{k} \right) U_i^j + \frac{a_{i+1}}{4h^2} U_{i+2}^j = \frac{1}{-k} U_i^{j+1} + M_i^j.$$
(20)

• For $3 \le i \le n_x - 2$ Now we consider

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{a(x_{i+\frac{1}{2}})\frac{\partial u}{\partial x}(t_j, x_{i+\frac{1}{2}}) - a(x_{i-\frac{1}{2}})\frac{\partial u}{\partial x}(t_j, x_{i-\frac{1}{2}})}{-h} + M_i^j,$$
(21)

where $x_{i+\frac{1}{2}} = x_i + \frac{h}{2}$ and $x_{i-\frac{1}{2}} = x_i - \frac{h}{2}$. Which leads to $\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{-1}{h} \left[a(x_{i+\frac{1}{2}}) \frac{u(t_j, x_{i+1}) - u(t_j, x_i)}{h} - a(x_{i-\frac{1}{2}}) \frac{u(t_j, x_i) - u(t_j, x_{i-1})}{h} \right] + M_i^j. \quad (22)$

By employing the natural notations $a_{i+\frac{1}{2}}=a(x_{i+\frac{1}{2}}),\,a_{i-\frac{1}{2}}=a(x_{i-\frac{1}{2}}),$ we arrive at

$$\frac{U_i^{j+1} - U_i^j}{k} = \frac{-1}{h^2} \left[a_{i+\frac{1}{2}} (U_{i+1}^j - U_i^j) - a_{i-\frac{1}{2}} (U_i^j - U_{i-1}^j) \right] + M_i^j$$
(23)

$$\Leftrightarrow \frac{a_{i-\frac{1}{2}}}{h^2} U_{i-1}^j - \left(\frac{1}{k} + \frac{1}{h^2} (a_{i+\frac{1}{2}} + a_{i-\frac{1}{2}})\right) U_i^j + \frac{a_{i+\frac{1}{2}}}{h^2} U_{i+1}^j = \frac{-1}{k} U_i^{j+1} + M_i^j.$$
(24)

• For $i = n_x - 1$ This is analogous to the case i = 2

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{a_{i+1} \frac{\partial}{\partial x} u(t_j, x_{i+1}) - a_{i-1} \frac{\partial}{\partial x} u(t_j, x_{i-1})}{-2h} + M_i^j \qquad (25)$$

Note that here

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$$a_{i+1} = a_{n_x} = a(x_{n_x}) = a(1) = 0.$$
(26)

Therefore we get from (25)

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{1}{2h} \left[a_{i-1} \frac{u(t_j, x_i) - u(t_j, x_{i-2})}{2h} \right] + M_i^j, \quad (27)$$

$$\Rightarrow \frac{U_i^{j+1} - U_i^j}{k} = \frac{a_{i-1}}{4h^2} (U_i^j - U_{i-2}^j) + M_i^j, \tag{28}$$

$$\Leftrightarrow \left(\frac{a_{i-1}}{-4h^2} - \frac{1}{k}\right) U_i^j + \frac{a_{i-1}}{4h^2} U_{i-2}^j = \frac{1}{-k} U_i^{j+1} + M_i^j.$$
(29)

For $\mathbf{i} = \mathbf{n}_{\mathbf{x}}$

This is analogous to the case i = 1,

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{a_{i-2}\frac{\partial}{\partial x}u(t_j, x_{i-2}) - 4a_{i-1}\frac{\partial}{\partial x}u(t_j, x_{i-1}) + 3a_i\frac{\partial}{\partial x}u(t_j, x_i)}{-2h} + M_i^j.$$
(30)

Note that here

$$a_i = a_{n_x} = a(x_{n_x}) = a(1) = 0.$$
 (31)

So we get from (30)

$$\frac{u(t_{j+1}, x_i) - u(t_j, x_i)}{k} \approx \frac{-1}{2h} \left[a_{i-2} \frac{u(t_j, x_{i-1}) - u(t_j, x_{i-3})}{2h} - 4a_{i-1} \frac{u(t_j, x_i) - u(t_j, x_{i-2})}{2h} \right] + M_i^j.$$
(32)

$$\Rightarrow \frac{U_i^{j+1} - U_i^j}{k} = \frac{-a_{i-2}}{4h^2} (U_{i-1}^j - U_{i-3}^j) + \frac{a_{i-1}}{h^2} (U_i^j - U_{i-2}^j) + M_i^j, \qquad (33)$$

$$\Leftrightarrow \left(\frac{a_{i-1}}{-h^2} - \frac{1}{k}\right) U_i^j = \frac{a_{i-2}}{-4h^2} \left(U_{i-1}^j - U_{i-3}^j\right) - \frac{a_{i-1}}{h^2} U_{i-2}^j - \frac{1}{k} U_i^{j+1} + M_i^j. \quad (34)$$

Equation (7), together with (9) is a final value problem, so we know the value of U_i^j when $j = n_t$. Now we will find the value of U_i^j when $j = n_t - 1$ (at t - T - k).

When $j = n_t - 1$ then we get from (20), (24) and (29) the following system of equations.

1. For
$$\mathbf{i} = 2$$

$$\left(\frac{a_{i+1}}{-4h^2} - \frac{1}{k}\right) U_i^{n_t - 1} + \frac{a_{i+1}}{4h^2} U_{i+2}^{n_t - 1} = \frac{1}{-k} U_i^{n_t} + M_i^{n_t - 1}, \quad (35)$$
2. For $3 \le i \le n_x - 2$

$$\frac{a_{i-\frac{1}{2}}}{h^2}U_{i-1}^{n_t-1} - \left(\frac{1}{k} + \frac{1}{h^2}(a_{i+\frac{1}{2}} + a_{i-\frac{1}{2}})\right)U_i^{n_t-1} + \frac{a_{i+\frac{1}{2}}}{h^2}U_{i+1}^{n_t-1} = \frac{-1}{k}U_i^{n_t} + M_i^{n_t-1},$$
(36)

and

3. For
$$\mathbf{i} = \mathbf{n}_{\mathbf{x}} - 1$$

$$\frac{a_{i-1}}{4h^2} U_{i-2}^{n_t-1} - \left(\frac{a_{i-1}}{4h^2} + \frac{1}{k}\right) U_i^{n_t-1} = \frac{1}{-k} U_i^{n_t} + M_i^{n_t-1}$$
(37)

accordingly.

We see from (35), (36) and (37) that the number of equations is $n_x -2$. We know the value of U_i^{nt} , for every $i = 1, 2 ..., n_x$ and the value of M_i^j for every $i = 1, 2 ..., n_x$, $j = 1, 2, ..., n_t$. therefore the right hand sides of the three equations (35), (36) and (37) are known and the number of unknowns is n_x-2 also. So we can write equations (35), (36) and (37) in a square matrix form easily:

$$\begin{bmatrix} -\frac{a_3}{4h^2} - \frac{1}{k} & 0 & \frac{a_3}{4h^2} & \cdots & 0 & 0 & 0 & 0 \\ \frac{3-\frac{1}{2}}{h^2} & -\left(\frac{1}{k} + \frac{1}{h^2}(a_{3+\frac{1}{2}} + a_{3-\frac{1}{2}})\right) & \frac{a_{3\frac{1}{4}h^2}}{h^2} & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \frac{a_{(nx-2)-\frac{1}{2}}}{h^2} & -\left(\frac{1}{k} + \frac{1}{h^2}(a_{(nx-2)+\frac{1}{2}} + a_{(nx-2)-\frac{1}{2}})\right) & \frac{a_{(nx-2)+\frac{1}{2}}}{h^2} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \frac{a_{n_x-2}}{4h^2} & 0 & -\left(\frac{1}{k} + \frac{1}{h^2}(a_{(nx-2)+\frac{1}{2}} + a_{(nx-2)-\frac{1}{2}})\right) & \frac{a_{(nx-2)+\frac{1}{2}}}{h^2} \\ \\ & & \\ 0 & 0 & 0 & \cdots & 0 & \frac{a_{n_x-2}}{4h^2} & 0 & -\left(\frac{a_{n_x-2}}{4h^2} + \frac{1}{k}\right) \end{bmatrix} \\ \times \begin{bmatrix} u_2^{n_t-1} \\ \vdots \\ u_{n_t-1}^{n_t-1} \\ \vdots \\ u_{n_x-1}^{n_t-1} \end{bmatrix} = \begin{bmatrix} \frac{-1}{k} u_{n_t}^{n_t} + M_{n_t-1}^{n_t-1} \\ \frac{-1}{k} u_{n_x-1}^{n_t} + M_{n_x-1}^{n_t-1} \\ \frac{-1}{k} u_{n_x-1}^{n_t-1} + M_{n_x-1}^{n_t-1} \end{bmatrix}$$

$$(38)$$

We solve the equation (38) and find

$$U_2^{n_t-1}, U_3^{n_t-1}, ..., U_{n_x-2}^{n_t-1} \text{ and } U_{n_x-1}^{n_t-1}.$$
 (39)

Again we get from (17) and (34) when $j = n_t - 1$.

1. For i = 1

$$\left(\frac{a_2}{-h^2} - \frac{1}{k}\right)U_1^{n_t - 1} = \frac{a_2}{-h^2}U_3^{n_t - 1} + \frac{a_3}{4h^2}\left(U_4^{n_t - 1} - U_2^{n_t - 1}\right) - \frac{1}{k}U_1^{n_t} + M_1^{n_t - 1},$$
(40)

and

2. For $i = n_x$

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$$\left(\frac{a_{n_x-1}}{-h^2} - \frac{1}{k}\right) U_{n_x}^{n_t-1} = \frac{a_{n_x-2}}{-4h^2} \left(U_{n_x-1}^{n_t-1} - U_{n_x-3}^{n_t-1}\right) - \frac{a_{n_x-1}}{h^2} U_{n_x-2}^{n_t-1} - \frac{1}{k} U_{n_x}^{n_t} + M_{n_x}^{n_t-1}$$

$$\tag{41}$$

accordingly.

From (40) and (41) we can find $U_1^{n_t-1}$ and $U_{n_x}^{n_t-1}$ respectively by using (39). Similarly we can find the value of U_i^j for all *i* and for $j = n_t - 2, n_t - 3, ..., 2, 1$.

4.1 Matlab code

I have made a MATLAB code to solve the equation (7) with the Final value condition (9) that means to solve (38), (40) and (41). The code is made of 4 m-files. The name of those m-files are benchmark, Exact2, FM2 and data.

- 1. In the benchmark m-file exact and approximate solutions are compared.
- 2. In the data m-file we give the input data for the program. Here we use the following notations.
 - (a) We use enx for the number of nodes in [x1, x2]. Where x1 is the lower limit and x2 is the upper limit of the range of x which is used in (7).
 - (b) We use ent where ent-1 is the number of time steps covering [t1, t2]. Where t1 is the lower limit and t2 is the upper limit of the range of t use in (7)
- 3. In Exact2 we put the exact solution u(t, x) for testing our Matlab code.
- 4. In FM2 we put function M(t, x). For exact test function M(t, x) is computed with (7) for a given u(t, x).

4.2 Numerical results

The present numerical scheme and matlab code is validated with some examples. We test our Matlab code for three exact tests. Let u(t, x) be a given function and put this u(t, x) in (7) in order to find the function M(t, x). By using M(t, x) we can find an approximate value of

 $u(t_j \ , \ x_i), \ where \ i=1, \ 2, \ ..., \ n_x \ and \ j=1, \ 2, \ ..., \ n_t \ \ -1.$

by using our Matlab code. Also we can find the exact value of $u(x_i, t_j)$ directly. We compare those two values of $u(t_j, x_i)$ and give the difference of the two values which is the error. We compute the error by means of the infinite norm over the grid (t_i, x_i) .

1. We take $u(t, x) = sin(t^2 + x^3)$ then we get by using (7)

 $M(t, x) = 2(t + 3x - 6x^3)\cos(t^2 + x^3) - 9x^4(1 - x^2)\sin(t^2 + x^3).$ (42)

n _x	n _t	Error	Time
11	11	0.2180	0.04 sec.
31	101	0.0426	0.08 sec.
91	1001	0.0037	1.64 sec.
271	10001	2.8624e-004	184 sec.

n _x	n _t	Error	Time		
11	11	0.2634	0.03 sec.		
31	101	1.0244	0.08 sec.		
91	1001	0.0022	1.56 sec.		
271	10001	2.0290e-004	177 sec.		
Table 2					

Table 1

Now we use this u(t, x) and M(t, x) in our Matlab code and find the error which we show in the table (1). Numerical results show that

error $\approx O(\triangle t) + O((\triangle x)^2)$, (43)

as expected. In here we see that if we reduce ten times the value of $\triangle t$ and ten times the value of $(\triangle x)^2$ then the error will reduce approximate ten times. But for reducing ten times the value of $(\triangle x)^2$ need to increase three times of n_x approximately. Which we represent in the following tables.

1. We see in the table $n_x = 11, 31, 91, 271$ because $\triangle x = h = \frac{x_2 - x_1}{n_x - 1}$ and also we use $n_t = 11, 101, 1001, 10001$ because $\triangle t = k = \frac{t_2 - t_1}{n_t - 1}$.

2. We take $u(t, x) = t^2 + x^3$ then we get by using (7) $M(t, x) = 2t + 6x + 12x^3$. (44)

Now we use this u(t, x) and M(t, x) in our Matlab code and find the error which we show in the table (2).

3. We take $u(t, x) = sin(x^2)$ then we get by using (7) M(t, x)

 $M(t, x) = 4x^{2}(x^{2} - 1)\sin(x^{2}) + 2(1 - 3x^{2})\cos(x^{2}).$ (45)

Now we use this u(t, x) and M(t, x) in our Matlab code and find the error which we show in the table (3).

5 Conclusion

The equation (7) contains a first order partial derivative with respect to t and a second order partial derivative with respect to x. Typically to solve this kind

n _x	n _t	Error	Time
11	11	0.1162	0.05 sec.
31	101	0.0152	0.08 sec.
91	1001	0.0011	1053 sec.
271	10001	8.4993e-005	177 sec.

Table 3

of equations, it is needed a final condition and two boundary conditions, one at x = -1 and other at x = 1. However, this is a degenerate parabolic PDE, it is degenerate because here a(x) = 0 at the boundary of [-1, 1], and for this reason the boundary values are not needed here. Therefore for choosing an appropriate numerical scheme we cannot choose any numerical scheme which is used to solve heat equation. We choose a numerical scheme which takes into account that a(x) = 0 at the boundary. As in the case of the heat equation, implicit schemes give better result than explicit ones. In this paper we present a numerical scheme of a degenerate parabolic partial differential equation which has been taken from the Fokker-Planck equation. Which may help to calculate the number of photons and

electrons for the dose calculation of radiotherapy of cancer treatment. Also, some examples are shown for proving the trueness of our MATLAB CODE in this paper.

6 Appendix

The coefficients are defined according to Pomraning [9]. Here ϵ'_e and ϵ_e indicate the energy of outgoing particle and incoming particle respectively.

6.1 Differential cross section for Møller scattering of primary electrons, i.e., $\epsilon_{\rm e} > (\epsilon'_{\rm e} - \epsilon_{\rm B})/2$

Literature.[14] and [15].

$$\tilde{\sigma}_{\mathsf{M}}(\epsilon'_{\mathsf{e}}, \epsilon_{\mathsf{e}}, \Omega'_{\mathsf{e}} \cdot \Omega_{\mathsf{e}}) = \sigma_{\mathsf{M}}(\epsilon'_{\mathsf{e}}, \epsilon_{\mathsf{e}}) \delta_{\mathsf{M}}(\mu_{\mathsf{e}}, \mu_{p}) \frac{1}{2\pi}, \quad \mu_{\mathsf{e}} = \Omega'_{\mathsf{e}} \cdot \Omega_{\mathsf{e}}$$
(46)

with

$$\sigma_{\mathsf{M}}(\epsilon'_{\mathsf{e}},\epsilon_{\mathsf{e}}) = \frac{2\pi r_{\mathsf{e}}^{2}(\epsilon'_{\mathsf{e}}+1)^{2}}{\epsilon'_{\mathsf{e}}(\epsilon'_{\mathsf{e}}+2)} \left[\frac{1}{\epsilon_{\mathsf{e}}^{2}} + \frac{1}{(\epsilon'_{\mathsf{e}}-\epsilon_{\mathsf{e}})^{2}} + \frac{1}{(\epsilon'_{\mathsf{e}}+1)^{2}} - \frac{2\epsilon'_{\mathsf{e}}+1}{(\epsilon'_{\mathsf{e}}+1)^{2}\epsilon_{\mathsf{e}}(\epsilon'_{\mathsf{e}}-\epsilon_{\mathsf{e}})} \right]$$
(47)

$$\delta_{\mathsf{M},\delta}(\mu_{\mathsf{e}},\mu_{\delta}) = \delta\left(\mu_{\mathsf{e}} - \sqrt{\frac{\epsilon_{\mathsf{e}}}{\epsilon'_{\mathsf{e}}}\frac{\epsilon'_{\mathsf{e}}+2}{\epsilon_{\mathsf{e}}+2}}\right), \ \epsilon_{\mathsf{e}} > (\epsilon'_{\mathsf{e}} - \epsilon_{\mathsf{B}})/2.$$
(48)

6.2 Differential cross section for Møller scattering of secondary electrons, i.e., $\epsilon_{\rm e} < (\epsilon_{\rm e}'-\epsilon_{\rm B})/2$

Literature.[14] and [15].

$$\tilde{\sigma}_{\mathsf{M},\delta}(\epsilon'_{\mathsf{e}},\epsilon_{\mathsf{e}},\mathbf{\Omega}'_{\mathsf{e}}\cdot\mathbf{\Omega}_{\mathsf{e}}) = \sigma_{\mathsf{M}}(\epsilon'_{\mathsf{e}},\epsilon_{\mathsf{e}})\delta_{\mathsf{M},\delta}(\mu_{\mathsf{e}},\mu_{\delta})\frac{1}{2\pi}, \quad \mu_{\mathsf{e}} = \mathbf{\Omega}'_{\mathsf{e}}\cdot\mathbf{\Omega}_{\mathsf{e}}$$
(49)

with

$$\sigma_{\mathsf{M}}(\epsilon_{\mathsf{e}}',\epsilon_{\mathsf{e}}) = \frac{2\pi r_{\mathsf{e}}^{2}(\epsilon_{\mathsf{e}}'+1)^{2}}{\epsilon_{\mathsf{e}}'(\epsilon_{\mathsf{e}}'+2)} \left[\frac{1}{\epsilon_{\mathsf{e}}^{2}} + \frac{1}{(\epsilon_{\mathsf{e}}'-\epsilon_{\mathsf{e}})^{2}} + \frac{1}{(\epsilon_{\mathsf{e}}'+1)^{2}} - \frac{2\epsilon_{\mathsf{e}}'+1}{(\epsilon_{\mathsf{e}}'+1)^{2}\epsilon_{\mathsf{e}}(\epsilon_{\mathsf{e}}'-\epsilon_{\mathsf{e}})} \right] (50)$$
$$\delta_{\mathsf{M},\delta}(\mu_{\mathsf{e}},\mu_{\delta}) = \delta \left(\mu_{\mathsf{e}} - \sqrt{\frac{\epsilon_{\mathsf{e}}}{\epsilon_{\mathsf{e}}'}\frac{\epsilon_{\mathsf{e}}'+2}{\epsilon_{\mathsf{e}}+2}} \right), \ \epsilon_{\mathsf{e}} < (\epsilon_{\mathsf{e}}'-\epsilon_{\mathsf{B}})/2. \tag{51}$$

6.3 Differential cross section for Mott scattering of electrons

Literature. [16] and [17].

 $\alpha \approx 1/137$ is the fine structure constant, Z is the atomic number of the irradiate medium. Z depends on r to account for heterogeneous media.

$$\sigma_{\text{Mott}}(\mathbf{r}, \epsilon_{\text{e}}, \mathbf{\Omega}_{\text{e}}' \cdot \mathbf{\Omega}_{\text{e}}) = \frac{Z^2(\mathbf{r})r_{\text{e}}^2(mc^2)^2}{4p^2c^2\beta^2\sin^4(\frac{\vartheta_{\text{e}}}{2})} \left[1 - \beta^2\sin^2\frac{\vartheta_{\text{e}}}{2} + Z\pi\alpha\beta\sin\frac{\vartheta_{\text{e}}}{2}(1 - \sin\frac{\vartheta_{\text{e}}}{2}) \right] \\ \approx \frac{Z^2(\mathbf{r})r_{\text{e}}^2(mc^2)^2}{4p^2c^2\beta^2\sin^4\frac{\vartheta_{\text{e}}}{2}} \left[1 - \beta^2\sin^2\frac{\vartheta_{\text{e}}}{2} \right],$$
(52)

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with $\beta^2 = \frac{\epsilon_e(\epsilon+2)}{(\epsilon+1)^2}$. The last approximation is justified, because in the energy range studied here and for typical low-Z media like water only small errors are made.

To avoid the singularity at $\vartheta_e = 0$ a screening parameter η can be introduced (see [18]) that models the screening effect of the electron and the atomic shell.

$$\sigma_{\rm Mott}(\mathbf{r},\epsilon_{\rm e},\Omega_{\rm e}'\cdot\Omega_{\rm e}) = \frac{Z^2(\mathbf{r})r_{\rm e}^2(1+\epsilon_{\rm e})^2}{4[\epsilon_{\rm e}(\epsilon_{\rm e}+2)]^2(1+2\eta(\mathbf{r},\epsilon_{\rm e})-\cos\vartheta_{\rm e})^2} \left[1-\frac{\epsilon_{\rm e}(\epsilon_{\rm e}+2)}{(1+\epsilon_{\rm e})^2}\sin^2\frac{\vartheta_{\rm e}}{2}\right],\tag{53}$$

where

$$\eta(\mathbf{r}, \epsilon_{\mathsf{e}}) = \frac{\pi^2 \alpha^2 Z^{\frac{2}{3}}(r)}{\epsilon_{\mathsf{e}}(\epsilon_{\mathsf{e}} + 2)}.$$
(54)

6.4 The Møller coefficient $T_{\rm M}$

Since the secondary (outgoing) electron has the lower energy $\epsilon'_e < \frac{\epsilon_e - \epsilon_B}{2}$, energy is restricted to $\left[\epsilon_{B, \frac{\epsilon_e - \epsilon_B}{2}}\right]$:

$$T_{\mathsf{M}}(\mathbf{r},\epsilon_{\mathsf{e}}) = \pi \rho_{\mathsf{e}}(\mathbf{r}) \int_{\epsilon_{\mathsf{B}}}^{(\epsilon_{\mathsf{e}}-\epsilon_{\mathsf{B}})/2} \int_{-1}^{1} (1-\mu) \tilde{\sigma}_{\mathsf{M}}(\epsilon_{\mathsf{e}},\epsilon_{\mathsf{e}}',\mu) d\mu \, d\epsilon_{\mathsf{e}}'.$$
(55)

Using the definition (see equations 46, 47 and 48) of the Møller scattering cross section one gets

$$T_{\mathsf{M}}(\mathbf{r},\epsilon_{\mathsf{e}}) = \frac{\rho_{\mathsf{e}}(\mathbf{r})}{2} \int_{\epsilon_{\mathsf{B}}}^{(\epsilon_{\mathsf{e}}-\epsilon_{\mathsf{B}})/2} \left(1 - \sqrt{\frac{\epsilon_{\mathsf{e}}-\epsilon_{\mathsf{e}}'}{\epsilon_{\mathsf{e}}}\frac{\epsilon_{\mathsf{e}}+2}{\epsilon_{\mathsf{e}}-\epsilon_{\mathsf{e}}'+2}}\right) \sigma_{\mathsf{M}}(\epsilon_{\mathsf{e}},\,\epsilon_{\mathsf{e}}')d\epsilon_{\mathsf{e}}'.$$
 (56)

This integral can in principle be calculated analytically.

6.5 The Mott coefficient $T_{ m Mott}$

$$T_{\mathsf{Mott}}(\mathbf{r},\,\epsilon_{\mathsf{e}}) = \pi \rho_{\mathsf{c}}(\mathbf{r}) \int_{-1}^{1} (1-\mu) \sigma_{\mathsf{Mott}}(\epsilon_{\mathsf{e}},\,\mu) d\mu.$$
(57)

The angular integration can be done analytically and one gets

$$T_{\text{Mott}}(\mathbf{r}, \epsilon_{\text{e}}) = -\frac{\pi Z^2(\mathbf{r}) r_{\text{e}}^2 \rho_{\text{c}}(\mathbf{r}) (\epsilon_{\text{e}} + 1)^2}{\epsilon_{\text{e}}^2 (\epsilon_{\text{e}} + 2)^2 (1 + \eta)}$$
(58)

× {1 +
$$\beta^2(1+2\eta)$$
 + (1 + η)(1 + 2 $\beta^2\eta$)[ln 2 η - ln(2 + 2 η)]}, (59)

with
$$\beta^2 = \frac{\epsilon_{e}(\epsilon_{e}+2)}{(\epsilon_{e}+1)^2}$$
 and $\eta = \eta(\mathbf{r}, \epsilon_{e})$ as defined in equation (54).

6.6 The Møller stopping power S_M

Insted of using the definition of Pomraning (1992) it is convenient to use the standard definition of the stopping power.

$$S_M(\mathbf{r}, \epsilon_{\mathbf{e}}) = \rho_{\mathbf{e}}(r) \int_{\epsilon_{\mathbf{B}}}^{(\epsilon_{\mathbf{e}} - \epsilon_{\mathbf{B}})/2} \epsilon'_{\mathbf{e}} \sigma_M(\epsilon_{\mathbf{e}}, \epsilon'_{\mathbf{e}}) \mathrm{d}\epsilon'_{\mathbf{e}}, \qquad (60)$$

Of course both definitions are equivalent.

This integral can be evaluated analytically, too, and one gets

$$S_{M}(\mathbf{r},\epsilon_{e}) = \frac{2\pi r_{e}^{2} \rho_{e}(r)(\epsilon_{e}+1)^{2}}{\epsilon_{e}(\epsilon_{e}+2)} \left[\frac{2\epsilon_{e}}{\epsilon_{e}-\epsilon_{B}} + 2ln \frac{\epsilon_{e}-\epsilon_{B}}{2} - ln\epsilon_{B} - \frac{\epsilon}{\epsilon-\epsilon_{B}} - ln(\epsilon-\epsilon_{B}) \right] + \frac{1}{2(\epsilon_{e}+1)^{2}} \left(\frac{(\epsilon_{e}-\epsilon_{B})^{2}}{4} - \epsilon_{B}^{2} \right) + \frac{2\epsilon_{e}+1}{(\epsilon_{e}+1)^{2}} \left(ln \frac{\epsilon_{e}-\epsilon_{B}}{2} - ln(\epsilon_{e}-\epsilon_{B}) \right)$$
(61)

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