A Space-Time Variational Method for Optimal Control Problems

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Abstract

We consider a space-time variational formulation of a PDE-constrained optimal control problem with box constraints on the control and a parabolic PDE with Robin boundary conditions. In this setting, the optimal control problem reduces to an optimization problem for which we derive necessary and sufficient optimality conditions. We propose to utilize a well-posed inf-sup stable framework of the PDE in appropriate Lebesgue-Bochner spaces.

Next, we introduce a conforming simultaneous space-time (tensorproduct) discretization in these Lebesgue-Bochner spaces. Using finite elements in space and piecewise linear functions in time, this setting is known to be equivalent to a Crank-Nicolson time stepping scheme for parabolic problems. The optimization problem is solved by a projected gradient method. We show numerical comparisons for problems in 1d, 2d and 3d in space. It is shown that the classical semi-discrete primal-dual setting is more efficient for small problem sizes and moderate accuracy. However, the simultaneous space-time discretization shows good stability properties and even outperforms the classical approach as the dimension in space and/or the desired accuracy increases.

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1. Introduction

PDE-constrained optimal control is an area of vast growing significance e.g. in fluid flows, crystal growths or heart medicine, see, e.g. [1, 2]. This explains the huge amount of literature concerning theoretical as well as numerical aspects. There are several approaches for the numerical solution of PDE-constrained optimal control problems. One of them is to first consider a variational formulation of the instationary partial differential equation (PDE) in space only and to discretize this e.g. by finite elements. In the second step, suitable time-stepping schemes are introduced for the primal (forward) and adjoint (backward) problem. This approach is often termed *semi-discrete*. A somewhat different approach is to keep the variational formulation of the optimal control problem in a space-time setting and to consider the reduced problem in this infinite-dimensional setting. The reduced space-time problem is then discretized and can efficiently be solved, see e.g. [2–7]. This approach is typically termed *space-time* in the literature and we stress that our approach is somewhat different.

In fact, our point of departure is a *space-time variational formulation* of the PDE, in which both time and space variables are treated in a variational manner. The corresponding theory dates back (at least) to the 1970s, see e.g. [8–10]. This yields (well-posed) infinite-dimensional problems of the form:

$$\text{find } y \in \mathcal{Y}: \quad b(y,z) = f(z) \quad \text{for all } z \in \mathcal{Z}, \tag{1.1}$$

where $f \in \mathcal{Z}'$ is a given right-hand side and $\mathcal{Y}$, $\mathcal{Z}$ are Bochner spaces depending on the particular problem, see (2.14) below. Existence, uniqueness and stability of (1.1) can then be analyzed by the Banach-Nečas theorem; the inf-sup-condition (2.16) plays an important role. In order to solve (1.1) numerically, a straightforward manner is a Petrov-Galerkin approach by determining finite-dimensional spaces $\mathcal{Y}_\delta \subset \mathcal{Y}$, $\mathcal{Z}_\delta \subset \mathcal{Z}$ and to consider (1.1) on those spaces, which need to be chosen carefully in the sense that the discrete inf-sup (also called LBB) condition holds, i.e.,

$$\inf_{y_\delta \in \mathcal{Y}_\delta} \sup_{z_\delta \in \mathcal{Z}_\delta} \frac{b(y_\delta, z_\delta)}{\|y_\delta\|_{\mathcal{Y}} \, \|z_\delta\|_{\mathcal{Z}}} \geq \beta > 0 \tag{1.2}$$

uniformly in δ (where β is independent of δ). The inf-sup constant β is particularly relevant as the Xu-Zikatanov lemma [11] yields an error/residual-relation with the multiplicative factor $\frac{1}{\beta}$. In some cases, one can realize *optimally stable* discretizations, i.e., $\beta = 1$. This is the main motiviation for our approach.

Until recent it has been believed that such a simultaneous discretization of time and space variables would be way too costly since problems in $d+1$ dimension need to be solved, where d denotes the space dimension. This has changed somehow since it is nowadays known that space-time discretizations yield good stability properties, can efficiently be used for model reduction and can also be treated by efficient numerical solvers, see [12–20], just to name a few papers in that direction. Concerning PDE-constrained optimal control problems it is known (see e.g. [21]) that such problems reduce to an optimization problem when using a space-time variational formulation. However, the issues of a suitable discretization and the question if the arising higher-dimensional problem can efficiently be solved remain. This is the point of departure for this paper. We consider the following control-constrained PDE-constrained optimal control problem. For simplicity, we do not apply any additional constraints to the state.

Problem 1.1 (Model problem in classical form)**.** *Let $I = (0,T) \subset \mathbb{R}$, $0 < T < \infty$ and $\Omega \subset \mathbb{R}^n$ be a bounded open Lipschitz domain. The normal vector of $\partial\Omega \coloneqq \Gamma$ is denoted by $\nu(x) \in \mathbb{R}^n$ for all $x \in \Gamma$.*

The state space $\mathcal{Y}$ consists of mappings $y : I \times \Omega \to \mathbb{R}$, the control space $\mathcal{U}$ of functions $u : I \times \Omega \to \mathbb{R}$. We are interested in determining a control $u^* \in \mathcal{U}$ and *a corresponding state* $y^* \in \mathcal{Y}$ *that solve the following optimization problem:*

$$\min_{(y,u)\in\mathcal{Y}\times\mathcal{U}} J(y,u) \coloneqq \frac{1}{2}\int_\Omega |y(T,x)-y_d(x)|^2\,\mathrm{d}x + \frac{\lambda}{2}\int_I\int_\Omega |u(t,x)|^2\,\mathrm{d}x\,\mathrm{d}t$$

$$\text{s.t.:}\quad \boxed{\begin{aligned} \partial_t y(t,x) - \Delta y(t,x) &= u(t,x) && \text{in } I\times\Omega\\ \partial_\nu y(t,x) + \mu(x)\cdot y(t,x) &= \eta(t,x) && \text{in } I\times\Gamma\\ y(0,x) &= y_0(x) && \text{in } \Omega \end{aligned}} \tag{1.3}$$

$$u_a(t,x) \le u(t,x) \le u_b(t,x) \qquad \text{in } I\times\Omega,$$

where the functions $\mu:\Gamma\to\mathbb{R}$, $\eta: I\times\Gamma\to\mathbb{R}$, $y_0, y_d:\Omega\to\mathbb{R}$ *and* $u_a, u_b: I\times\Omega\to\mathbb{R}$ *with* $u_a(t,x) < u_b(t,x)$ *for all* $(t,x)\in I\times\Omega$ *as well as a scalar* $\lambda > 0$ *are given. We shall always assume that* $\mu(x) > 0$ *for all* $x\in\Omega$ *a.e.*

Remark 1.2. *We could easily extend to a cost function of the form*

$$J(y,u) = \frac{\omega_1}{2}\|y-y_d\|^2_{L_2(I;L_2(\Omega))} + \frac{\omega_2}{2}\|y(T)-y_d(T)\|^2_{L_2(\Omega)} + \frac{\omega_3}{2}\|u\|^2_{L_2(I;L_2(\Omega))},$$

with real constants ω_1, $\omega_2 \ge 0$, $\omega_1+\omega_2 > 0$, $\omega_3 > 0$ *and* $y_d: I\times\Omega\to\mathbb{R}$.

As already indicated, the numerical solution of Problem 1.1 typically requires a suitable discretization. In the *semi-discretization*, the spatial and the temporal variable are sequentially discretized (also known as *method of lines*). In this case, we obtain the solution for each time step based on the corresponding previous time step. On the other hand, we consider an alternative approach and apply a *space-time discretization* based upon a space-time variational formulation, where both variables are treated in a variational sense. This means that the treatment is different from the very beginning on. In fact, the concrete form of necessary and sufficient optimality conditions depends on the weak formulation in which the initial boundary value problem is incorporated into the optimal control problem. Hence, we obtain a different system for the semi-discrete and the space-time approach. In particular, special attention should be paid to the adjoint problem that occurs within the optimality system and, in the case of time-dependent optimal control problems, is again a time-dependent partial differential equation (but typically backward in time). This circumstance generally leads the solution of the adjoint problem to be numerically challenging and motivates the use of the space-time discretization as an alternative approach.

The remainder of this paper is organized as follows. In Section 2, we recall and collect some preliminaries on constrained optimization problems in Banach spaces and on space-time variational formulations of parabolic PDEs. The space-time variational formulation of the optimal control problem under consideration is developed in Section 3. In particular, we derive necessary and sufficient optimality conditions. Section 4 is devoted to the space-time discretization of the PDE, the discretization of the control as well as of the adjoint problem. The latter one turns out to be much simpler in the space-time context as we obtain a linear system whose matrix is just the transposed of the matrix appearing in the primal problem. The fully discretized optimal control problem is then solved by a projected gradient method. We report on our numerical experiments in Section 5 and conclude by a summary, conclusions and an outlook in Section 6.

2. Preliminaries

Let us start by collecting some preliminaries that we will need in the sequel.

2.1. Optimal control problems

In this section, we recall the abstract framework for optimal control problems which we will later apply within the space-time setting.

Problem 2.1. *Let $\mathcal{Y}$, $\mathcal{U}$, $\mathcal{Z}$ be some real Banach spaces and $\mathcal{U}_{ad} \subset \mathcal{U}$, $\mathcal{Y}_{ad} \subset \mathcal{Y}$ some subspaces of admissible states and controls. Given an* objective function $J : \mathcal{Y} \times \mathcal{U} \to \mathbb{R}$ *and the* state operator $e : \mathcal{Y} \times \mathcal{U} \to \mathcal{Z}'$, *we consider the problem*

$$\min_{(y,u)\in\mathcal{Y}\times\mathcal{U}} J(y,u) \quad \textit{subject to (s.t.) the constraint } e(y,u) = 0.$$

Remark 2.2. *Note, that $e(y,u) = 0$ is an equation in the dual space $\mathcal{Z}'$ of $\mathcal{Z}$, which means that the constraint is to be interpreted as*

$$\langle e(y,u), z\rangle_{\mathcal{Z}'\times\mathcal{Z}''} = 0 \qquad \textit{for all } z \in \mathcal{Z}'', \tag{2.1}$$

where $\langle\cdot,\cdot\rangle_{\mathcal{Z}'\times\mathcal{Z}''}$ is the dual pairing. This is also the reason why we use $\mathcal{Z}'$ as opposed to the standard notation – i.e., the adjoint state will be in $\mathcal{Z}''$, which is $\mathcal{Z}$, if $\mathcal{Z}$ is reflexive, which is often the case.

A pair $(\overline{y},\overline{u}) \in \mathcal{Y}_{ad} \times \mathcal{U}_{ad}$ is called *local optimum* of problem (2.1) if

$$J(\overline{y},\overline{u}) \le J(y,u) \qquad \forall (y,u) \in \mathcal{N}(\overline{y},\overline{u}) \cap (\mathcal{Y}_{ad} \times \mathcal{U}_{ad}), \tag{2.2}$$

for some neighborhood $\mathcal{N}(\overline{y},\overline{u})$ of $(\overline{y},\overline{u})$; the pair is called *global optimum* of problem (2.1) if equation (2.2) is satisfied for all $(y,u) \in \mathcal{Y}_{ad} \times \mathcal{U}_{ad}$. We will be investigating the well-posedness of such optimal control problems in a space-time variational setting. This requires to consider the well-posedness of the state equation $e(y,u) = 0$, namely the question if a unique state can be assigned to each admissible control. If so, one defines the *control-to-state operator*

$$G : \mathcal{U} \to \mathcal{Y},\ u \mapsto y(u) = Gu, \tag{2.3}$$

which allows one to consider the *reduced objective functional*

$$\hat{J} : \mathcal{U} \to \mathbb{R},\ \hat{J}(u) := J(Gu,u) \tag{2.4}$$

and the corresponding *reduced problem*

$$\min_{u\in\mathcal{U}} \hat{J}(u) \qquad \text{s.t.:} \qquad u \in \mathcal{U}_{ad}. \tag{2.5}$$

The following result is well-known, we recall it for later reference. For extensions with state constraints, we refer e.g. to [8].

Theorem 2.3. *Let $U \supset \mathcal{U}_{ad} \neq \varnothing$ be weakly sequentially compact and $\hat{J} : \mathcal{U} \to \mathbb{R}$ be a weakly lower semi-continuous functional such that there exists a constant $c > -\infty$ so that $\hat{J}(u) \geq c$ for all $u \in \mathcal{U}_{ad}$. Then,* (2.5) *has at least one solution $\overline{u}$. If $\hat{J}$ is in addition strictly convex, then the optimal solution is unique.*

Necessary optimality conditions for optimal control problems are based upon a *variational inequality* of the type $\langle \hat{J}'(\overline{u}), u - \overline{u} \rangle_{\mathcal{U}' \times \mathcal{U}} \geq 0$ for all $u \in \mathcal{U}_{ad}$, e.g. [1]. This, however, involves the derivative of $\hat{J}$, which is often difficult to determine exactly. The well-known way-out is through the adjoint problem. In fact, if $e_y(Gu, u) : \mathcal{Y} \to \mathcal{Z}'$ (the partial derivative w.r.t. y) is a bijection, then,

$$\hat{J}'(u) = J_u(Gu, u) - e_u(Gu, u)^* \left(e_y(Gu, u)^*\right)^{-1} J_y(Gu, u), \tag{2.6}$$

for any $u \in \mathcal{U}$, where $e_y(Gu, u)^*$ and $e_u(Gu, u)^*$ denote the adjoint operators of $e_y(Gu, u)$ and $e_u(Gu, u)$, respectively. In order to avoid the determination of the inverses of the adjoints, one considers the *adjoint equation*

$$e_y(y, u)^* p = J_y(y, u), \tag{2.7}$$

whose solution $p \in \mathcal{Z}$ is called *adjoint state*. Then,

$$\hat{J}'(u) = J_u(y(u), u) - e_u(y(u), u)^* p = J_u(Gu, u) - e_u(Gu, u)^* p. \tag{2.8}$$

In order to detail first-order necessary optimality conditions, we need to specify the constraints under consideration. As in Problem 1.1 we use *box constraints*, which can be modeled by

$$\mathcal{U}_{ad} := \{u \in \mathcal{U} : u_a(t, x) \leq u(t, x) \leq u_b(t, x) \quad \text{a.e. in } I \times \Omega\} \tag{2.9}$$

with u_a, u_b such that $u_a(t, x) < u_b(t, x)$ for $(t, x) \in I \times \Omega$, a.e. This means that we will always consider the case

$$\mathcal{U} := L_2(I; H), \qquad \text{where we abbreviate } H := L_2(\Omega). \tag{2.10}$$

In this special case, the variational inequality can be replaced as follows.

Theorem 2.4. *Let $\overline{u}$ be a solution of* (2.5) *and $\overline{y} := y(\overline{u})$ the related state. Then, there exist an adjoint state $\overline{p} \in \mathcal{Z}$ and multipliers $\overline{\lambda}_a, \overline{\lambda}_b \in \mathcal{U}$, such that the following KKT system is satisfied: for all $(t, x) \in I \times \Omega$ a.e.:*

$$e(\overline{y}, \overline{u}) = 0 \tag{2.11a}$$

$$e_y(\overline{y}, \overline{u})^* \overline{p} = J_y(\overline{y}, \overline{u}) \tag{2.11b}$$

$$J_u(\overline{y}, \overline{u}) - e_u(\overline{y}, \overline{u})^* \overline{p} = \overline{\lambda}_b - \overline{\lambda}_a \tag{2.11c}$$

$$u_a(t, x) \leq \overline{u}(t, x) \leq u_b(t, x) \tag{2.11d}$$

$$\overline{\lambda}_a(t, x) \geq 0, \quad \overline{\lambda}_b(t, x) \geq 0 \tag{2.11e}$$

$$\overline{\lambda}_a(t, x)(u_a(t, x) - \overline{u}(t, x)) = \overline{\lambda}_b(t, x)(u_b(t, x) - \overline{u}(t, x)) = 0. \tag{2.11f}$$

The Lagrange function $\mathcal{L} : \mathcal{Y} \times \mathcal{U} \times \mathcal{Z} \times \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ to Problem 2.1 reads

$$\mathcal{L}(y, u, p, \lambda_a, \lambda_b) := J(y, u) - \langle p, e(y, u) \rangle_{\mathcal{Z} \times \mathcal{Z}'} - (\lambda_a, u_a - u)_{\mathcal{U}} - (\lambda_b, u - u_b)_{\mathcal{U}}.$$

Then, (2.11a-2.11c) can equivalently be written as $\mathcal{L}_p(\overline{y}, \overline{u}, \overline{p}) = 0$, $\mathcal{L}_y(\overline{y}, \overline{u}, \overline{p}) = 0$ and $\mathcal{L}_u(\overline{y}, \overline{u}, \overline{p}) = 0$.

2.2. Space-time variational formulation of parabolic problems

We review a variational formulation of the initial boundary value problem (1.3) in space and time, which yields the specific form of the state operator $e(\cdot,\cdot)$. To this end, we start by testing the first equation in (1.3) with functions $z_1(t) \in X := H^1(\Omega)$, $t \in I$ a.e., integrate over time, perform integration by parts in space and insert the Robin boundary condition. Denoting by $a : X \times X \to \mathbb{R}$ the bilinear form in space, i.e., $a(\phi,\psi) := (\nabla\phi,\nabla\psi)_{L_2(\Omega)} + (\mu, \phi\cdot\psi)_{L_2(\Gamma)}$, we get

$$\langle \partial_t y(t), z_1(t)\rangle_{X',X} + a(y(t), z_1(t)) = \ell(z_1(t); u)(t), \quad t \in I \text{ a.e.,} \tag{2.12}$$

where we used the abbreviations $\langle z, w\rangle_{X',X} := \int_\Omega z(x)\, w(x)\,\mathrm{d}x$, $z \in X'$, $w \in X$ as well as $\ell(\phi; u)(t) := (u(t),\phi)_{L_2(\Omega)} + (\eta(t),\phi)_{L_2(\Gamma)}$ for $\phi \in X$, i.e., $\ell \in X'$. To obtain a variational formulation in space and time we integrate (2.12) in time:

$$\int_I \langle \partial_t y(t), z_1(t)\rangle_{X',X}\,\mathrm{d}t + \int_I a(y(t), z_1(t))\,\mathrm{d}t = \int_I \ell(z_1(t); u)(t)\,\mathrm{d}t,$$

which is well-defined in view of (2.10). Finally, in order to enforce the initial condition (in a weak sense), we test the second equation by $z_2 \in H = L_2(\Omega)$ and add that term yielding the test space

$$\mathcal{Z} := L_2(I; X) \times H, \tag{2.13}$$

such that for all $z = (z_1, z_2) \in \mathcal{Z}$

$$\begin{aligned} b(y,z) &= f(z;u), \qquad \text{where} && (2.14)\\ b(y,z) &:= \int_I \langle \partial_t y(t), z_1(t)\rangle_{X',X}\,\mathrm{d}t + \int_I a(y(t), z_1(t))\,\mathrm{d}t + (y(0), z_2)_H \\ f(z;u) &:= \int_I \ell(z_1(t);u)(t)\,\mathrm{d}t + (y_0, z_2)_H, \ \text{ and } (\phi,\psi)_H := \int_\Omega \phi(x)\,\psi(x)\,dx. \end{aligned}$$

The trial space in which we seek y is a Bochner space defined as

$$\mathcal{Y} := \{y \in L_2(I;X) : \partial_t y \in L_2(I;X')\} = L_2(I;X) \cap H^1(I;X'), \tag{2.15}$$

where X' is the dual space of X induced by the inner product of H, i.e., the Gelfand triple $X' \hookrightarrow H \hookrightarrow X$. Obviously, (2.14) is a variational problem, $b : \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$ a bilinear and $f : \mathcal{Z} \to \mathbb{R}$ a linear form.

It was proven in [10, 14] that (2.14) is well-posed, which can be shown by verifying the conditions of the Banach-Nečas theorem. The key point also for numerical purposes is the inf-sup condition

$$\inf_{y\in\mathcal{Y}} \sup_{z\in\mathcal{Z}} \frac{b(y,z)}{\|y\|_{\mathcal{Y}}\,\|z\|_{\mathcal{Z}}} \geq \beta > 0. \tag{2.16}$$

In [22, 23], estimates for the inf-sup constant β have been derived allowing for sharp error/residual relations for a posteriori error control.

3. Space-Time Variational Optimal Control Problem

We adopt the above notation, in particular (2.10), (2.13), (2.15) for $\mathcal{U}$, $\mathcal{Y}$ as well as (2.14) for the space-time variational form of the constraint. We note that the dual of $\mathcal{Z}$ defined in (2.13) reads $\mathcal{Z}' = L_2(I;X') \times H$. Moreover, being a Hilbert space, $\mathcal{Z}$ is reflexive, i.e. we have $\mathcal{Z}'' \cong \mathcal{Z}$.

3.1. Formulation

We are now going to derive a space-time variational formulation of Problem 1.1. Recall, that both state and control are functions of space and time and that we are facing a problem with distributed control with box constraints

$$\mathcal{U}_{ad} \coloneqq \{u \in \mathcal{U} : u_a(t,x) \le u(t,x) \le u_b(t,x) \quad \text{a.e. in } I \times \Omega\} \tag{3.1}$$

where $u_a, u_b \in \mathcal{U}$, $u_a(t,x) < u_b(t,x)$ for $(t,x) \in I \times \Omega$, a.e.. The state space is determined by the PDE, i.e., we choose $\mathcal{Y}$ defined in (2.15). Since we do not consider state constraints in Problem 1.1, we choose $\mathcal{Y}_{ad} = \mathcal{Y}$.

In view of Remark 2.2 and recalling that $\mathcal{Z}'' \cong \mathcal{Z}$, we are now in position to formulate the PDE constraint in space-time variational form as follows

$$\langle e(y,u), z\rangle_{\mathcal{Z}'\times\mathcal{Z}} \coloneqq b(y,z) - f(z;u), \qquad z \in \mathcal{Z}, \tag{3.2}$$

i.e., $e(y,u) \coloneqq f(\cdot;u) - b(y,\cdot) \in \mathcal{Z}'$. For later reference, it will be convenient to reformulate the constraint in operator form. To this end, we define

$$\begin{aligned}
B : \mathcal{Y} \to \mathcal{Z}', &\qquad \langle By, z\rangle_{\mathcal{Z}'\times\mathcal{Z}} \coloneqq b(y,z),\\
F : \mathcal{U} \to \mathcal{Z}', &\qquad \langle Fu, z\rangle_{\mathcal{Z}'\times\mathcal{Z}} \coloneqq \int_I \int_\Omega u(t,x)\, z_1(t,x)\, \mathrm{d}x\, \mathrm{d}t,\\
C \in \mathcal{Z}', &\qquad \langle C, z\rangle_{\mathcal{Z}'\times\mathcal{Z}} \coloneqq \int_I \int_\Gamma \eta(t,s)\, z_1(t,s)\, \mathrm{d}s\, \mathrm{d}t + (y_0, z_2)_H,
\end{aligned}$$

so that $e(y,u) = 0$ is equivalent to $By - Fu - C = 0$. Note, that both operators B and F are linear and that B is an isomorphism as long as the space-time variational form of the PDE constraint is well-posed. This means that we can detail the control-to-state operator $G : \mathcal{U} \to \mathcal{Y}$ as follows $Gu = B^{-1}(Fu + C)$, where $B^{-1} : \mathcal{Z}' \to \mathcal{Y}$ is the inverse. Finally, the objective function $J : \mathcal{Y} \times \mathcal{U} \to \mathbb{R}$ in Problem 1.1 can now be written as $J(y,u) = \frac{1}{2}\|y(T) - y_d\|_H^2 + \frac{\lambda}{2}\|u\|_{L_2(I;H)}^2$, where $\lambda > 0$ is the regularization parameter.

3.2. Existence of an optimal solution

Problem 3.1 (Reduced form of Problem 1.1)**.** *Find a control $u \in \mathcal{U}$ such that*

$$\min_{u\in\mathcal{U}} \hat{J}(u), \quad \hat{J}(u) \coloneqq \frac{1}{2}\|(Gu)(T) - y_d\|_H^2 + \frac{\lambda}{2}\|u\|_{\mathcal{U}}^2 \qquad \textit{s.t. } u \in \mathcal{U}_{ad}. \tag{3.3}$$

We are going to prove that Problem 3.1 admits a unique solution.

Lemma 3.2. *The reduced objective function* (3.3) *is strictly convex.*

Proof. Let $u, v \in \mathcal{U} = L_2(I; H)$, $u \neq v$ and $\alpha \in (0,1)$. Then, it is readily seen that $\|\alpha u + (1-\alpha)v\|_{\mathcal{U}}^2 = \alpha\|u\|_{\mathcal{U}}^2 + (1-\alpha)\|v\|_{\mathcal{U}}^2 - (\alpha - \alpha^2)\|u - v\|_{\mathcal{U}}^2 < \alpha\|u\|_{\mathcal{U}}^2 + (1-\alpha)\|v\|_{\mathcal{U}}^2$, since $\mathcal{U}$ is a Hilbert space. In a similar way, the linearity of G yields

$$\|G(\alpha u + (1-\alpha)v)(T) - y_d\|_H^2 < \alpha\|Gu(T) - y_d\|_H^2 + (1-\alpha)\|Gv(T) - y_d\|_H^2.$$

Then, we get

$$\begin{aligned}
\hat{J}(\alpha u + (1-\alpha)v) &= \frac{1}{2}\|G(\alpha u + (1-\alpha)v)(T) - y_d\|_H^2 + \frac{\lambda}{2}\|\alpha u + (1-\alpha)v\|_{\mathcal{U}}^2 \\
&< \frac{1}{2}\left[\alpha\|u\|_{\mathcal{U}}^2 + (1-\alpha)\|v\|_{\mathcal{U}}^2\right] + \frac{\lambda}{2}\left[\alpha\|Gu(T) - y_d\|_H^2 + (1-\alpha)\|Gv(T) - y_d\|_H^2\right] \\
&= \frac{1}{2}\alpha\|Gu(T) - y_d\|_H^2 + \frac{\lambda}{2}\alpha\|u\|_{\mathcal{U}}^2 + \frac{1}{2}(1-\alpha)\|Gv(T) - y_d\|_H^2 + \frac{\lambda}{2}(1-\alpha)\|v\|_{\mathcal{U}}^2 \\
&= \alpha\hat{J}(u) + (1-\alpha)\hat{J}(v)
\end{aligned}$$

which proves the claim. □

Lemma 3.3. *The set $\mathcal{U}_{ad}$ in* (3.1) *of admissible controls is strictly convex.*

Proof. Let $u_1, u_2 \in \mathcal{U}_{ad}$ and $\alpha \in (0,1)$. Then, $\alpha u_1 + (1-\alpha)u_2 \geq \alpha u_a + (1-\alpha)u_a = u_a$ as well as $\alpha u_1 + (1-\alpha)u_2 \leq \alpha u_b + (1-\alpha)u_b = u_b$, i.e., $\alpha u_1 + (1-\alpha)u_2 \in \mathcal{U}_{ad}$. □

Proposition 3.4. *Problem 3.1 admits a unique solution.*

Proof. In order to apply Theorem 2.3 we need to verify that $\mathcal{U}_{ad}$ is weakly sequentially compact. Since $\mathcal{U}_{ad} \subset \mathcal{U}$ and $\mathcal{U}$ is reflexive, it is sufficient to show that $\mathcal{U}_{ad}$ is bounded, closed and convex. The boundedness is obvious and the convexity is given by Lemma 3.3.

Since $\hat{J}$ is non-negative there exists a constant $c > -\infty$ so that $\hat{J}(u) \geq c$ for all $u \in \mathcal{U}_{ad}$. It remains to show that $\hat{J}$ is weakly lower semi-continuous. To this end, we need convexity (strict convextiy guaranteed by Lemma 3.2) and continuity of $\hat{J}$ (valid by continuity of G and the norms). Thus, Theorem 2.3 proves the claim. □

3.3. First-order necessary optimality conditions

Adopting the previous notation, we start by detailing the Lagrange function $\mathcal{L} : \mathcal{Y} \times \mathcal{U} \times \mathcal{Z} \times \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ for Problem 1.1, namely

$$\begin{aligned}
\mathcal{L}(y, u, p, \lambda_a, \lambda_b) = &\frac{1}{2}\|y(T) - y_d\|_H^2 + \frac{\lambda}{2}\|u\|_{L_2(I;H)}^2 \\
&- \langle p, By - Fu - C\rangle_{\mathcal{Z}\times\mathcal{Z}'} - (\lambda_a, u_a - u)_{\mathcal{U}} - (\lambda_b, u - u_b)_{\mathcal{U}}.
\end{aligned} \tag{3.4}$$

The partial derivatives can easily be derived as follows: $\mathcal{L}_p(y, u, p, \lambda_a, \lambda_b) = -By + Fu + C$, $\mathcal{L}_y(y, u, p, \lambda_a, \lambda_b) = y(T) - y_d - B^*p$ and $\mathcal{L}_u(y, u, p, \lambda_a, \lambda_b) = F^*p + \lambda u + \lambda_a - \lambda_b$. This yields the KKT conditions.

Proposition 3.5 (KKT system). *Let $(\overline{y},\overline{u}) \in \mathcal{Y}\times\mathcal{U}$ be an optimal solution of Problem 1.1. Then, there exist an adjoint state $\overline{p} \in \mathcal{Z}$ and multipliers $\overline{\lambda}_a, \overline{\lambda}_b \in L_2(I;H)$ such that the following optimality system holds:*

$$B\overline{y} = F\overline{u} \qquad \textit{in } \mathcal{Z}' \qquad \text{(state equation)}, \tag{3.5a}$$
$$B^*\overline{p} = \overline{y}(T) - y_d \qquad \textit{in } \mathcal{Y}_T' \qquad \text{(adjoint problem)}, \tag{3.5b}$$
$$F^*\overline{p} + \lambda\overline{u} = \overline{\lambda}_b - \overline{\lambda}_a \qquad \textit{in } \mathcal{U}' \qquad \text{(optimality)}, \tag{3.5c}$$

as well as the complementarity conditions *a.e. in $I\times\Omega$*

$$u_a(t,x) \le \overline{u}(t,x) \le u_b(t,x), \tag{3.6a}$$
$$\overline{\lambda}_a(t,x) \ge 0, \quad \overline{\lambda}_b(t,x) \ge 0, \tag{3.6b}$$
$$\overline{\lambda}_a(t,x)(u_a(t,x) - \overline{u}(t,x)) = \overline{\lambda}_b(t,x)(u_b(t,x) - \overline{u}(t,x)) = 0. \qquad \square \tag{3.6c}$$

In the space-time variational framework, the above equations read:

$$b(\overline{y},\delta p) = f(\delta p;\overline{u}) \qquad \forall \delta p \in \mathcal{Z}, \tag{3.5a'}$$
$$b(\delta y,\overline{p}) = (\overline{y}(T) - y_d, \delta y(T))_H \qquad \forall \delta y \in \mathcal{Y}, \tag{3.5b'}$$
$$\lambda\,(\overline{u},\delta u)_{\mathcal{U}} + \int_I (\delta u(t), \overline{p}_1(t))_H \,\mathrm{d}t = \big(\overline{\lambda}_b - \overline{\lambda}_a, \delta u\big)_{\mathcal{U}} \qquad \forall \delta u \in \mathcal{U}, \tag{3.5c'}$$

where $\mathcal{U} = L_2(I;H)$. From (3.5b') we see that the adjont problem arises from the primal one by exchanging the roles of trial and test spaces – and by a different right-hand side, of course. We note that this is a major difference to a standard approach for optimal control problems, where the adjoint problem is backward in time. Moreover, the well-posedness of the adjoint problem follows directly from the Banach-Nečas theorem, even with the same inf-sup constant as in (2.16).

Remark 3.6. *Due to the convexity of the objective functional and of the set of admissible controls (see Lemma 3.2 and 3.3, resp.) as well as the linearity of the state equation, the Problem 1.1 is convex. Hence, every control satisfying* (3.5) *is an optimal solution of the problem, [1].*

4. Space-Time Discretization

In this section, we are going to describe a conforming discretization of the optimal control problem in space and time. We start by reviewing space-time Petrov-Galerkin methods for parabolic problems from [16, 22, 23].

4.1. Petrov-Galerkin discretization of the PDE

We consider and construct finite-dimensional spaces $\mathcal{Y}_\delta \subset \mathcal{Y}$ and $\mathcal{Z}_\delta \subset \mathcal{Z}$, where – for simplicity – we assume that $n_\delta := \dim(\mathcal{Y}_\delta) = \dim(\mathcal{Z}_\delta)$. The Petrov-Galerkin approximation to (2.14) then amounts determining $y_\delta \in \mathcal{Y}_\delta$ such that

$$b(y_\delta, z_\delta) = f(z_\delta; u) \qquad \forall z_\delta \in \mathcal{Z}_\delta. \tag{4.1}$$

We may think of $\delta = (\Delta t, h)$, where Δt is the temporal and h the spatial mesh width. We recall, that there are several ways to select such discrete spaces so that the arising discrete problem is well-posed and stable in the sense of (1.2). An overview of conditionally and unconditionally stable variants can be found in [15, 16, 24]. In [25] a finite element approach is described, [22, 23] show that linear ansatz and constant test functions w.r.t. time lead to the *Crank-Nicolson* time integration scheme for the special case of homogeneous Dirichlet boundary conditions if the right-hand side is approximated with the trapezoidal rule. A similar approach, but for the case of Robin boundary condition, is briefly presented in the sequel, where we basically follow [16]. It is convenient (and also efficient from the numerical point of view) to choose the approximation spaces to be of tensor product form,

$$\mathcal{Y}_\delta = V_{\Delta t} \otimes X_h, \quad \mathcal{Z}_\delta = (Q_{\Delta t} \otimes X_h) \times X_h$$

with the temporal subspaces $V_{\Delta t} \subset H^1(I)$ und $Q_{\Delta t} \subset L_2(I)$ as well as the spatial subspace $X_h \subset X = H^1(\Omega)$. Our particular choice is as follows: The time interval $I = (0, T)$ is discretized according to

$$\mathcal{T}_{\Delta t} \coloneqq \{0 =: t^{(0)} < t^{(1)} < \dots < t^{(K)} \coloneqq T\} \subset [0, T], \quad t^{(k)} = k \cdot \Delta t,$$

where $K \in \mathbb{N}$ denotes the number of time steps, i.e., $\Delta t \coloneqq T/K$ is the time step size. The temporal subspaces $V_{\Delta t}$, $Q_{\Delta t}$ and the spatial subspace X_h read

$$V_{\Delta t} \coloneqq \operatorname{span} \Theta_{\Delta t} \subset H^1(I), \quad Q_{\Delta t} \coloneqq \operatorname{span} \Xi_{\Delta t} \subset L_2(I), \quad X_h \coloneqq \operatorname{span} \Phi_h \subset H^1(\Omega)$$

with piecewise linear functions $\Theta_{\Delta t} = \{\theta^k \in H^1(I) : k = 0, \dots, K\}$, piecewise constants $\Xi_{\Delta t} = \{\xi^\ell \in L_2(I) : \ell = 0, \dots, K-1\}$ in time and piecewise linear basis functions in space $\Phi_h = \{\phi_i \in H^1(\Omega) : i = 1, \dots, n_h\}$. Doing so, we obtain $\dim(\mathcal{Y}_\delta) = \dim(\mathcal{Z}_\delta) = n_\delta = (K+1)n_h$.

The linear system. Such a Petrov-Galerkin discretization for solving (4.1) amounts determining

$$y_\delta = \sum_{k=0}^{K} \sum_{i=1}^{n_h} y_i^k \theta^k \otimes \phi_i \in \mathcal{Y}_\delta, \tag{4.2}$$

with the coefficient vector $\boldsymbol{y}_\delta \coloneqq (y_1^0, \dots, y_{n_h}^0, \dots, y_1^K, \dots, y_{n_h}^K)^\top \in \mathbb{R}^{n_\delta}$. The corresponding initial value is given by $y_\delta(0) = \sum_{i=1}^{n_h} y_i^0 \otimes \phi_i = \sum_{i=1}^{n_h} y_i^0 \cdot \phi_i$. We are going to derive the arising linear system of equations for (4.1)

$$\boldsymbol{B}_\delta \, \boldsymbol{y}_\delta = \boldsymbol{f}_\delta(u), \tag{4.3}$$

with the stiffness matrix $\boldsymbol{B}_\delta \in \mathbb{R}^{n_\delta \times n_\delta}$ and the right-hand side $\boldsymbol{f}_\delta(u) \in \mathbb{R}^{n_\delta}$. To this end, we use the basis functions for the test space and obtain for $\ell = 0, \dots, K-1$, $j = 1, \dots, n_h$ and $m = 1, \dots, n_h$

$$b(y_\delta, (\xi^\ell \otimes \phi_j, \phi_m)) = \int_I \langle \dot{y}_\delta(t), \xi^\ell \otimes \phi_j \rangle_{X' \times X} + a(y_\delta(t), \xi^l \otimes \phi_j) \, \mathrm{d}t + (y_\delta(0), \phi_m)_H$$

$$= \sum_{k=0}^{K} \sum_{i=1}^{n_h} y_i^k \left[\langle \dot\theta^k \otimes \phi_i, \xi^\ell \otimes \phi_j \rangle_{X' \times X} + a(\theta^k \otimes \phi_i, \xi^\ell \otimes \phi_j)\, \mathrm{d}t \right] + \sum_{i=1}^{n_h} y_i^0\, (\phi_i, \phi_m)_H$$
$$= \sum_{k=0}^{K} \sum_{i=1}^{n_h} y_i^k \left[\big(\dot\theta^k, \xi^\ell\big)_{L_2(I)}\, (\phi_i, \phi_j)_H + \big(\theta^k, \xi^\ell\big)_{L_2(I)}\, a(\phi_i, \phi_j) \right] + \sum_{i=1}^{n_h} y_i^0\, (\phi_i, \phi_m)_H\,,$$

and $f((\xi^\ell \otimes \phi_j, \phi_m); u) = f^1_{\ell,j}(u) + f^2_m$, where $f^1_{\ell,j}(u) := \int_I \{(u(t), \xi^\ell \otimes \phi_j)_H + (\eta(t), \xi^\ell \otimes \phi_j)_{L_2(\Gamma)}\}\, \mathrm{d}t$ and $f^2_m = (y_0, \phi_m)_H$. In order to derive a compact form, we introduce a number of matrices

$$\underline{C}^{\text{time}}_{\Delta t} := [c_{k,\ell}]_{k=0,\ell=0}^{K,K-1} \in \mathbb{R}^{(K+1)\times K} \quad \text{with} \quad c_{k,\ell} := (\dot\theta^k, \xi^\ell)_{L_2(I)}$$

$$\underline{N}^{\text{time}}_{\Delta t} := [n_{k,\ell}]_{k=0,\ell=0}^{K,K-1} \in \mathbb{R}^{(K+1)\times K} \quad \text{with} \quad n_{k,\ell} := (\theta^k, \xi^\ell)_{L_2(I)}$$

$$\underline{M}^{\text{time}}_{\Delta t} := [m_{k,\ell}]_{k=0,\ell=0}^{K-1,K-1} \in \mathbb{R}^{K\times K} \quad \text{with} \quad m_{k,\ell} := (\xi^k, \xi^\ell)_{L_2(I)}$$

$$\underline{A}^{\text{space}}_{h} := [a_{i,j}]_{i,j=1}^{n_h} \in \mathbb{R}^{n_h\times n_h} \quad \text{with} \quad a_{i,j} := a(\phi_i, \phi_j)$$

$$\underline{M}^{\text{space}}_{h} := [m_{i,j}]_{i,j=1}^{n_h} \in \mathbb{R}^{n_h\times n_h} \quad \text{with} \quad m_{i,j} := (\phi_i, \phi_j)_H$$

as well as a column vector $\underline{e}^{\text{time}} := [1, 0, \ldots, 0]^\top \in \mathbb{R}^{K+1}$. Based on this, we define

$$\boldsymbol{B}_\delta := \begin{pmatrix} \underline{C}^{\text{time}}_{\Delta t} \otimes \underline{M}^{\text{space}}_h + \underline{N}^{\text{time}}_{\Delta t} \otimes \underline{A}^{\text{space}}_h \\ \big(\underline{e}^{\text{time}}_{\Delta t}\big)^\top \otimes \underline{M}^{\text{space}}_h \end{pmatrix} \in \mathbb{R}^{n_\delta \times n_\delta}, \quad \boldsymbol{f}_\delta(u) := (\boldsymbol{f}^1_\delta(u), \boldsymbol{f}^2_\delta)^\top \in \mathbb{R}^{n_\delta}$$

with $\boldsymbol{f}^1_\delta(u) := \big[f^1_{\ell,j}(u)\big]_{j=1,\ell=0}^{n_h,K-1} \in \mathbb{R}^{K\cdot n_h}$ and $\boldsymbol{f}^2_\delta := \big[f^2_j\big]_{j=1}^{n_h} \in \mathbb{R}^{n_h}$ defined above.

4.2. Discretization of the control

So far, we did not yet discretize the control $u \in L_2(I;H) = \mathcal{U}$. Keeping the above discretizations in mind, it seems natural to choose $\mathcal{U}_\delta := Q_{\Delta t} \otimes S_h$, where $S_h := \operatorname{span} \Sigma_h \subset L_2(\Omega)$ and $\Sigma_h = \{\sigma_i \in L_2(\Omega) : i = 1, ..., \tilde n_h\}$ is a set of piecewise constant basis functions in space. Then, we consider $u_\delta = \sum_{k=0}^{K-1} \sum_{i=1}^{\tilde n_h} u_{k,i}\, \xi^k \otimes \sigma_i$ with the coefficient vector $\boldsymbol{u}_\delta := (u_{k,i})_{k=0,\ldots,K-1; i=1,\ldots,\tilde n_h} \in \mathbb{R}^{K \tilde n_h}$.

The next step is to detail $\boldsymbol{f}^1_\delta(u_\delta)$ based upon this discretization. We start with the first term, i.e.,

$$\int_I \big(u_\delta(t), \xi^\ell \otimes \phi_j\big)_H = \sum_{k=0}^{K-1} \sum_{i=1}^{\tilde n_h} u_{k,i}\, (\xi^k, \xi^\ell)_{L_2(I)}\, (\sigma_i, \phi_j)_H = \sum_{i=1}^{\tilde n_h} u_{\ell,i}\, (\sigma_i, \phi_j)_H$$
$$= [\underline{M}^{\text{time}}_{\Delta t} \otimes \underline{N}^{\text{space}}_h \boldsymbol{u}_\delta]_{\ell,j},$$

where $\underline{M}^{\text{time}}_{\Delta t}$ is the $(K \times K)$-dimensional identity (for piecewise constants) and $\underline{N}^{\text{space}}_h := [n_{i,j}]_{i=1,j=1}^{n_h, \tilde n_h}$ with $n_{i,j} := (\phi_i, \sigma_j)_H$. For later reference, we note that

$$\|u_\delta\|^2_{L_2(I;H)} = \sum_{k,\ell=0}^{K-1} \sum_{i,j=1}^{\tilde n_h} u_{k,i}\, u_{\ell,j}\, (\xi^k, \xi^\ell)_{L_2(I)}\, (\sigma_i, \sigma_j)_H = \boldsymbol{u}_\delta^\top\, [\underline{M}^{\text{time}}_{\Delta t} \otimes \underline{M}^{\text{control}}_h]\, \boldsymbol{u}_\delta,$$

where $\underline{M}_h^{\text{control}} \coloneqq [m_{i,j}]_{i=1,j=1}^{n_h,\tilde{n}_h} \in \mathbb{R}^{n_h \times \tilde{n}_h}$ with $m_{i,j} \coloneqq (\sigma_i, \sigma_j)_H$. Using piecewise constants for ξ^k and σ_i yields the identity, i.e., $\|u_\delta\|_{L_2(I;H)} = \|\boldsymbol{u}_\delta\|$. Finally, we detail the right-hand side of the primal problem as follows

$$\begin{aligned} f^1_{\ell,j}(u_\delta) &= (u_\delta, \xi^\ell \otimes \phi_j)_{L_2(I;H)} + (\eta, \xi^\ell \otimes \phi_j)_{L_2(I;L_2(\Gamma))} \\ &= \sum_{k=0}^{K-1} \sum_{i=1}^{\tilde{n}_h} u_{k,i}\, (\xi^k, \xi^\ell)_{L_2(I)}\, (\phi_j, \sigma_i)_H + (\eta, \xi^\ell \otimes \phi_j)_{L_2(I;L_2(\Gamma))} \\ &= \left([\underline{M}_{\Delta t}^{\text{time}} \otimes \underline{N}_h^{\text{space}}] \boldsymbol{u}_\delta + \boldsymbol{\eta}_\delta \right)_{\ell,j}, \end{aligned}$$

where $\boldsymbol{\eta}_\delta \coloneqq [(\eta, \xi^\ell \otimes \phi_j)_{L_2(I;L_2(\Gamma))}]_{\ell=0,\dots,K-1; j=1,\dots,n_h}$.

Remark 4.1. *We stress the fact that we could use any other suitable discretization of the control, both w.r.t. time and space, in particular including adaptive techniques or a discretization arising from implicitly utilizing the optimality conditions and the discretization of the state and adjoint equation, [26]. In our numerical experiments, we consider the case* $\mathcal{U}_\delta \coloneqq Q_{\Delta t} \otimes X_h$*, i.e., the same spatial discretization for state and control (which is of course not necessary here).*

4.3. Petrov-Galerkin discretization of the adjoint problem

We are now going to derive the discrete form of the adjoint problem (3.5b) or (3.5b'). Since this problem involves the adjoint operator, it seems reasonable to use the same discretization, so that the discrete problem amounts finding $\boldsymbol{p}_\delta \in \mathbb{R}^{n_\delta}$ such that

$$\boldsymbol{B}_\delta^\top \boldsymbol{p}_\delta = \boldsymbol{g}_\delta(y_\delta),$$

i.e., the stiffness matrix is the transposed of the stiffness matrix of the primal problem. The unknown coefficient vector can be decomposed as $\boldsymbol{p}_\delta = (\boldsymbol{p}_\delta^1, \boldsymbol{p}_\delta^2)^\top$, where $\boldsymbol{p}_\delta^1 = (p_{k,i}^1)_{k=0,\dots,K-1, i=1,\dots,n_h} \in \mathbb{R}^{K n_h}$ and $\boldsymbol{p}_\delta^2 = (p_i^2)_{i=1,\dots,n_h}$ such that

$$\mathcal{Z}_\delta \ni p_\delta = (p_\delta^1, p_\delta^2) = \left(\sum_{k=0}^{K-1} \sum_{i=1}^{n_h} p_{k,i}^1\, \xi^k \otimes \phi_i, \sum_{i=1}^{n_h} p_i^2\, \phi_i \right).$$

Let us now detail the right-hand side. To this end, we abbreviate the coefficient vector of $y_\delta(T)$ in terms of the basis Φ_h as $\boldsymbol{y}_{\delta;K} \coloneqq (y_1^K, \dots, y_{n_h}^K)^\top$. By (4.2) we obtain

$$y_\delta(T) = \theta^K(T) \sum_{i=1}^{n_h} y_i^K \phi_i. \tag{4.4}$$

Moreover, we discretize (or approximate) y_d in Problem 1.1 as $y_d \approx y_{d,h} = \sum_{i=1}^{n_h} y_{d,i}\, \phi_i$ and $\boldsymbol{y}_{d;h} \coloneqq (y_{d,1}, \dots, y_{d,n_h})^\top$. With these notations at hand, the right-hand side can be written as $\boldsymbol{g}_\delta(y_\delta) = (\boldsymbol{0}, \boldsymbol{g}_\delta^2(y_\delta))^\top$, $\boldsymbol{0} \in \mathbb{R}^{K n_h}$ and $\boldsymbol{g}_\delta^2(y_\delta) \coloneqq \underline{M}_h^{\text{space}} (\theta^K(T)\, \boldsymbol{y}_{\delta;K} - \boldsymbol{y}_{d;h}) \in \mathbb{R}^{n_h}$.

4.4. Optimal control problem

Next, we detail the specific form of the space-time discretization of the cost function, i.e., $J_\delta(y_\delta, u)$[1]. We have

$$\hat{\boldsymbol{J}}_\delta(\boldsymbol{u}_\delta) := J_\delta(y_\delta, u_\delta) := \frac{1}{2}\int_\Omega |y_\delta(T,x) - y_{d;h}(x)|^2 \,\mathrm{d}x + \frac{\lambda}{2}\int_I \int_\Omega |u_\delta(t,x)|^2 \,\mathrm{d}x\,\mathrm{d}t$$

$$= \frac{1}{2}(\theta^K(T)\,\boldsymbol{y}_{\delta;K} - \boldsymbol{y}_{d;h})^\top \underline{M}_h^{\text{space}}(\theta^K(T)\,\boldsymbol{y}_{\delta;K} - \boldsymbol{y}_{d;h}) + \frac{\lambda}{2}\boldsymbol{u}_\delta^\top\,[\underline{M}_{\Delta t}^{\text{time}} \otimes \underline{M}_h^{\text{control}}]\,\boldsymbol{u}_\delta.$$

We solve the optimal control problem using a standard approach, namely the projected gradient method.[2] To this end, we need to detail the search direction. Given some current iteration $u_\delta^{(\ell)}$ for the control and the corresponding adjoint $p_\delta^{(\ell)}$, by (2.7) and recalling that $e(y_\delta, u_\delta) = By_\delta - Fu_\delta - C$ we get $\hat{J}'(u_\delta^{(\ell)}) = J_u(Gu^{(\ell)_\delta}, u_\delta^{(\ell)}) - e_u(Gu_\delta^{(\ell)}, u_\delta^{(\ell)})^*\, p_\delta^{(\ell)} = \lambda u_\delta^{(\ell)} + F^* p_\delta^{(\ell)}$ and set $s_\delta^{(\ell)} := -\hat{J}(u_\delta^{(\ell)})$. It remains to detail $F^* p_\delta^{(\ell)}$. Recalling that $\langle Fu, z\rangle_{\mathcal{Z}'\times\mathcal{Z}} = (u, z_1)_{L_2(I;H)}$, we obtain that $\langle F^* p, \tilde{u}\rangle_{\mathcal{U}'\times\mathcal{U}} = (p_1, \tilde{u})_{L_2(I;H)}$ for all $\tilde{u} \in \mathcal{U}' \cong \mathcal{U} = L_2(I;H)$ by (2.10) and $p = (p_1, p_2) \in \mathcal{Z}$. i.e., $p_1 \in L_2(I;X)$. This means that $F^* p = p_1$. For the discrete version, we obtain $\hat{\boldsymbol{J}}'(\boldsymbol{u}_\delta^{(\ell)}) = \lambda \boldsymbol{u}_\delta^{(\ell)} + \boldsymbol{p}_\delta^1 \in \mathbb{R}^{Kn_h}$.

Algorithm 4.1 Projected gradient algorithm for Problem 1.1 in space-time

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Input: $\mathcal{U}_{ad}$ in (3.1), $\boldsymbol{B}_\delta$, $\boldsymbol{f}_\delta(u_\delta)$ as in §4.1, $\lambda > 0$, $\boldsymbol{y}_{d;h}$, $\mathbb{P}_{\text{ad}} : \mathcal{U} \to \mathcal{U}_{ad}$ and its discrete version $\boldsymbol{P}_{\text{ad}}$, $\boldsymbol{u}_\delta^{(0)} \in \mathbb{R}^{Kn_h}$ such that $u^{(0)} \in \mathcal{U}_{ad}$

1: **for** $\ell = 0, 1, 2, \ldots$ **do**
2: solve $\boldsymbol{B}_\delta \boldsymbol{y}_\delta^{(\ell)} = \boldsymbol{f}_\delta(u_\delta^{(\ell)})$ // state equation
3: solve $\boldsymbol{B}_\delta^T \boldsymbol{p}^{(\ell)} = (\boldsymbol{0},\ \underline{M}_h^{\text{space}}(\theta^K(T)\,\boldsymbol{y}_{\delta;K} - \boldsymbol{y}_{d;h}))^\top$ // adjoint equation
4: $\boldsymbol{v}_\delta^{(\ell)} := -\lambda \boldsymbol{u}_\delta^{(\ell)} - \boldsymbol{p}_\delta^1$ // search direction
5: determine admissible step size $s^{(\ell)}$ // step size
6: $\boldsymbol{u}_\delta^{(\ell+1)} := \boldsymbol{P}_{\text{ad}}(\boldsymbol{u}_\delta^{(\ell)} + s^{(\ell)}\,\boldsymbol{v}_\delta^{(\ell)})$ // update
7: **if** stopping criterion satisfied **stop**; **return** $(\boldsymbol{u}_\delta^{(\ell+1)}, \boldsymbol{y}_\delta^{(\ell+1)}, \boldsymbol{p}_\delta^{(\ell+1)})$
8: **end for**

Remark 4.2. *Some remarks concerning our choices in Algorithm 4.1 are in order. We stress the fact that other choices are of course also possible.*

(a) *We choose the step size in line 5 by a standard resetting algorithm.*
(b) *The projection in line 6 was realized by computing the point values and then performing a cut-off w.r.t. the given box constraints.*
(c) *As stopping criterion in line 7 we used two conditions and stopped as soon as one of the two is satisfied:*

[1] We use the notation J_δ since u_d needs to be discretized.
[2] Of course, other methods could be used as well, which is not the topic of this paper.

(1) $\|\boldsymbol{u}_\delta^{(\ell-1)} - \boldsymbol{u}_{\delta;0}^{(\ell)}\|_{\mathcal{U}} \le \tau_{rel} \|\boldsymbol{u}_\delta^{(0)} - \boldsymbol{u}_{\delta;0}^{(\ell)}\|_{\mathcal{U}} + \tau_{abs}$ *with tolerances* $0 < \tau_{\text{rel}} \le \tau_{\text{abs}}$ *where* $\mathbf{u}_{\delta;0}^{(\ell)}$ *denotes the control computed in the* ℓ*-th step using the initial step size* $s_0^{(\ell)}$*.*

(2) $\boldsymbol{J}^{(\ell-1)} - \boldsymbol{J}^{(\ell)} \le \tau_{\text{stagnation}}$ *with some tolerance* $\tau_{\text{stagnation}} > 0$*, which ensures a proper reduction of the objective functional.*

4.5. Numerically solving primal and dual problems

To finalize the realization of Algorithm 4.1, it remains to numerically solve primal and dual problems in lines 2 and 3. Since the adjoint system matrix is the transposed of the primal one, it suffices to detail the primal problem. Recall, that $\boldsymbol{B}_\delta$ is a block matrix of sums of tensor products of sparse matrices. Also the right-hand sides in lines 2 and 3 are of tensor product structure. This allows us to use specific numerical solvers for such linear systems, see e.g. [19, 20]

5. Numerical Results

In this section, we present some results of our numerical experiments. Our main goal is to compare the above presented space-time variational approach with the standard semi-discretization (see also [27] for such comparisons for parabolic problems). We do not compare with other state-of-the-art methods as we are mainly interested in investigating the effect of simultaneous space-time discretization. In order to make the comparison fair, we used the Crank-Nicolson scheme for the semi-discrete problem since our choice for trial and test spaces for the primal problem is equivalent to this time-stepping scheme, [22, 23]. Thus, in the semi-discrete setting, primal and dual problems amount for a comparable number of operations, with a stability issue for the dual problem, of course. All results were obtained with Matlab R2018b on a machine with a quad core with 2.3 GHz and 8 GB of RAM.

5.1. One-dimensional examples

We consider Problem 1.1 on $I = (0, 1)$ with the data shown in Table 1.

The tolerances are chosen as $\tau_{\text{stagnation}} = 10^{-8}$, $\tau_{\text{abs}} = 10^{-8}$ and $\tau_{\text{rel}} = 10^{-4}$. Table 2 shows the value of the objective function and the number of iterations in Algorithm 4.1 with regard to the discretization sizes for case 1. It can be observed that both approaches yield similar results. The results for case 2 were similar.

In Figure 1, we show the convergence history of the objective function, its summands and the step size. We see no significant differences between the space-time and the semi-discrete approach. This is similar for all cases.

	case 1	case 2
Ω	$(0,1)$	$(-1,1)$
Dirichlet BC y_0	0	0
Robin BC μ	1	x^2
η	0.2	$-xt$
Desired state y_d	0.2	$\begin{cases} 1, & x \le -\varepsilon \\ -\frac{1}{\varepsilon}x, & -\varepsilon < x < \varepsilon \\ -1, & x \ge \varepsilon \end{cases}$
Regularization λ	0.01	0.01
Constr. u_a, u_b	$-0.1, 0.1$	$-30, 30$
Initial value $u^{(0)}$	-0.1	0

Table 1: Data for the 1d example.

		semi-discrete		space-time	
n_h	K	#its.	$J(y,u)$	#its.	$J(y,u)$
11	40	25	$2.2828 \cdot 10^{-5}$	25	$2.2823 \cdot 10^{-5}$
26	100	25	$2.2904 \cdot 10^{-5}$	25	$2.2903 \cdot 10^{-5}$
51	200	25	$2.2914 \cdot 10^{-5}$	25	$2.2914 \cdot 10^{-5}$
101	400	25	$2.2917 \cdot 10^{-5}$	25	$2.2917 \cdot 10^{-5}$

Table 2: Objective functional for different discretizations, case 1, 1d.

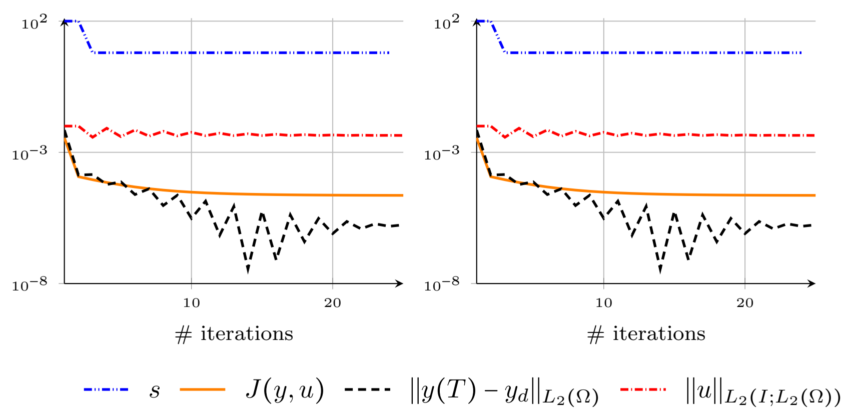

Figure 1: Case 1, 1d: Convergence, $n_h = 51$, $K = 200$, left: semi-discrete, right: space-time.

We are now going to indicate some differences between the schemes that we observed. Figures 2 (semi-discretization) and 3 (space-time) show the final control for different numbers of time steps. We observe a better stability for the space-time approach.

Finally, in Figure 4, we monitor the value of the objective function at the final time for different mesh sizes in space. We show the results for case 2, where y_d is close to a jump function and $\varepsilon = 10^{-3}$. We see that the space-time discretization reaches small values for J almost independent of the temporal

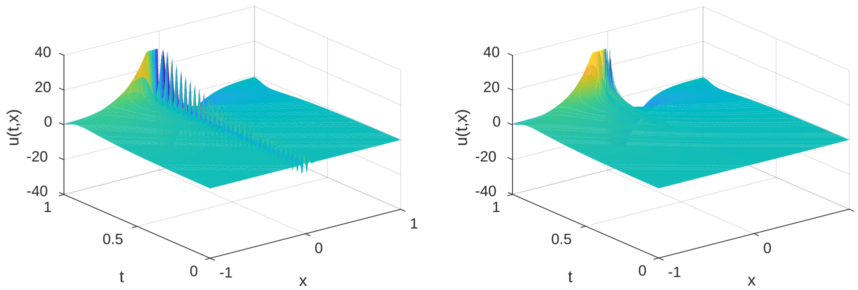

Figure 2: Final control (semi-discrete), $n_h = 128$, left: $K = 64$, right: $K = 256$, case 2, 1d.

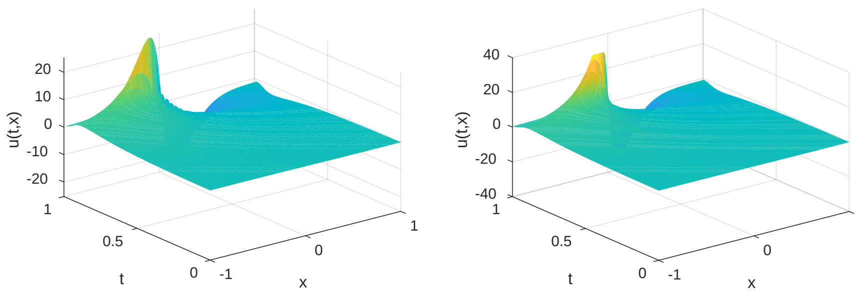

Figure 3: Final control (space-time), $n_h = 128$, left: $K = 64$, right: $K = 256$, case 2, 1d.

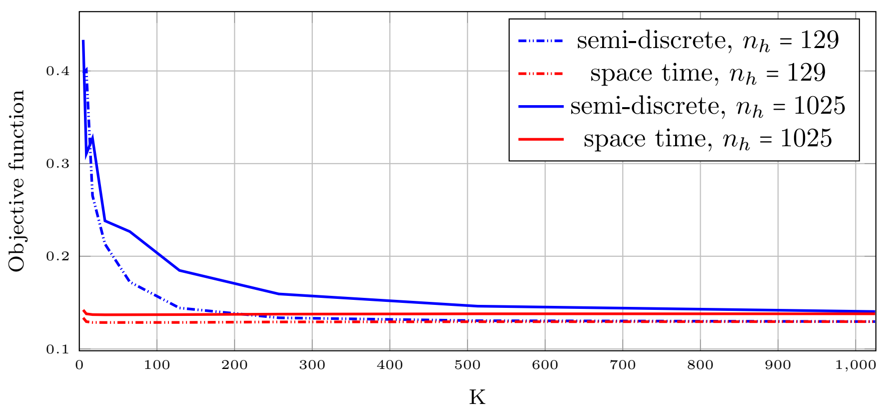

Figure 4: Case 3, $\varepsilon = 10^{-3}$: Value of objective function at final time over number of time steps.

discretization, whereas in the semi-discrete case we need many time steps to reach the same accuracy. Hence, we compare the CPU times in that light. In Table 3, we compare the CPU times to reach (almost) the same values for the objective function. We see that the semi-discrete discretization outperforms the space-time setting, but the difference is not that severe.

n_h	semi-discrete K	obj. fct.	CPU [sec]	space-time K	obj. fct.	CPU [sec]
129	1025	1.295e-01	0.44	9	1.294e-01	1.94
1025	1025	1.403e-01	1.76	5	1.421e-01	4.66

Table 3: Case 2, 1d, $\varepsilon = 10^{-3}$: CPU-times for comparable values of the objective function.

5.2. *Two-dimensional example*

Next, we consider $\Omega = (0,1)^2$, $I = (0,1)$ and choose different data for the boundary conditions and the desired state. In particular, we investigated smooth and non-smooth functions for those data. The qualitative results, however, showed a quite similar trend.

We start by comparing the CPU times for the same number of unknowns in space and time. As we see in Figure 5, semi-discrete scales linearly with the number of time-steps, as expected. For coarse meshes in space, the space-time approach (which also scales linearly) is way too expensive, see the left part of Figure 5. The situation changes with increasing spatial resolution. For $n_h = 4821$, we see a break even point for about $K = 250$. From that point on, as the number of time steps increases, space-time outperforms the semi-discrete discretization. This makes the comparison of the values of the objective function at the final time even more interesting, see Figure 6. Again, as in the 1d-case, space-time reaches the same value for the objective function with much fewer time steps. In Table 4, we fix the value of the objective function and see that space-time is more efficient by a factor of more than 4.

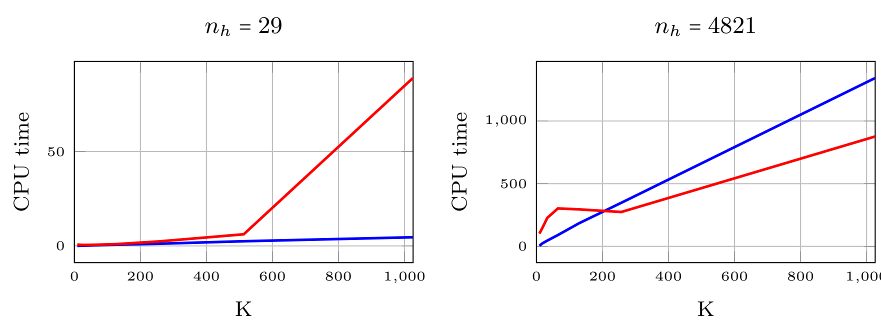

Figure 5: 2d-case, CPU-timings: coarse and fine space discretizations: $n_h = 29$ (left) and $n_h = 4821$ (right). Semi-discrete in blue, space-time in red.

n_h	semi-discrete K	obj. fct.	CPU [sec]	space-time K	obj. fct.	CPU [sec]
4821	33	1.44e-02	46.28	5	1.44e-02	10.19

Table 4: 2d: CPU-time comparisons for comparable values of the objective function.

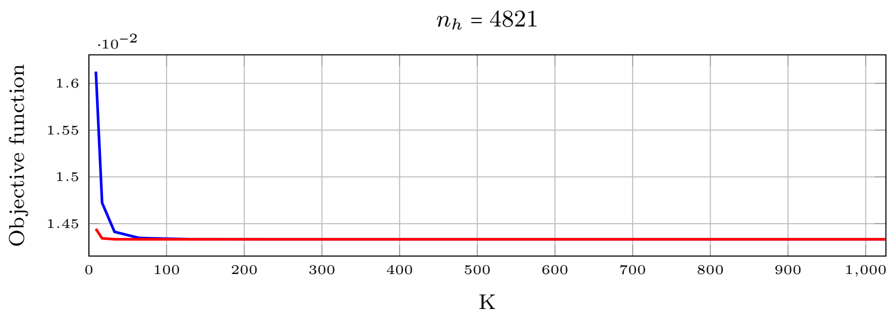

Figure 6: 2d-case, value of objective function for $n_h = 4821$. Semi-discrete in blue, space-time in red.

5.3. Three-dimensional example

Finally, we consider a spatially three-dimensional setting $\Omega = (0,1)^3$, $I = (0,1)$ and choose different smooth data for the boundary conditions and the desired state. Again, we compare runtime and the value of the objective function. As we can see from Figure 7 space-time and semi-discrete discretization are already comparable concerning runtime for a coarse mesh in space ($n_h = 93$), whereas for fine discretizations, we see a break-even point for about $K = 170$.

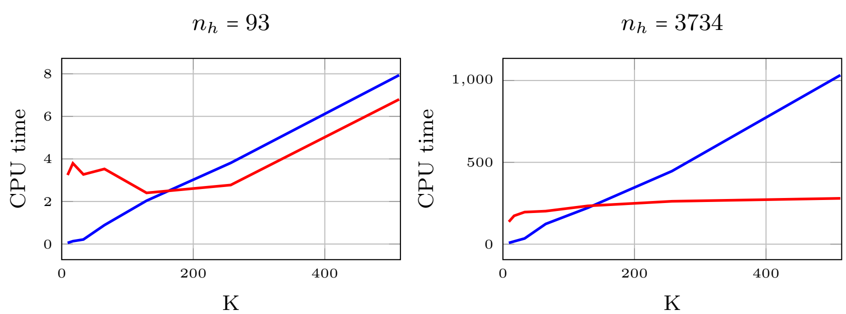

Figure 7: 3d-case, CPU-timings: coarse and fine space discretizations: $n_h = 93$ (left) and $n_h = 3734$ (right). Semi-discrete in blue, space-time in red.

The behavior of the values of the objective function in Figure 8 is similar to the previous cases, the space-time approach yields good results for much smaller number of time steps as also the comparison of CPU-times for comparable values of the objective function in Table 5 shows.

6. Summary, conclusions and outlook

We have considered a space-time variational formulation for a PDE-constrained optimal control problem with box constraints. Necessary and sufficient optimality conditions have been derived. Primal and dual problem are linear

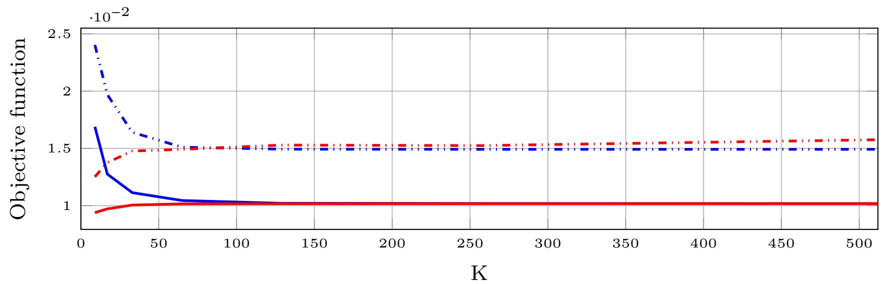

Figure 8: 3d-case, value of objective function. Semi-discrete in blue, space-time in red; $n_h = 93$ (dash-dotted), $n_h = 3734$ (solid).

	semi-discrete			space-time		
n_h	K	obj. fct.	CPU [sec]	K	obj. fct.	CPU [sec]
93	129	1.492e-02	2.04	9	1.252e-02	3.24
4821	513	1.017e-02	1032.59	33	1.005e-02	196.08

Table 5: 3d: CPU-time comparisons for comparable values of the objective function.

systems with the transposed system matrix. A simple projected gradient method has been used for solving the optimal control problem. Next, we introduced a space-time discretization which is equivalent to a Crank-Nicolson semi-discrete discretization, which allows us to perform numerical comparisons. We reported on such experiments in 1d, 2d and 3d.

In 1d, the semi-discrete discretization is much more efficient concerning runtime, most likely since the stiffness matrix is tridiagonal. However, we could already see the good stability properties of the space-time setting in the sense that we obtained stable solutions with much fewer time steps. Also the reachable value of the objective function was lower for the space-time approach. This trend is more pronounced in the 2d case and even more in the 3d example. Depending on the desired accuracy, the space-time discretization can outperform the classical semi-discrete approach significantly.

We conclude that it might in fact pay off to further investigate space-time formulations and discretizations for PDE-constrained optimal control problems. This might involve a number of topics such as state constraints, other types of PDEs for the constraints, improved schemes for solving the optimality system, adaptive discretization of the control, etc. Finally, the above setting seems to be a very good starting point for investigating model reduction [23]. We will address these issues in the future.

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