Optimal Control Model for Inverse Radiation Therapy Treatment Planning

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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].

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

\[
\begin{align*}
\Omega \cdot \nabla \psi_1 + K_1(\psi_1, \psi_2, \psi_3) &= Q_1(x, E, \Omega) \\
\Omega \cdot \nabla \psi_2 + K_2(\psi_1, \psi_2, \psi_3) &= Q_2(x, E, \Omega) \\
\Omega \cdot \nabla \psi_3 + K_3(\psi_1, \psi_2, \psi_3) &= Q_3(x, E, \Omega)
\end{align*}
\]

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 \(\phi, \theta\) are the standard spherical coordinates on \(S\). In the following the integral \(\int_S f(\Omega) d\Omega\) denotes the surface integral \(\int_S f(\Omega) d\Omega = \int_W (f \circ h)(\phi, \theta) \sin \theta d\phi d\theta\), where \(W := [0, 2\pi] \times [0, \pi]\). \(I\) is the energy interval, say \([E_0, E_f]\). \(\nabla\) is the gradient with respect to the \(x\)-variable. We are able to identify \(S\) with \(W\). Hence the solution \(\psi\) 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

\[
K_j \psi = -\sum_{k=1}^{3} \Sigma_{j,k}(x, E)\psi_k + \sum_{k=1}^{3} \int_{S} \int_{U} \sigma_{j,k}(x, E', E, \Omega', \Omega)\psi_k(x, E', \Omega')dE'd\Omega'.
\]

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 \(\partial V\) is a Lipschitz-boundary [6]. Then the outward normal \(n(x)\) exists and it is continuous on \(\partial V\) possibly except a set with surface measure zero.

Let \(\Gamma_l, l = 1, ..., L\) be (sufficiently smooth) patches of \(\partial V\). 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 \(\psi\) are of the form

\[
\psi_2(x, E, \Omega) = \psi_3(x, E, \Omega) = 0, \quad \text{for} \quad (x, E, \Omega) \in \partial V \times I \times S \quad \text{such that} \quad n(x) \cdot \Omega < 0;
\]

\[
\psi_1(x, E, \Omega) = 0, \quad \text{for} \quad (x, E, \Omega) \in \Gamma_1 \times I \times S \quad \text{such that} \quad n(x) \cdot \Omega < 0;
\]

\[
\psi_1(x, E, \Omega) = 0, \quad \text{for} \quad (x, E, \Omega) \in (\partial V \setminus \Gamma_1) \times I \times S \quad \text{such that} \quad n(x) \cdot \Omega < 0.
\]

Above \(n(x)\) is the unit outward normal vector on the boundary surface \(\partial V\) and \(\psi_1\) is the flux per unit area incident on \(\Gamma_1\). The condition \(\psi_1 = 0\) for \(n(x) \cdot \Omega < 0, \ x \in \Gamma_1\) means that the beam (the flux \(\psi_1\)) is incoming from outwards on the patch \(\Gamma_1\). The conditions \(\psi_2 = \psi_3 = 0\) for \(n(x) \cdot \Omega < 0, \ x \in \partial V\), \(\psi_1 = 0\) for \(n(x) \cdot \Omega < 0, \ x \in \partial V \setminus \Gamma_1\) mean that no outward fluxes (of corresponding particles) exist on \(\partial V\) and on \(\partial V \setminus \Gamma_1\), 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

\[
\Omega \cdot \nabla \psi := (\Omega \cdot \nabla \psi_1, \Omega \cdot \nabla \psi_2, \Omega \cdot \nabla \psi_3)
\]

and

\[
K \psi := (K_1 \psi, K_2 \psi, K_3 \psi)
\]

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

\[
(\Omega \cdot \nabla + K) \psi = Q(x, E, \Omega)
\]

where \(\psi\) 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. \(\Sigma_{j,k} \in L_\infty(V \times I),\)
2. \(\sigma_{j,k} \in L_\infty(V \times I^2 \times S^2),\)
3. \(Q_j \in L_2(G), \ u_l \in L_2(\Gamma_1 \times I \times S).\)

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

\[
B(\psi, v) = F(v), \ v \in H^3
\]

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

\[
B(\psi, v) = -\langle \psi, \Omega \cdot \nabla v \rangle_{L_2(G)^3} + \langle K \psi, v \rangle_{L_2(G)^3} + \sum_{j=1}^{3} \int_{S} \int_{U} (\Omega \cdot n)_{j,k} \psi_j v_j d\sigma dE d\Omega,
\]

Define a norm for \(\psi \in H\) by

\[
||\psi||_H^2 = \sum_{j=1}^{3} \int_{S} \int_{U} \Omega \cdot n \psi_j^2 d\sigma dE d\Omega + ||\psi||_{L_2(G)^3}^2.
\]

For \(\psi \in H^3\) we define \(||\psi||_{H_1^3}^2 = \sum_{j=1}^{3} \int_{S} \int_{U} \Omega \cdot n \psi_j^2 d\sigma dE d\Omega + ||\psi||_{L_2(G)^3}^2\). By the Trace Theorem [6] we find that \(||\psi||_{H_1^3} \leq C ||\psi||_H\). Hence also \(||\psi||_{H_1^3} \leq C ||\psi||_H\) 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 exists \(\kappa > 0\) such that for \(\psi \in H^3\)

\[
(k \psi, \psi)_{L_2(G)^3} \geq \kappa ||\psi||_{L_2(G)^3}^2
\]

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

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

for \(\psi, \ v \in H^3\) and

\[
B(\psi, \psi) \geq c ||\psi||_{H_1^3}^2 \quad (H_1^3-\text{coercitivity})
\]
for $\psi \in H^3$. In addition, $F \in (H_1^3)^*$ and there exists $C > 0$ such that
\[
\|\psi\|_{H_1^3} \leq C \|F\| \tag{15}
\]
where
\[
\|F\| := \|Q\|_{L_2(G)^3} + \sum_{i=1}^L \int_S \int_{I_1} \int_{I_2} |(\Omega \cdot n)_-u_1^2| d\sigma dEd\Omega.
\]

The assumptions of Theorem 2 imply a sufficient condition for the unique existence of the (variational) solution $\psi \in H^3$. We remark that also the adjoint problem $B(v, \psi^*) = F^*v$, $v \in H^3$ has a unique solution $\psi^* \in H^3$ 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 coercitivity assumption (12)

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

\[
\Sigma_{j,i}(x, E, \Omega) - \int_S \int_{I_1} \int_{I_2} \int_{I_3} \sigma_{k,j}(x, E', \Omega', \Omega) dE' d\Omega' \geq \gamma \tag{16}
\]

\[
\Sigma_{j,k}(x, E, \Omega) - \int_S \int_{I_1} \int_{I_2} \int_{I_3} \sigma_{j,k}(x, E', \Omega', \Omega) dE' d\Omega' \geq \gamma \tag{17}
\]

for $j = 1, 2, 3$. Then the inequality
\[
\langle K\psi, \psi \rangle_{L_2(G)^3} \geq \gamma \|\psi\|_{L_2(G)^3}^2, \ \psi \in H^3 \tag{18}
\]
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 $V = T \cup C \cup N$. Assume that we have $L$ fields $S_l$, $l = 1, \ldots, L$. 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 $l$-th field $S_l$ be $u_l$. Denote the corresponding (disjoint) patches of $\partial V$ by $\Gamma_l$.

We have no internal sources. So $Q_l = 0$ for each field $S_l$.

The effect of incoming flux is given by the functional
\[
F(v) = \sum_{l=1}^L \int_S \int_{I_1} \int_{I_2} (\Omega \cdot n)_-u_l v_1 d\sigma dEd\Omega. \tag{19}
\]

The bilinear form $B$ is independent of the incoming flux.

The total dose $D = D(x) = D(x, \psi)$ is obtained from the functional
\[
D(x) = \sum_{j=2}^3 \int_S \int_{I_1} \kappa_j(x, E)\psi_j(x, E, \Omega) dE d\Omega =: L\psi(x) \tag{20}
\]
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 $l = 1, \ldots, L$ determine the incoming flux $u_l \in L_2(\Gamma_l \times I \times S)$ such that
\[
\begin{align*}
D(x) &= D_0, \ x \in T \\
D(x) &\leq D_C, \ x \in C \\
D(x) &\leq D_N, \ x \in N.
\end{align*} \tag{21}
\]

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 $u = (u_1, \ldots, u_L) \in L_2(\Gamma \times I \times S)$ 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 $\tilde{F} : L_2(\Gamma \times I \times S) \rightarrow (H^3)^*$ be the operator defined by
\[
(\tilde{F}u)(v) = \sum_{l=1}^L \int_S \int_{I_1} \int_{I_2} (\Omega \cdot n)_-u_l v_1 d\sigma dEd\Omega.
\]

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 $\psi$ is a linear function of $u$ as well. Furthermore, $L$ (defined by (20)) is a linear function of $\psi$.

**Lemma 1:** $\psi$ is a bounded operator $L_2(\Gamma \times I \times S) \rightarrow L_2(G)^3$ and $L$ is a bounded operator $L_2(G)^3 \rightarrow L_\infty(V)$ that is,
\[
\|\psi(u)\|_{L_2(G)^3} \leq C_1 \|u\|_{L_2(\Gamma \times I \times S)} \tag{22}
\]
for $u \in L_2(\Gamma \times I \times S)$ and
\[
\|L\psi\|_{L_\infty(V)} \leq C_2 \|\psi\|_{L_2(G)^3} \tag{23}
\]
for $\psi \in L_2(G)^3$.

Since $L$ and $\psi$ 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
\[
J(u) = c_1 ||D_0 - D(\cdot, \psi(u))||_{L^2(T)}^2 (24) + c_2 ||D_C - D(\cdot, \psi(u))||_{L^2(C)}^2 \\
+ c_3 ||D_N - D(\cdot, \psi(u))||_{L^2(N)}^2 \\
+ c_4 ||(u) - (u)||_{L^2(\Gamma \times I \times S)}^2 + a ||u||_{L^2(\Gamma \times I \times S)}^2,
\]
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 \(D(x) \leq D_C, x \in C\) and \(D(x) \leq D_N, x \in N\). 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 \(c_4 ||(u) - (u)||_{L^2(\Gamma \times I \times S)}^2\) which hinders the violation of the constraint \(u \geq 0\). The last (convex) term regularizes the schemes and helps the optimization process in theory and in numerical considerations. To diminish (that is, minimization of \(||u||_{L^2(\Gamma \times I \times S)}^2\)) 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
\[
\min_{u \in U} J(u) (25)
\]
such that
\[
B(\psi(u), v) = (\tilde{F}u)(v), \ v \in H^3. (26)
\]

B. Optimal solution

The optimal control \(u_0\) minimizes the functional \(J\) among the set \(U_{ad}\), 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
\[
J'(u_0)(u - u_0) \geq 0 \text{ for all } u \in U_{ad}. (27)
\]
In the case where \(U_{ad}\) is the linear space \(U\) (as in our case) the condition (27) reduces to
\[
J'(u_0) = 0. (28)
\]
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
\[
L^* w = (k_1 w, k_2 w, k_3 w), \ w \in L^1(V).
\]
In addition, the adjoint \(\tilde{F}^*: H^3 \rightarrow L^2(\Gamma \times I \times S)\) of \(\tilde{F}\) is
\[
\tilde{F}^* v = (r_{\Gamma_1}, ((\Omega \cdot n) - v_1), ..., r_{\Gamma_L}, ((\Omega \cdot n) - v_1))\]
where \(r_{\Gamma_j}\) is the restriction operator on \(\Gamma_j\).

We replace the negative part of a function by a Fréchet differentiable approximation. This can be done as follows, for example. Let \(H_\epsilon\) be some approximation of the Heaviside function. We can choose
\[
H_\epsilon(x) = \text{erf}_\epsilon(x) = \frac{1}{\sqrt{\pi \epsilon}} \int_{-\infty}^{\infty} e^{-s^2/\epsilon^2} ds. (30)
\]
Then the negative part \(f_-\) of a function \(f \in L^2(V)\) is approximately given by
\[
f_- \approx -(H_\epsilon \circ (-f))f. (31)
\]
Note that \(H_\epsilon \in L^\infty(\mathbb{R})\).

Let \(A\) be a Lebesgue measurable subset of \(V\). Furthermore, let \(r_\Lambda\) be the restriction operator \(r_\Lambda f = f_{|_{\Lambda}}\) and let \(e_\Lambda\) be the "extension by zero operator" from a set \(A\) on \(V\).

**Lemma 2:** The function \(g_A : L^\infty(V) \rightarrow L^2(\Lambda)\) defined by \(g_A(f) = r_\Lambda (-H_\epsilon \circ (-f))f\) is Fréchet differentiable and
\[
g_A'(f)h = r_\Lambda (([H_\epsilon \circ (-f)] \cdot f - H_\epsilon \circ (-f)) \cdot h). (32)
\]
In addition, \(g_A'(f) = w \in L^2(V)\) and
\[
g_A'(f)(w) = e_\Lambda (([H_\epsilon \circ (-f)] \cdot f - H_\epsilon \circ (-f)) \cdot w), (33)
\]
where \(w \in L^2(\Lambda)\).

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
\[
J(u) = c_1 ||(r_{\Gamma_1}(D_0 - L\psi(u)))||_{L^2(T)}^2 (34) + c_2 ||g_C(D_C - L\psi(u))||_{L^2(C)}^2 \\
+ c_3 ||g_N(D_N - L\psi(u))||_{L^2(N)}^2 \\
+ c_4 ||g_0(u)||_{L^2(\Gamma \times I \times S)}^2 + a ||u||_{L^2(\Gamma \times I \times S)}^2.
\]

Define
\[
N_1(\psi) := c_1 L^* (e_\epsilon(D_0 - L\psi)) + c_2 L^* (g_C(D_C - L\psi)) + c_3 L^* (g_N(D_N - L\psi)) + c_4 L^* (g_0(u))u + a u. (35)
\]

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
\[
B(\psi(u_0), v) = (\tilde{F}u_0)(v), \ v \in H^3 \quad (37)
\]
\[
B(v, \psi'^*(u_0)) = (v, N_1(\psi(u_0)))_{L^2(G)^3}, \ v \in H^3 \quad (38)
\]
\[
\tilde{F}^* \psi'^*(u_0) = N_2(u_0) \quad (39)
\]

**Proof.** Denote
\[
J_1(u) := (D_0 - L\psi(u), D_0 - L\psi(u))_{L^2(T)}, \\
J_2(u) := (g_C(D_C - L\psi(u)), g_C(D_C - L\psi(u)))_{L^2(C)}, \\
J_3(u) := (g_N(D_N - L\psi(u)), g_N(D_N - L\psi(u)))_{L^2(N)}, \\
J_4(u) := (g_0(u), g_0(u))_{L^2(\Gamma \times I \times S)}, \\
J_5(u) := (u, u)_{L^2(\Gamma \times I \times S)}.
\]
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
\[ J'_1(u) = -2 \langle L^* e_T (D_0 - L \psi(u)), \psi(u) \rangle_{L_2(G)^3}, \]
\[ J'_2(u) = -2 \langle L^* [g_C(D_C - L \psi(u))^* \cdot (g_C(D_C - L \psi(u)))], \psi(u) \rangle_{L_2(G)^3}, \]
\[ J'_3(u) = -2 \langle L^* [g_N(D_N - L \psi(u))^* \cdot (g_N(D_N - L \psi(u)))], \psi(u) \rangle_{L_2(G)^3}, \]
\[ J'_4(u) = 2 \langle g_0(u)^* g_0(u), w \rangle_{L_2(\Gamma \times I \times S)}, \]
\[ J'_5(u) = 2 \langle u, w \rangle_{L_2(\Gamma \times I \times S)}. \]

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

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
\[ \langle \psi(w), N_1(\psi) \rangle_{L_2(G)^3} = B(\psi(w), \psi^*) = (\tilde{F}^* \psi^*, u) \]
\[ = \langle \tilde{F}^* \psi^*, w \rangle_{L_2(\Gamma \times I \times S)}. \]

From the previous equations we see that
\[ 2 \langle \tilde{F}^* \psi^* - N_2(u), w \rangle_{L_2(\Gamma \times I \times S)} = 0, \forall w \in L_\infty(\Gamma \times I \times S), \]
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
\[ (\tilde{F}^*)(\psi^*(u_0)) = \langle \tilde{F}^* \psi^*(u_0), w \rangle_{L_2(\Gamma \times I \times S)} = \langle N_2(u_0), w \rangle_{L_2(\Gamma \times I \times S)}. \]

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 nonlinearities. One possibility to help the computations is to diminish the required restrictions. For example, we can at first consider simply the cost functional
\[ J(u) = c ||D_0 - L \psi(u)||_{L_2(\Gamma)}^2 + a ||u||_{L_2(\Gamma \times I \times S)}. \]

In this case, the optimal boundary control is
\[ u_0 = -\frac{1}{a} \tilde{F}^* \psi^* , \]
where \( \psi^* \) is uniquely obtained from the equations (note that \( J \) is convex)
\[ B(\psi, v) = -\frac{1}{a} \tilde{F}(\tilde{F}^* \psi^*)(v), v \in H^3 \]
\[ B(v, \psi^*) = -c \langle v, L^* e_T (D_0 - L \psi) \rangle_{L_2(G)^3}, v \in H^3 \]

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 \( \psi^h \) and \( \psi^{*h} \) of the solutions \( \psi \) and \( \psi^* \) are
\[ \psi^h(x, E, \theta) = \sum_{k=1}^N \alpha_k \phi_k(x, E, \theta) \]
\[ \psi^{*h}(x, E, \theta) = \sum_{k=1}^N \alpha_k^* \phi_k(x, E, \theta) \]
where \( \phi_k \) are the basis functions for fluxes \( \psi(x, E, \theta) \) and \( \psi^*(x, E, \theta), \theta \in [0, 2\pi] \). The unknown parameters \( \alpha_k \) and \( \alpha_k^* \) are found by demanding
\[ B(\psi^h, v) = -\frac{1}{a} \tilde{F}(\tilde{F}^* \psi^{*h})(v), \]
\[ B(v, \psi^{*h}) = -c \langle v, L^* e_T (D_0 - L \psi^h) \rangle_{L_2(G)^3}, \]
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 \( Ac = b \) 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
\[ \begin{pmatrix} A & M_T \\ M_T^T & A^* \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^* \end{pmatrix} = \begin{pmatrix} 0 \\ b_T \end{pmatrix}, \]
where \( * \) denotes the matrix transpose operation,
\[ M_T(t, k) = -\frac{1}{a} \sum_{l=1}^L \int_{\Gamma} \int_{S, 1} \int_{I} \int_{J} (\sin \theta, \cos \theta) \cdot n)^2 \phi_t \phi_k dE \theta d\theta d\sigma, \]
\[ b_T(t) = -c \int_{J} \int_{S, 1} \int_{I} \int_{J} \kappa \phi_t \phi_k dE \theta d\theta d\sigma \]
and \( \int_{J} \) 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
The first 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 $\psi^h$, is shown in figure 1.

The second simulation was also done in a $[-5, 5] \times [0, 10]$ cm² homogeneous domain. Now the target was located at $[0.5, 4.5] \times [3, 6]$ cm² 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 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
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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