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Optimal Control Model for
Inverse Radiation Therapy Treatment Planning

Jouko Tervo, Marko Vauhkonen, Eeva Boman, Petri Kokkonen, and Markku Nihtilä

Abstract— **A model for the inverse radiotherapy treatment planning is studied and discussed here. The dose calculation (forward problem) is based on the Boltzmann transport equation for charged particles. The required treatment optimization (inverse problem), which is always present in the real situations, is solved by the boundary control optimization theory for variational forms. We obtain the variational equations, where finite element methodology can be directly applied. Two finite element simulations are presented to show how boundary control optimization works in practice.**

I. INTRODUCTION

The Boltzmann transport equation (BTE) models various kind of transport phenomena of particles. The equation takes rigorously into account the scattering effects in inhomogeneous material. In the general situation, the transport of particles (photons, electrons, positrons) is covered by a system of three coupled Boltzmann transport (partial integro-differential) equations. Although the incoming radiation involves only one type of particles the interactions in media mobilize other types of particles. Hence it is necessary to consider at the same time the above mentioned three species of particles. For the transport theory of particles we refer to the monographs [3], [5], [7], [13]. The mathematical analysis related to the BTE can be found in [6]. Typical applications can be found *e.g.* in nuclear processes, cosmic radiation, material physics, and radiation therapy. Here we consider the inverse radiation treatment planning, where the inflow of particles is on the boundary of the region. We deduce the variational equations whose solution contains the optimal control. We suppose that the equations are linear. This assumption neglects some interactions between the particles which are not essential in our application.

Our application contains a problem arising in radiation therapy. In the radiation therapy treatment planning one tries to optimize the dose distribution to ensure high and homogeneous dose in the tumor, but on the other hand to spare the normal tissue and critical organs. This is called the inverse treatment planning problem which is mathematically a typical inverse problem. The dose distributions can be generated with different techniques. The most recent of them is the so-called multileaf collimator (MLC) delivery technique. For some reviews of radiation treatment planning we refer to [2], [4], [14], [18].

J. Tervo, P. Kokkonen and M. Nihtilä are with the Faculty of Business and Information Technology, Department of Mathematics and Statistics, and M. Vauhkonen and E. Boman are with the Faculty of Natural and Environmental Sciences, Department of Applied Physics, University of Kuopio, P.O.Box 1627, FI-70211 Kuopio, Finland {jouko.tervo; marko.vauhkonen; eeva.boman; petri.kokkonen; markku.nihtila}@uku.fi

Calculation of the dose distribution from the given incoming radiation is a forward problem. Its solving demands some dose calculation model. The present paper applies the BTE in dose calculation which has solid physical foundations. In [1] we have preliminarily studied the dose calculation applying the BTE model. The inverse problem is considered as an optimal boundary control problem. To our knowledge this approach is not previously applied in the literature. In [15], [16], [17] we have modeled and solved the related problems utilizing (global) optimization. In practice, the arising (variational) equations must be handled numerically. The discretization leads to very large dimensional problems.

II. TRANSPORT MODEL

A. Boltzmann transport equation

In the case where elastic collision, inelastic collision and "bremsstrahlung" are taken into account the stationary particle transport model consists of the following coupled system of partial integro-differential equations

$$\begin{aligned}
\Omega \cdot \nabla \psi_1 + K_1(\psi_1, \psi_2, \psi_3) &= Q_1(x, E, \Omega) \\
\Omega \cdot \nabla \psi_2 + K_2(\psi_1, \psi_2, \psi_3) &= Q_2(x, E, \Omega) \\
\Omega \cdot \nabla \psi_3 + K_3(\psi_1, \psi_2, \psi_3) &= Q_3(x, E, \Omega)
\end{aligned} \quad (1)$$

for $(x, E, \Omega) \in V \times I \times S$. In (1) $\psi_j = \psi_j(x, E, \Omega)$, $j = 1, 2, 3$ are the phase space densities of (angular) fluxes for photons, electrons and positrons, respectively. $x = (x_1, x_2, x_3)$ is the point in a domain $V \subset \mathbb{R}^3$ which is assumed to be open and bounded. S is the surface of the unit sphere in $\mathbb{R}^3$. $\Omega = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta) := h(\phi, \theta)$ is a point on S, where ϕ, θ are the standard spherical coordinates on S. In the following the integral $\int_S f(\Omega)\mathrm{d}\Omega$ denotes the surface integral $\int_S f(\Omega)\mathrm{d}\Omega = \int_W (f \circ h)(\phi, \theta)\sin\theta\mathrm{d}\phi\mathrm{d}\theta$, where $W := [0, 2\pi[\times [0, \pi[$. I is the energy interval, say $[E_0, E_f]$. ∇ is the *gradient with respect to the x-variable*. We are able to identify S with W. Hence the solution ψ is essentially defined in the 6-dimensional state space $G := V \times I \times S$.

The functions $K_j(\psi_1, \psi_2, \psi_3)$, $j = 1, 2, 3$ are collision terms resulting from different kinds of interactions. As mentioned above we assume that the model is linear. Hence the terms K_1, K_2, K_3 are linear functions of $\psi := (\psi_1, \psi_2, \psi_3)$. The interactions can be described by the differential and total

cross sections $\sigma_{j,k}(x,E',E,\Omega',\Omega)$, $\Sigma_{j,k}(x,E)$ as follows

$$K_j\psi = -\sum_{k=1}^{3}\Sigma_{j,k}(x,E)\psi_k$$

$$+\sum_{k=1}^{3}\int_S\int_I\sigma_{j,k}(x,E',E,\Omega',\Omega)\psi_k(x,E',\Omega')\mathrm{d}E'\mathrm{d}\Omega'.$$

Some analytical expressions and /or numerical values for the cross sections $\sigma_{j,k}(x,E',E,\Omega',\Omega)$, $\Sigma_{j,k}(x,E)$ can be found in the radiation therapy literature.

Finally, $Q_j(x,E,\Omega)$ are the source terms. These describe sources in V.

Physically the given Boltzmann equation (1) is based on a simple particle balance in an infinitesimal volume element expressed by the above concepts, see *e.g.* [13].

B. Inflow boundary condition for photon invasion

We consider especially the photon invasion in the stationary case. We assume that the boundary ∂V is a Lipschitz-boundary [6]. Then the outward normal $n(x)$ exists and it is continuous on ∂V possibly except a set with surface measure zero.

Let Γ_l, $l=1,...,L$ be (sufficiently smooth) patches of ∂V. To take into account the incoming external flux we must put some *(boundary) conditions* for the solution. In applications the typical conditions for the solution ψ are of the form

$$\psi_2(x,E,\Omega) = \psi_3(x,E,\Omega) = 0, \text{ for}$$
$$(x,E,\Omega) \in \partial V \times I \times S \text{ such that } n(x)\cdot\Omega < 0;$$
$$\psi_1(x,E,\Omega) = u_l(x,E,\Omega), \text{ for} \qquad (2)$$
$$(x,E,\Omega) \in \Gamma_l \times I \times S \text{ such that } n(x)\cdot\Omega < 0;$$
$$\psi_1(x,E,\Omega) = 0, \text{ for}$$
$$(x,E,\Omega) \in (\partial V \setminus \Gamma_l) \times I \times S \text{ such that } n(x)\cdot\Omega < 0.$$

Above $n(x)$ is the unit outward normal vector on the boundary surface ∂V. u_l is the photon flux per unit area incident on Γ_l. The condition $\psi_1 = u_l$ for $n(x)\cdot\Omega < 0$, $x \in \Gamma_l$ means that the beam (the flux u_l) is incoming from outwards on the patch Γ_l. The conditions $\psi_2 = \psi_3 = 0$ for $n(x)\cdot\Omega < 0$, $x \in \partial V$, $\psi_1 = 0$ for $n(x)\cdot\Omega < 0$, $x \in \partial V \setminus \Gamma_l$ mean that no outward fluxes (of corresponding particles) exist on ∂V and on $\partial V \setminus \Gamma_l$, respectively.

C. Variational formulation of the problem

Let $L_2(G)$ be the Lebesque space of (real-valued) square integrable functions on G with the usual inner product. Furthermore, let H be the linear (Sobolev) space

$$H = \{f \in L_2(G) | \Omega\cdot\nabla f \in L_2(G)\}.$$

H is a Hilbert space equipped with the inner product

$$\langle f,g\rangle_H = \langle f,g\rangle_{L_2(G)} + \langle \Omega\cdot\nabla f,\Omega\cdot\nabla g\rangle_{L_2(G)}.$$

In the product space H^3 the usual inner product

$$\langle f,g\rangle_{H^3} = \sum_{j=1}^{3}\langle f_j,g_j\rangle_H$$

for $f=(f_1,f_2,f_3)$, $g=(g_1,g_2,g_3) \in H^3$ is defined.

Define further linear operators $\Omega\cdot\nabla : H^3 \to L_2(G)^3$ and $K : L_2(G)^3 \to L_2(G)^3$ by

$$\Omega\cdot\nabla\psi := (\Omega\cdot\nabla\psi_1,\Omega\cdot\nabla\psi_2,\Omega\cdot\nabla\psi_3) \qquad (3)$$

and

$$K\psi := (K_1\psi,K_2\psi,K_3\psi) \qquad (4)$$

for $\psi = (\psi_1,\psi_2,\psi_3) \in H^3$. We find that $\Omega\cdot\nabla$ is a linear partial differential operator and K is a linear integral operator.

We assume the boundary conditions (2). Denote $Q = (Q_1,Q_2,Q_3)$. Then the problem gets the form

$$(\Omega\cdot\nabla + K)\psi = Q(x,E,\Omega) \qquad (5)$$

where ψ satisfies the boundary conditions (2).

In the following the subscripts " $-$ " and " $+$ " refer to the negative part and to the positive part of a function, respectively. The variational formulation of the problem (5) & (2) under physically relevant assumptions is given by

Theorem 1: Assume that

1. $\quad \Sigma_{j,k} \in L_\infty(V \times I)$, $\qquad\qquad\qquad$ (6)
2. $\quad \sigma_{j,k} \in L_\infty(V \times I^2 \times S^2)$, $\qquad\quad$ (7)
3. $\quad Q_j \in L_2(G)$, $u_l \in L_2(\Gamma_l \times I \times S)$. $\quad$ (8)

Then the variational form of the equation (5) with the stated boundary conditions (2) is given by

$$B(\psi,v) = F(v), \; v \in H^3 \qquad (9)$$

where $B(\cdot,\cdot) : H^3 \times H^3 \to \mathbb{R}$ is the bilinear form

$$B(\psi,v) = -\langle\psi,\Omega\cdot\nabla v\rangle_{L_2(G)^3} + \langle K\psi,v\rangle_{L_2(G)^3} \quad (10)$$
$$+ \sum_{j=1}^{3}\int_S\int_I\int_{\partial V}(\Omega\cdot n)_+\psi_j v_j\mathrm{d}\sigma\mathrm{d}E\mathrm{d}\Omega,$$

$$F(v)=\langle Q,v\rangle_{L_2(G)^3}+\sum_{l=1}^{L}\int_S\int_I\int_{\Gamma_l}(\Omega\cdot n)_- u_l v_1\mathrm{d}\sigma\mathrm{d}E\mathrm{d}\Omega. \;(11)$$

Define a norm for $\psi_j \in H$ by

$$||\psi_j||_{H_1}^2 = \int_S\int_I\int_{\partial V}|\Omega\cdot n|\psi_j^2\mathrm{d}\sigma\mathrm{d}E\mathrm{d}\Omega + ||\psi_j||_{L_2(G)}^2.$$

For $\psi \in H^3$ we define $||\psi||_{H_1^3}^2 = \sum_{j=1}^{3}||\psi_j||_{H_1}^2$. By the Trace Theorem [6] we find that $||\psi_j||_{H_1} \leq C||\psi_j||_H$. Hence also $||\psi||_{H_1^3} \leq C||\psi||_{H^3}$ for $\psi \in H^3$.

The adjoint (dual) spaces and operators are indicated by the superscript *. We formulate the following theorem

Theorem 2: Assume that (6), (7), (8) are valid, and that there exits $\kappa > 0$ such that for $\psi \in H^3$

$$\langle K\psi,\psi\rangle_{L_2(G)^3} \geq \kappa||\psi||_{L_2(G)^3}^2 \qquad (12)$$

Then the bilinear form $B(\psi,v)$ satisfies

$$B(\psi,v) \leq C||\psi||_{H^3}||v||_{H^3} \quad (H^3-\text{boundedness}) \quad (13)$$

for ψ, $v \in H^3$ and

$$B(\psi,\psi) \geq c||\psi||_{H_1^3}^2 \quad (H_1^3-\text{coercitivity}) \qquad (14)$$

for $\psi \in H^3$. In addition, $F \in (H_1^3)^*$ and there exists $C > 0$ such that

$$||\psi||_{H_1^3} \leq C||F|| \qquad (15)$$

where

$$||F|| := ||Q||_{L_2(G)^3} + \sum_{l=1}^{L} \sqrt{\int_S \int_I \int_{\Gamma_l} |(\Omega \cdot n)_-| u_l^2 \mathrm{d}\sigma \mathrm{d}E \mathrm{d}\Omega}.$$

The assumptions of Theorem 2 imply a sufficient condition for the unique existence of the (variational) solution $\psi \in H_1^3$. We remark that also the adjoint problem $B(v, \psi^*) = F'v$, $v \in H^3$ has a unique solution $\psi^* \in H_1^3$ for $F' \in (H_1^3)^*$ (below F' is given by the inner product).

In [1] we have proved the following sufficient algebraic criterion for the coercivity assumption (12)

Theorem 3: Assume that $\Sigma_{j,j}(x, E, \Omega) \in L_\infty(V \times I \times S)$ and $\sigma_{k,j}(x, E', E, \Omega', \Omega) \in L_\infty(V \times I^2 \times S^2)$. Suppose that there exists $\gamma > 0$ such that almost everywhere $(x, E, \Omega) \in G$

$$\Sigma_{j,j}(x, E, \Omega) - \int_S \int_I \sum_{k=1}^{3} \sigma_{k,j}(x, E', E, \Omega', \Omega) \mathrm{d}E' \mathrm{d}\Omega' \geq \gamma \quad (16)$$

$$\Sigma_{j,j}(x, E, \Omega) - \int_S \int_I \sum_{k=1}^{3} \sigma_{j,k}(x, E', E, \Omega', \Omega) \mathrm{d}E' \mathrm{d}\Omega' \geq \gamma \quad (17)$$

for $j = 1, 2, 3$. Then the inequality

$$\langle K\psi, \psi \rangle_{L_2(G)^3} \geq \gamma ||\psi||_{L_2(G)^3}^2, \ \psi \in H^3 \qquad (18)$$

is valid.

The assumptions (16)-(17) have physical foundations.

III. INVERSE RADIATION TREATMENT PLANNING

A. Optimal boundary control problem

The patient domain $V \subset \mathbb{R}^3$ contains tumor's (target's) region T, the region of critical organs C, and normal tissue's region N, whose disjoint union is $V = \mathrm{T} \cup \mathrm{C} \cup \mathrm{N}$. Assume that we have L fields S_l, $l = 1, ..., L$. This means that gantry, couch and collimator angles are determined and the whole treatment contains L different angle settings. Let the incoming (initial) flux distribution of the lth field S_l be u_l. Denote the corresponding (disjoint) patches of ∂V by Γ_l.

We have no internal sources. So $Q_l = 0$ for each field S_l. The effect of incoming flux is given by the functional

$$F(v) = \sum_{l=1}^{L} \int_S \int_I \int_{\Gamma_l} (\Omega \cdot n)_- u_l v_1 \mathrm{d}\sigma \mathrm{d}E \mathrm{d}\Omega. \qquad (19)$$

The bilinear form B is independent of the incoming flux.

The total dose $D = D(x) = D(x, \psi)$ is obtained from the functional

$$D(x) = \sum_{j=2}^{3} \int_S \int_I \kappa_j(x, E) \psi_j(x, E, \Omega) \mathrm{d}E \mathrm{d}\Omega =: L\psi(x) \quad (20)$$

where $\kappa_j(x, E)$ are known factors (so-called stopping powers). We assume that $\kappa_j \in L_\infty(V \times I)$.

Applying the above concepts the inverse radiation treatment planning problem is stated as:

Suppose that D_0 is the prescribed (uniform) dose in tumor T and that D_C and D_N are the upper bounds of dose in the critical organs C and in the normal tissue N, respectively. Furthermore, suppose that the number L and the gantry, coach and collimator angles of fields S_l are given.

For each $l = 1, ..., L$ determine the incoming flux $u_l \in L_2(\Gamma_l \times I \times S)$ such that

$$\begin{aligned} D(x) &= D_0, \ x \in \mathrm{T} \\ D(x) &\leq D_\mathrm{C}, \ x \in \mathrm{C} \qquad (21) \\ D(x) &\leq D_\mathrm{N}, \ x \in \mathrm{N}. \end{aligned}$$

subject to the constraints $u_l \geq 0$.

Besides the requirements (21) one often demands that so-called *dose volume constraints*, see [2] & [18], are fulfilled. In addition, the tumor, critical organs and normal tissue may be divided into many separate parts.

We denote

$$L_2(\Gamma \times I \times S) = L_2(\Gamma_1 \times I \times S) \times \cdots \times L_2(\Gamma_L \times I \times S).$$

Furthermore we denote $u = (u_1, ..., u_L) \in L_2(\Gamma \times I \times S)$ where $u_l \in L_2(\Gamma_l \times I \times S)$. The space $L_2(\Gamma \times I \times S)$ is equipped with the inner product

$$\langle u, u' \rangle_{L_2(\Gamma \times I \times S)} = \sum_{l=1}^{L} \langle u_l, u_l' \rangle_{L_2(\Gamma_l \times I \times S)}.$$

To clarify the u-dependence of variables we denote $\psi = \psi(u)$.

Let $\tilde{F} : L_2(\Gamma \times I \times S) \to (H^3)^*$ be the operator defined by

$$(\tilde{F}u)(v) = \sum_{l=1}^{L} \int_S \int_I \int_{\Gamma_l} (\Omega \cdot n)_- u_l v_1 \mathrm{d}\sigma \mathrm{d}E \mathrm{d}\Omega.$$

Note that $F(v) = (\tilde{F}u)(v)$.

Using these notations the solution $\psi = \psi(u)$ satisfies the variational equation $B(\psi(u), v) = (\tilde{F}u)(v)$, $v \in H^3$. Since $\tilde{F}$ is a linear function of u one can show by the uniqueness of solutions that the solution ψ is a linear function of u as well. Furthermore, L (defined by (20)) is a linear function of ψ.

Lemma 1: ψ is a bounded operator $L_2(\Gamma \times I \times S) \to L_2(G)^3$ and L is a bounded operator $L_2(G)^3 \to L_\infty(V)$ that is,

$$||\psi(u)||_{L_2(G)^3} \leq C_1 ||u||_{L_2(\Gamma \times I \times S)} \qquad (22)$$

for $u \in L_2(\Gamma \times I \times S)$ and

$$||L\psi||_{L_\infty(V)} \leq C_2 ||\psi||_{L_2(G)^3} \qquad (23)$$

for $\psi \in L_2(G)^3$.

Since L and ψ are bounded operators $L \circ \psi$ is Fréchet differentiable and $(L \circ \psi)'(u) = L \circ \psi$

The dose $D(x)$ must be as near as possible the described dose D_0 in tumor and the upper bounds of dose in critical organs and normal tissue may not be violated. Hence we try to optimize the incoming fluxes u_l so that this holds. The concrete implementation of this leads to the following optimization problem.

Define a cost functional by

$$
\begin{aligned}
J(u) \;=\; & c_1||D_0 - D(\cdot, \psi(u))||^2_{L_2(\mathrm{T})} \qquad\qquad (24)\\
+\; & c_2||(D_\mathrm{C} - D(\cdot, \psi(u)))_-||^2_{L_2(\mathrm{C})}\\
+\; & c_3||(D_\mathrm{N} - D(\cdot, \psi(u)))_-||^2_{L_2(\mathrm{N})}\\
+\; & c_4||(u)_-||^2_{L_2(\Gamma \times I \times S)} + a||u||^2_{L_2(\Gamma \times I \times S)},
\end{aligned}
$$

where c_1, c_2, c_3, c_4, a are positive weights. In this contribution, we do not present any mathematical theory to choose the weights c_j. In simulations, these parameters are chosen experimentally. The minimization of the second and the third terms tries to take care of the requirements $D(x) \leq D_\mathrm{C}$, $x \in \mathrm{C}$ and $D(x) \leq D_\mathrm{N}$, $x \in \mathrm{N}$. To keep the admissible control set as the whole space $L_2(\Gamma \times I \times S)$ or its suitable linear subspace U we added a penalty term $c_4||(u)_-||^2_{L_2(\Gamma \times I \times S)}$ which hinders the violation of the constraint $u_l \geq 0$. The last (convex) term regularizes the schemes and helps the optimization process in theory and in numerical considerations. To diminish (that is, minimization of $||u||^2_{L_2(\Gamma \times I \times S)}$) the incoming fluency u may also be of practical importance. Also the dose volume constraints can be added to the cost function.

As a conclusion we find that the corresponding optimization problem states : *Find the minimum*

$$
\min_{u \in U} J(u) \qquad\qquad (25)
$$

such that

$$
B(\psi(u), v) = (\tilde{F}u)(v), \;\; v \in H^3. \qquad\qquad (26)
$$

B. Optimal solution

The optimal control u_0 minimizes the functional J among the set, say U_{ad}, of admissible controls u. The well known necessary condition for the optimal control u_0 is that [6]

$$
B(\psi(u_0), v) = (\tilde{F}u_0)(v), \;\; v \in H^3
$$

and that

$$
J'(u_0)(u - u_0) \geq 0 \text{ for all } u \in U_{ad}. \qquad (27)
$$

In the case where U_{ad} is the linear space U (as in our case) the condition (27) reduces to

$$
J'(u_0) = 0. \qquad\qquad (28)
$$

In the case where J is a convex function the condition (28) is also sufficient for the optimal control. Our functional J, however contains also nonconvex terms.

The adjoint $L^* : L_\infty(V)^* \rightarrow L_2(G)^3$ of L can be computed and

$$
L^*w = (\kappa_1 w, \kappa_2 w, \kappa_3 w), \quad w \in L_1(V).
$$

In addition, the adjoint $\tilde{F}^* : H^3 \rightarrow L_2(\Gamma \times I \times S)$ of $\tilde{F}$ is

$$
\tilde{F}^*v = \left(r_{\Gamma_1}((\Omega \cdot n)_- v_1), ..., r_{\Gamma_L}((\Omega \cdot n)_- v_1) \right) \qquad (29)
$$

where r_{Γ_l} is the restriction operator on Γ_l.

We replace the negative part of a function by a Fréchet differentiable approximation. This can be done as follows, for example. Let H_ϵ be some approximation of the Heaviside function. We can choose

$$
H_\epsilon(x) = \mathrm{erf}_\epsilon(x) = \frac{1}{\sqrt{\pi}\epsilon} \int_{-\infty}^{x} e^{-s^2/\epsilon^2} \mathrm{d}s. \qquad (30)
$$

Then the negative part f_- of a function $f \in L_2(V)$ is approximately given by

$$
f_- \approx -(H_\epsilon \circ (-f))f. \qquad\qquad (31)
$$

Note that $H_\epsilon \in L_\infty(\mathbb{R})$.

Let A be a Lebesgue measurable subset of V. Furthermore, let r_A be the restriction operator $r_A f = f_{|A}$ and let e_A be the "extension by zero operator" from a set A on V.

Lemma 2: The function $g_A : L_\infty(V) \rightarrow L_2(A)$ defined by $g_A(f) = r_A(-H_\epsilon \circ (-f))f)$ is Fréchet differentiable and

$$
g_A'(f)h = r_A([(H_\epsilon' \circ (-f)) \cdot f - H_\epsilon \circ (-f)] \cdot h). \quad (32)
$$

In addition, $g_A'(f)^*w \in L_1(V)$ and

$$
g_A'(f)^*w = e_A([(H_\epsilon' \circ (-f)) \cdot f - H_\epsilon \circ (-f)] \cdot w), \quad (33)
$$

where $w \in L_2(A)$.

Similarly we approximate $u_- \approx -(H_\epsilon \circ (-u))u =: g_0(u)$. The function $g_0 : L_\infty(\Gamma \times I \times S) \rightarrow L_2(\Gamma \times I \times S)$ is Fréchet differentiable and its derivative $g_0'(u)$ and the adjoint $g_0'(u)^*$ are calculated analogously to Lemma 2. Using these approximations the object function is

$$
\begin{aligned}
J(u) \;=\; & c_1||r_\mathrm{T}(D_0 - L\psi(u))||^2_{L_2(\mathrm{T})} \qquad\qquad (34)\\
+\; & c_2||g_\mathrm{C}(D_\mathrm{C} - L\psi(u))||^2_{L_2(\mathrm{C})}\\
+\; & c_3||g_\mathrm{N}(D_\mathrm{N} - L\psi(u))||^2_{L_2(\mathrm{N})}\\
+\; & c_4||g_0(u)||^2_{L_2(\Gamma \times I \times S)} + a||u||^2_{L_2(\Gamma \times I \times S)}.
\end{aligned}
$$

Define

$$
\begin{aligned}
N_1(\psi) \;:=\; & c_1 L^*(e_T(D_0 - L\psi)) \qquad\qquad (35)\\
+\; & c_2 L^*(g_C'(D_C - L\psi)^* g_C(D_C - L\psi))\\
+\; & c_3 L^*(g_N'(D_N - L\psi)^* g_N(D_N - L\psi)),\\
N_2(u) \;:=\; & c_4 g_0'(u)^* g_0(u) + au. \qquad\qquad (36)
\end{aligned}
$$

Replacing the objective function (24) by (34) and assuming that $u_0 \in L_\infty(\Gamma \times I \times S)$ (this is always true in practice) we have, see [8],

Theorem 4: Suppose that the assumptions of Theorem 2 are valid. Then the optimal control $u_0 \in L_\infty(\Gamma \times I \times S)$ satisfies the following equations

$$
\begin{aligned}
B(\psi(u_0), v) &= (\tilde{F}u_0)(v), \;\; v \in H^3 \qquad\qquad (37)\\
B(v, \psi^*(u_0)) &= \langle v, N_1(\psi(u_0)) \rangle_{L_2(G)^3}, \;\; v \in H^3 \quad (38)\\
\tilde{F}^*\psi^*(u_0) &= N_2(u_0) \qquad\qquad (39)
\end{aligned}
$$

Proof. Denote

$$
\begin{aligned}
J_1(u) &:= \langle D_0 - L\psi(u), D_0 - L\psi(u) \rangle_{L_2(T)},\\
J_2(u) &:= \langle g_C(D_C - L\psi(u)), g_C(D_C - L\psi(u)) \rangle_{L_2(C)},\\
J_3(u) &:= \langle g_N(D_N - L\psi(u)), g_N(D_N - L\psi(u)) \rangle_{L_2(N)},\\
J_4(u) &:= \langle g_0(u), g_0(u) \rangle_{L_2(\Gamma \times I \times S)},\\
J_5(u) &:= \langle u, u \rangle_{L_2(\Gamma \times I \times S)}.
\end{aligned}
$$

Then
$$J(u) = c_1 J_1(u) + c_2 J_2(u) + c_3 J_3(u) + c_4 J_4(u) + a J_5(u).$$

From these we calculate
$$
\begin{aligned}
J_1'(u)w &= -2\left\langle L^* e_T(D_0 - L\psi(u)), \psi(w)\right\rangle_{L_2(G)^3}, \\
J_2'(u)w &= -2\langle L^*[g_C'(D_C - L\psi(u))^* \cdot \\
&\quad \cdot (g_C(D_C - L\psi(u)))], \psi(w)\rangle_{L_2(G)^3}, \\
J_3'(u)w &= -2\langle L^*[g_N'(D_N - L\psi(u))^* \cdot \\
&\quad \cdot (g_N(D_N - L\psi(u)))], \psi(w)\rangle_{L_2(G)^3}, \\
J_4'(u)w &= 2\left\langle g_0'(u)^* g_0(u), w\right\rangle_{L_2(\Gamma \times I \times S)}, \\
J_5'(u)w &= 2\left\langle u, w\right\rangle_{L_2(\Gamma \times I \times S)}.
\end{aligned}
$$

We see that $J'(u)w = 0$ if and only if
$$2\left\langle N_1(\psi), \psi(w)\right\rangle_{L_2(G)^3} - 2\left\langle N_2(u), w\right\rangle_{L_2(\Gamma \times I \times S)} = 0.$$

Suppose that $\psi^* = \psi^*(w)$ is the solution of the dual problem $B(v, \psi^*) = \langle v, N_1(\psi)\rangle_{L_2(G)^3}$, $v \in H^3$. Then we find that
$$
\begin{aligned}
\langle \psi(w), N_1(\psi)\rangle_{L^2(G)^3} &= B(\psi(w), \psi^*) = (\tilde{F}w)(\psi^*) \\
&= \left\langle \tilde{F}^* \psi^*, w\right\rangle_{L_2(\Gamma \times I \times S)}.
\end{aligned}
$$

From the previous equations we see that
$$2\left\langle \tilde{F}^* \psi^* - N_2(u), w\right\rangle_{L_2(\Gamma \times I \times S)} = 0, \ \forall w \in L_\infty(\Gamma \times I \times S),$$

and by denseness of $L_\infty(\Gamma \times I \times S)$ in $L_2(\Gamma \times I \times S)$ we have
$$\tilde{F}^* \psi^* - N_2(u) = 0$$

which completes the proof.

Note that the equation (39) can be given in the variational form
$$
\begin{aligned}
(\tilde{F}w)(\psi^*(u_0)) &= \left\langle \tilde{F}^*(\psi^*(u_0)), w\right\rangle_{L_2(\Gamma \times I \times S)} \quad (40) \\
&= \langle N_2(u_0), w\rangle_{L_2(\Gamma \times I \times S)}.
\end{aligned}
$$

The derivatives and their adjoints are calculated along Lemma 2. In general, the equations (37)-(39) may have many solutions u_0 corresponding to local extrema. After an appropriate discretization the equations (37)-(39) form a system of nonlinear algebraic equations. This system must be solved with some iterative scheme (Newton, quasi-Newton,...). To help the search of the (global) minimum it is useful to apply some kind of initial solution.

C. Initial solution

The above equations for the optimal control contain non-linearities. One possibility to help the computations is to diminish the required restrictions. For example, we can at first consider simply the cost functional
$$J(u) = c\|D_0 - L\psi(u)\|_{L_2(T)}^2 + a\|u\|_{L_2(\Gamma \times I \times S)}^2. \quad (41)$$

In this case, the optimal boundary control is
$$u_0 = -\frac{1}{a}\tilde{F}^*\psi^*, \quad (42)$$

where ψ^* is uniquely obtained from the equations (note that J is convex)
$$B(\psi, v) = -\frac{1}{a}\tilde{F}(\tilde{F}^*\psi^*)(v), \ v \in H^3 \quad (43)$$
$$B(v, \psi^*) = -c\left\langle v, L^* e_T(D_0 - L\psi)\right\rangle_{L_2(G)^3}, \ v \in H^3 \quad (44)$$

IV. NUMERICAL SIMULATIONS

In simulations, we solve for simplicity only the control problem (42-44) using finite element method (FEM) and one Boltzmann equation for one type of particles in two dimensional (2D) spatial domain. We define a linear hull $[\phi_1, ..., \phi_N]$ in a finite dimensional subspace of H. The finite element approximations ψ^h and ψ^{*h} of the solutions ψ and ψ^* are
$$\psi^h(x, E, \theta) = \sum_{k=1}^{N} \alpha_k \phi_k(x, E, \theta) \quad (45)$$
$$\psi^{*h}(x, E, \theta) = \sum_{k=1}^{N} \alpha_k^* \phi_k(x, E, \theta) \quad (46)$$

where ϕ_k are the basis functions for fluxes $\psi(x, E, \theta)$ and $\psi^*(x, E, \theta)$, $\theta \in [0, 2\pi[$. The unknown parameters α_k and α_k^* are found by demanding
$$
\begin{aligned}
B(\psi^h, v) &= -\frac{1}{a}\tilde{F}(\tilde{F}^*\psi^{*h})(v), \\
B(v, \psi^{*h}) &= -c\left\langle v, L^* e_T(D_0 - L\psi^h)\right\rangle_{L_2(G)^3}.
\end{aligned}
$$

for all $v \in [\phi_1, ..., \phi_N]$. The basis functions are used as a test functions $v = \phi_t$, $t = 1, ..., N$.

For FEM matrix definitions we refer to [1], in which we have solved BTE forward problem using FEM. If the problem $A\alpha = b$ describes the linear forward BTE problem (9), in which $\psi^h(x, E, \theta) = \sum_{k=1}^{N} \alpha_k \phi_k(x, E, \theta)$, then the control problem (43-44) can be written in a matrix form
$$
\begin{pmatrix} A & M_\Gamma \\ M_T & A^* \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} = \begin{pmatrix} 0 \\ b_T \end{pmatrix},
$$

where $*$ denotes the matrix transpose operation,
$$M_\Gamma(t, k) = -\frac{1}{a}\sum_{l=1}^{L}\int_{\Gamma_l}\int_S\int_I ((\sin\theta, \cos\theta)\cdot n)_-^2 \phi_t \phi_k \mathrm{d}E \mathrm{d}\theta \mathrm{d}\sigma,$$

$$M_T(t, k) = -c\int_T\int_S\int_I \left[\kappa\phi_t\int_S\int_I \kappa\phi_k \mathrm{d}E'\mathrm{d}\theta'\right] \mathrm{d}E\mathrm{d}\theta\mathrm{d}x,$$

$$b_T(t) = -c\int_T\int_S\int_I D_0\kappa\phi_t \mathrm{d}E\mathrm{d}\theta\mathrm{d}x$$

and $\int_T$ is the integration over the target.

V. SIMULATION RESULTS

The simulations demonstrate the use of control in BTE problems. The used parameters for particle cross sections and stopping powers are artificial.

The first simulation was done in a $[-5, 5] \times [0, 10]$ cm^2 domain, which was assumed to be homogeneous. The target was located at $[-1, 4] \times [1, 6]$ cm^2. Two radiation fields are assumed to locate on the surface. The geometry and source nodes for the fields are shown in figure 1. The same

figure also shows the spatial grid (100 evenly distributed elements) and optimized dose distribution in the spatial domain. Angular domain $\theta \in [0, 2\pi[$ was divided into 16 evenly distributed elements and energy domain $E \in [0.01, 1]$ MeV was divided into 6 evenly distributed elements. The used control parameters were $c = 100000$, $a = 0.1$ and for desired dose in the target $D_0 = 10$ (in arbitrary units).

The simulation was run in a normal PC (2GHz IV Pentium with 2GB memory) using MATLAB®. It took 4 hours to run the simulation. The control $u_0 = (u_1, u_2)$ was computed from equation (42). The field intensities can be computed by integrating the control flux $u_l(x, E, \Omega)$ ($l = 1, 2$) over energy and angle. Those intensities I_l are shown in figure 2. Figure 3 shows the control fluxes $u_l(x, E, \Omega)$ for selected energies $E = 0.2, 0.7, 1$ MeV. The controlled dose distribution, which is computed from ψ^h, is shown in figure 1.

The second simulation was also done in a $[-5, 5] \times [0, 10]$ cm^2 homogeneous domain. Now the target was located at $[0.5, 4.5] \times [3, 6]$ cm^2 and three control fields were used as shown in figure 4. Same values for c, a and D_0 were used as in the first simulation. Also the same energy and angle discretizations were used. Spatial domain were divided into 225 evenly distributed elements. Simulation took 5 hours to run in a normal PC using MATLAB®. The field intensities are shown in figure 5. The control fluxes $u_l(x, E, \Omega)$ for selected energies $E = 0.2, 0.7, 1$ MeV are shown in figure 6. The controlled dose distribution is shown in figure 4.

VI. Simulation discussion

The dose distributions, shown in figures 1 and 4, are in a good agreement with the used cost function (41), in which the desired dose $D_0 = 10$ was demanded into the target.

In the first simulation, one would except to obtain wedge-like intensity distributions, in which in the field 1 the intensity profile would increase in positive x_2 direction and in the field 2 the intensity profile would decrease in positive x_1 direction. In our results, this is not the case. In fact, the intensity profiles in figure 2 behave in opposite way. This is because the directions of the control fluxes are not constrained. It can be seen from figure 3 that for the field 2 the flux is directed mainly to the left (see for example the point (4,0)) and similarly for the field 1 the flux is directed mainly to the right (see for example the point (5,1)) to ensure homogeneous dose in the target area. However, in the real treatment planning, these control fluxes could not been used, since with the present technology it is not possible to control the particle directions or energies for the radiation fields. The directions should be constrained based on the actual treatment direction. Also the incoming particle energy distribution should be constrained to be the same that is obtained from the treatment unit. These restrictions are fairly easy to add in the method we have used here.

In the second simulation, fields 2 and 3 were selected not to be directly under and over the target, respectively. Now it is interesting to see that the direction of the particles is towards the target (figure 6). The treatment plan is better in
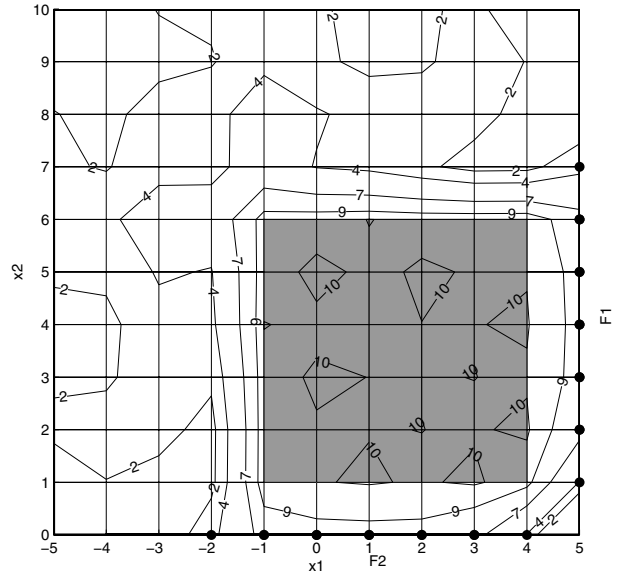

Fig. 1. The first 2D FEM control simulation. The spatial grid is drawn with straight lines. Black circles at the boundaries are the source nodes for the fields 1 and 2. The gray box inside the grid is the target. The optimized dose profile is presented with contour lines describing the dose of 2, 4, 7, 9 and 10 in arbitrary units.
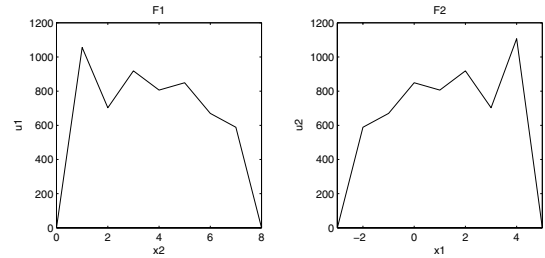

Fig. 2. The control field intensity for different fields I_l ($l = 1, 2$) in the first simulation.
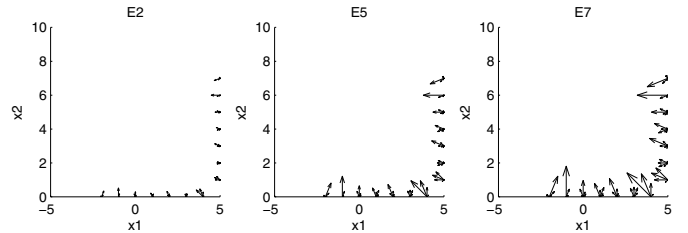

Fig. 3. Control fluxes $u_0(x, E, \theta)$ for different energies $E = 0.2, 0.7, 1$ MeV in the first simulation. The same scale is used for all the energies.

the second simulation, which is consistent with the practice (because we have three fields instead of two).

VII. Concluding remarks

Optimal dosing of radiation on tumors without affecting too much the other parts of the body is a necessity in successful radiation therapy treatment. Planning of the treatment is here based on the Boltzmann transport equation model. In the treatment planning, the cost functional minimization is applied. A necessary ingredient in optimization is the
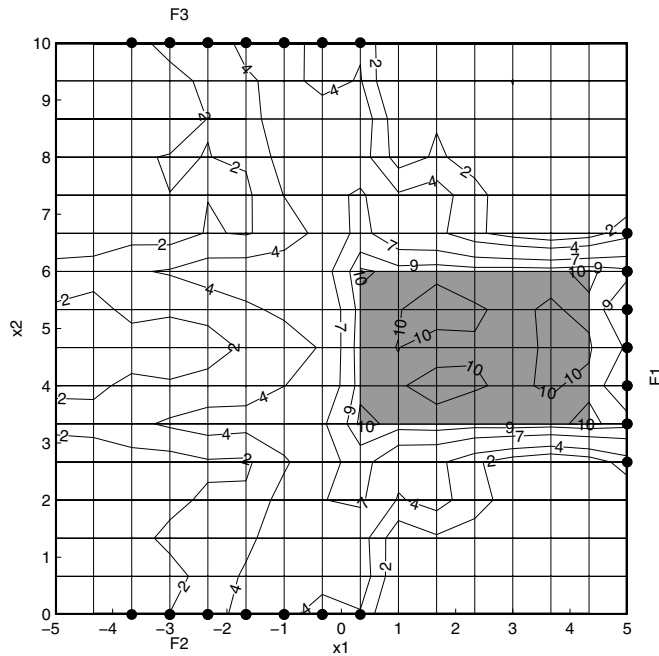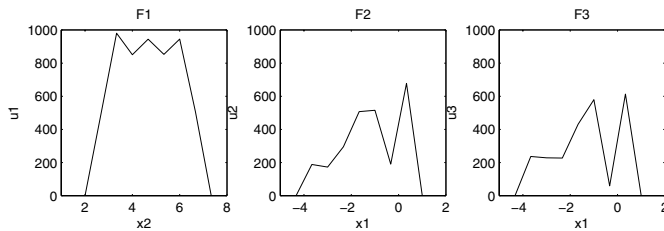
Fig. 4. The second 2D FEM control simulation. The spatial grid is drawn with straight lines. Black circles at the boundaries are the source nodes for the fields 1, 2 and 3. The gray box inside the grid is the target. The optimized dose profile is presented with contour lines describing the dose of 2, 4, 7, 9 and 10 in arbitrary units.

Fig. 5. Controlled field intensities I_l ($l = 1, 2, 3$) in the second simulation.
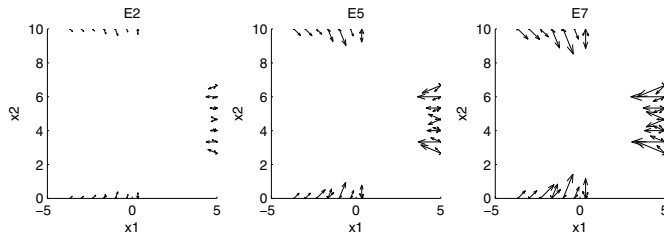

Fig. 6. Control fluxes $u_0(x, E, \theta)$ for different energies $E = 0.2,\ 0.7,\ 1$ MeV in the second simulation. The same scale is used for all the energies.

appearance of the adjoint variables.

By the simulations we have shown that it is possible to control the field intensities in optimization problem. The simulations give a good overview about the problem, although they are done in 2D and only for one Boltzmann equation to simplify the computational burden.

Besides using the adjoint variables, one also could study the elimination of the adjoint variables. This elimination

is based on the "compatibility operators". Their existence can be studied e.g. by homological-algebraic methodology [12]. The compatibility conditions and their solution form the essential part of the solution of the overall dosing optimization problem. We shall consider this idea elsewhere in the near future. Similar compatibility condition issues were used also in open-loop control design for PDE systems under the concept called parametrization, see [10] and [11].

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1637