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Optimal Control for a Class of Infinite Dimensional Systems Involving an L^∞-term in the Cost Functional

Sébastien Court* Karl Kunisch† Laurent Pfeiffer†

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Abstract

An optimal control problem with a time-parameter is considered. The functional to be optimized includes the maximum over time-horizon reached by a function of the state variable, and so an L^∞-term. In addition to the classical control function, the time at which this maximum is reached is considered as a free parameter. The problem couples the behavior of the state and the control, with this time-parameter. A change of variable is introduced to derive first and second-order optimality conditions. This allows the implementation of a Newton method. Numerical simulations are developed, for selected ordinary differential equations and a partial differential equation, which illustrate the influence of the additional parameter and the original motivation.

Keywords: Optimality conditions, PDE-constrained optimization, Transversality conditions, hybrid optimal control problem.

AMS subject classifications (2010): 49K20, 49K15, 49K21, 93C30, 90C46.

Contents

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1 Introduction

We consider optimal control problems with the objective of optimizing a function of the state variable at some time τ during its time evolution. The time τ itself is free to move within the time-span $(0, T)$ of the whole experiment. As a very first thought, one might think of the prototype of a new vehicle and ask what is the highest reachable speed on the race track. Our original motivation for the class of problems under consideration stems from the domain of cardiac electro-physiology. The problem of fibrillation of a part of the heart can be mechanically tackled with the use of electric shocks acting on this muscle, leading to the re-oxygenation of the ill area, and by this means forcing this area to recover a healthy electric activity. The efficiency of the defibrillation is known to be related to the maximum reached over time by the derivative of a pressure in the heart. This quantity can be mathematically formulated as the maximum taken by a function of the state variable of the problem. We refer to [CKP16] for more details on related optimal control problems arising in electro-cardiology. While we continue to work on this challenging problem, we focus in this article on the methodology enabling to derive optimality conditions for such a problem, for a simpler class of partial differential equations.

The optimal control problem that we shall investigate can be formulated as follows:

$$\max_{\tau\in(0,T),\, u\in \mathrm{L}^2(0,T;U)} \int_0^T \ell(y(t),u(t))\mathrm{d}t + \phi_1(y(\tau)) + \phi_2(y(T)), \quad \text{subject to:} \quad \dot{y} = f(y,u), \quad y(0) = y_0,$$

where the state variable y is the solution of an evolution equation controlled by u. In this problem, ℓ denotes the cost functional, ϕ_1 the functional we want to maximize at some time τ, and ϕ_2 is the terminal cost. The analytical framework will be specified later. The specificity of this kind of problem lies in the fact that a time parameter, namely τ, can be optimized. Not only do we maximize $\phi_1 \circ y$ with the help of the control u, but we also optimize the time τ for which the maximum is reached. Note that, when ϕ_1 is nonnegative, the problem can be equivalently formulated in the following way:

$$\max_{u\in \mathrm{L}^2(0,T;U)} \int_0^T \ell(y(t),u(t))\mathrm{d}t + \|\phi_1(y(\cdot))\|_{\mathrm{L}^\infty(0,T;Y)} + \phi_2(y(T)), \quad \text{subject to:} \quad \dot{y} = f(y,u), \quad y(0) = y_0.$$

In this fashion, the cost function incorporates the L^∞-norm of a given function of the state variable.

With appropriate technical modifications, the results provided in this paper can be extended to the following hybrid control problem:

$$\begin{cases} \displaystyle\max_{\substack{0=\tau_0<\tau_1<\ldots<\tau_K=T\\ u\in\mathrm{L}^2(0,T;U)}} \sum_{k=1}^K \int_{\tau_{k-1}}^{\tau_k} \ell_k(y(t),u(t))\mathrm{d}t + \phi_k(y(\tau_k)), \\ \text{subject to:} \quad \dot{y}(t) = f_k(y(t),u(t)), \ \text{for a. e.}\ t\in(\tau_{k-1},\tau_k), \quad y(0) = y_0. \end{cases} \tag{1}$$

The above problem incorporates time parameters (or switching times) $\tau_1,\ldots,\tau_{K-1}$ which can be optimized. The term *hybrid* refers here to the fact that at the switching times τ_k, the system move from a given regime (described here by the dynamics f_k) to another one (described by the dynamics f_{k+1}). At the switching times, the integral cost changes and a function of the state is also incorporated into the cost function. There are many ways to generalize problem (1) (see e.g. [GP05]). For example, one can consider a formulation of the problem for which the dynamics f_k (used during the interval (τ_{k-1},τ_k)) can be itself chosen into a finite set of functions. Such generalizations are beyond the scope of the paper.

In the optimal control literature, many problems include time parameters that have to be optimized. Among them, time-optimal control problems have probably attracted the most the attention. These problems basically consist in minimizing the time needed to reach a given target. We refer to the early reference [HL69] on this topic. Time-optimal control problems have been studied for various models: See for example [KW13] for the wave equation, [KR15, KPR16] for the monodomain system, [Bar97] for the Navier-Stokes equations, [MRT12] for the heat equation. We also mention the time-crisis management problem studied in [BR16]; For such a problem, the time spent out of a certain closed domain must be minimized.

For our problem, the first-order optimality conditions consist of a weak maximum principle for the control control, and a transversality condition for the optimality of the time parameter. The derivation of the transversality condition is difficult, in so far as the Lagrangian of the problem is not differentiable with respect to the time-parameters. In e.g. [IK10, RZ99, RZ00], a change of variables (in time) is performed to derive the transversality condition in the case of a time-optimal control problem. This is the approach that we adopt here. It also enables us to derive second-order optimality conditions, as in [KPR16] and [LGW15] for finite-dimensional hybrid control problems. In this last reference, a numerical test based on a Riccati equation is provided to check the sufficient second-order conditions. In [GP05], specific needle variations are designed, for hybrid systems. Other approaches can also be considered. In [BR16], the time-crisis management problem is regularized and optimality conditions are derived by Γ-convergence.

One novelty of our work lies in the fact that this class of hybrid problems is addressed in infinite dimensions, theoretically as well as for numerical applications (with an example dealing with a partial differential equation). Another novelty is the derivation of second-order optimality conditions, which is – as far as we know – addressed in few articles (except for instance [LGW15]).

The paper is organized as follows: In section 2 the functional framework is specified, and the problem is transformed with a change of variables. Section 3 is devoted to the derivation of first and second-order optimality conditions. The abstract framework proposed here is shown to be satisfied, as an example, by the Navier-Stokes equations in dimension 2. The issue of numerical resolution is addressed in section 4: We use the theoretical expressions of the optimality condition in order to perform an algorithm which solves the problem, mixing Barzilai-Borwein gradient steps with newton's steps. As illustrations, we consider two classical examples of ordinary differential systems, and one example dealing with the Burgers equation.

Notation. First and second-order partial derivatives are denoted with the use of indexes. When there is no ambiguity, the time variable is sometimes omitted, or written only once (e.g. $H(y,u,p)(s)$, instead of $H(y(s),u(s),p(s))$. The first and second-order derivatives with respect to all variables (except the adjoint state, in the case of the Hamiltonian) are denoted by D and D^2, respectively. When a function h is left- and right-continuous at a given time t, the left- and right-limits are denoted by $h(t^-)$ and $h(t^+)$, respectively, and the jump is denoted by $[h]_t$.

2 Formulation of the problem

2.1 Setting

Let X be a real Hilbert space, and Y be a reflexive Banach space forming with X a Gelfand triple $Y \subseteq X \equiv X' \subseteq Y'$, with Y densely contained in X. We denote $Z = Y'$, so that Z' is isomorphic to Y. Let U be the Banach space of controls. Further let $\ell : X \times U \to \mathbb{R}$ and $f : Y \times U \to Y'$ be two twice Fréchet-differentiable mappings. For $\tilde{u} \in \mathrm{L}^2(0,T;U)$, the state is governed by the autonomous control system

$$\left\{ \begin{array}{l} \dot{\tilde{y}} = f(\tilde{y},\tilde{u}) \quad \text{on } (0,T), \\ \tilde{y}(0) = y_0, \end{array} \right. \tag{2}$$

where the initial condition $y_0 \in X$ is given. We assume that for all $y_0 \in X$ and $\tilde{u} \in \mathrm{L}^2(0,T;U)$ this system has a unique solution $\tilde{y}$ in the space:

$$W(0,T;Y) := \mathrm{L}^2(0,T;Y) \cap \mathrm{W}^{1,2}(0,T;Y').$$

Recall the continuous embedding $W(0,T;Y) \hookrightarrow \mathcal{C}([0,T];X)$, so that in particular the initial condition makes sense in X. Let ϕ_1 and $\phi_2 : X \to \mathbb{R}$ be two twice continuously Fréchet-differentiable mappings. We consider the following problem:

$$\left\{ \begin{array}{l} \displaystyle\max_{\tau \in (0,T),\ \tilde{u} \in \mathrm{L}^2(0,T;U)} \int_0^T \ell(\tilde{y}(t),\tilde{u}(t))\mathrm{d}t + \phi_1(\tilde{y}(\tau)) + \phi_2(\tilde{y}(T)) \\ \text{subject to:} \quad \dot{\tilde{y}} = f(\tilde{y},\tilde{u}) \text{ in } Y', \quad \tilde{y}(0) = y_0 \text{ in } X. \end{array} \right. \tag{3}$$

Throughout the paper, we consider the following set of assumptions on f and ℓ.

A0 The mapping $\ell : W(0,T;Y) \times \mathrm{L}^2(0,T;U) \to \mathrm{L}^1(0,T;\mathbb{R})$ is twice continuously Fréchet-differentiable.

A1 The mapping $f : W(0,T;Y) \times \mathrm{L}^2(0,T;U) \to \mathrm{L}^2(0,T;Y')$ is twice continuously Fréchet-differentiable.

A2 For all $\tilde{u} \in \mathrm{L}^2(0,T;U)$, $y_0 \in X$, system (2) admits a unique weak solution in $W(0,T;Y)$.

A3 For all $(\tilde{y},\tilde{u}) \in W(0,T;Y) \times \mathrm{L}^2(0,T;U)$, $\xi \in \mathrm{L}^2(0,T;Y')$, $z_0 \in X$, there exists a unique $z \in W(0,T;Y)$ solution to the following system

$$\begin{cases} \dot{z} = f_{\tilde{y}}(\tilde{y},\tilde{u}).z + \xi & \text{on } (0,T), \\ z(0) = z_0. \end{cases}$$

2.2 Transformation of the problem

The formulation of problem (3) does not enable us to derive optimality conditions. Indeed, the control is not continuous at the optimal time τ, in general. Therefore, the trajectory is not differentiable at τ and the cost is not differentiable with respect to τ. This difficulty can be circumvented by introducing the following change of variables, $\pi(\cdot,\tau) : [0,2] \to [0,T]$, for all $\tau \in (0,T)$,

$$\pi(s,\tau) \quad = \quad \begin{cases} \tau s & \text{if } s \in [0,1], \\ (T-\tau)s + 2\tau - T & \text{if } s \in [1,2]. \end{cases}$$

Observe that $\pi(1,\tau) = \tau$. For future reference we introduce the time-derivative $\dot{\pi}$ of π (with respect to s), as well its the partial derivative $\dot{\pi}_\tau$ with respect to τ:

$$\dot{\pi}(s,\tau) = \begin{cases} \tau & \text{if } s \in [0,1], \\ (T-\tau) & \text{if } s \in [1,2], \end{cases} \qquad \dot{\pi}_\tau(s,\tau) = \begin{cases} 1 & \text{if } s \in [0,1], \\ -1 & \text{if } s \in [1,2]. \end{cases}$$

Observe that $\dot{\pi}_\tau$ is actually independent of τ. To simplify the notation, we will simply write $\dot{\pi}_\tau(s)$. Given $\pi(\cdot,\tau)$ we introduce the following change of unknowns

$$y : s \mapsto \tilde{y} \circ \pi(s,\tau), \quad u : s \mapsto \tilde{u} \circ \pi(s,\tau), \quad s \in [0,2]. \tag{4}$$

Then, for $(u,\tau) \in \mathrm{L}^2(0,2;U) \times (0,T)$, we are lead to consider the following system

$$\begin{cases} \dot{y} = \dot{\pi}(\cdot,\tau) f(y,u) & \text{on } (0,2), \\ y(0) = y_0, \end{cases} \tag{5}$$

and the following reformulated optimal control problem:

$$\begin{cases} \max\limits_{\tau \in (0,T),\ u \in \mathrm{L}^2(0,2;U)} & J(u,\tau) := \displaystyle\int_0^2 \dot{\pi}(s,\tau)\ell(y(s),u(s))\mathrm{d}s + \phi_1(y(1)) + \phi_2(y(2)) \\ \text{subject to:} & \dot{y} = \dot{\pi}(\cdot,\tau) f(y,u) \text{ in } Y', \quad y(0) = y_0 \text{ in } X. \end{cases} \tag{6}$$

Using the fact that $\pi(\cdot,\tau) \in \mathrm{W}^{1,\infty}(0,2;\mathbb{R})$, we can verify that assumptions **A0**–**A3** imply the following ones.

A0′ The mapping $\ell : W(0,2;Y) \times \mathrm{L}^2(0,2;U) \to \mathrm{L}^1(0,2;\mathbb{R})$ is twice continuously Fréchet-differentiable.

A1′ The mapping $f : W(0,2;Y) \times \mathrm{L}^2(0,2;U) \to \mathrm{L}^2(0,2;Y')$ is twice continuously Fréchet-differentiable.

A2′ For all $(u,\tau) \in \mathrm{L}^2(0,2;U) \times (0,T)$, $y_0 \in X$, system (5) admits a unique weak solution in $W(0,2;Y)$.

A3′ For all $(y,u) \in W(0,2;Y) \times \mathrm{L}^2(0,2;U)$, $\xi \in \mathrm{L}^2(0,2;Y')$, $z_0 \in X$, there exists a unique $z \in W(0,2;Y)$ solution to the following system

$$\begin{cases} \dot{z} = \dot{\pi}(\cdot,\tau) f_y(y,u).z + \xi & \text{on } (0,2), \\ z(0) = z_0. \end{cases}$$

The change of unknown (4) modifies the nature of the optimal control problem under investigation: While (3) looks like a shape optimization problem with variable domains $(0,\tau)$ and (τ,T), problem (6) has the nature of a parametric optimization problem.

The equivalence of problems (3) and (6) is straightforward because, on one hand, the time-derivative of $\tilde{y} \circ \pi(\cdot,\tau)$ is expressed with the chain rule as $\dot{\pi}(\cdot,\tau)\dot{\tilde{y}} \circ \pi(\cdot,\tau) = \dot{\pi}(\cdot,\tau) f(\tilde{y} \circ \pi(\cdot,\tau), \tilde{u} \circ \pi(\cdot,\tau))$. On the other hand, the integral on $(0,T)$ can be split on $(0,\tau) \cup (\tau,T)$, and the change of variables $\pi(\cdot,\tau)$ is used for transforming the integrals on $(0,\tau)$ and (τ,T) into the integrals on $(0,1)$ and $(1,2)$, respectively. To sum up, if $\tilde{u} \in \mathrm{L}^2(0,T;U)$, $\tau \in (0,T)$ and $u = \tilde{u} \circ \pi(\cdot,\tau)$, the pair $(\tilde{u},\tau)$ is an optimal solution of the original problem (3) if and only if the pair (u,τ) is an optimal solution of the reformulated problem (6).

3 First and second-order optimality conditions

In this section we derive necessary optimality conditions for the reformulated problem (6). Throughout this section, $\bar{u} \in \mathrm{L}^2(0,2;U)$ is a fixed value of the control and $\bar{\tau} \in (0,T)$ a fixed value of the variable τ. Note that we do not follow up the special cases which arise for $\bar{\tau} = 0$ and $\bar{\tau} = T$. We denote by $\bar{y} \in W(0,2;Y)$ the corresponding state variable, which is the solution of (5) for $(u,\tau) = (\bar{u},\bar{\tau})$.

The approach we use for deriving optimality conditions is classical, as described in [HK01, HPUU09], for instance. However, due to the time transformation and the additional optimization variable, special attention is required. Considering the state equation as a constraint of the optimization problem (6), our approach mainly consists in computing the first- and second-order derivatives of the associated Lagrangian.

3.1 Linearization of the system

We introduce the control-to-state mapping $(u,\tau) \in \mathrm{L}^2(0,2;U) \times (0,T) \mapsto S(u,\tau) \in W(0,2;Y)$, where $S(u,\tau)$ is the solution of (5). We have denoted $\bar{y} = S(\bar{u},\bar{\tau})$. The differentiability properties for this mapping S derive from assumptions $\mathbf{A1'}$–$\mathbf{A3'}$.

Lemma 1. *The mapping S is twice continuously Fréchet-differentiable on $\mathrm{L}^\infty(0,2;U) \times (0,T)$. For $v \in \mathrm{L}^2(0,2;U)$, the derivatives $z = S_u(\bar{u},\bar{\tau}).v$ and $w = S_\tau(\bar{u},\bar{\tau})$ are the respective solutions – in the weak sense – of the following systems:*

$$\left\{ \begin{array}{l} \dot{z} = \dot{\pi}(\cdot,\bar{\tau}) f_y(\bar{y},\bar{u}).z + \dot{\pi} f_u(\bar{y},\bar{u}).v \quad \text{on } (0,2), \\ z(0) = 0, \end{array} \right. \qquad \left\{ \begin{array}{l} \dot{w} = \dot{\pi}(\cdot,\bar{\tau}) f_y(\bar{y},\bar{u}).w + \dot{\pi}_\tau f(\bar{y},\bar{u}) \quad \text{on } (0,2), \\ w(0) = 0. \end{array} \right.$$

Proof. Consider the mapping

$$\begin{array}{rccl} e: & W(0,2;Y) \times \mathrm{L}^2(0,2;U) \times (0,T) & \to & \mathrm{L}^2(0,2;Y') \times X, \\ & (y,u,\tau) & \mapsto & (\dot{y} - \dot{\pi}(\cdot,\tau) f(y,u), y(0) - y_0). \end{array}$$

Since we have the identity $e(S(u,\tau),u,\tau) = 0$, assumptions $\mathbf{A1'}$–$\mathbf{A3'}$ enable us to apply the implicit function theorem. In fact, surjectivity of the mapping $e_y(y,u,\tau)$ is a consequence of $\mathbf{A3'}$, and the required smoothness conditions follow from $\mathbf{A1'}$. The result then follows. □

3.2 Comments on the functional framework

3.2.1 Example

The variational framework $W(0,T;Y)$ is applicable, for instance, to the Burgers system (see section 4.2.3), or to the unsteady Navier-Stokes system (see [HK01, HK04]). Assumptions **A1**–**A3** can be easily verified for the Burgers system, if we refer to the analysis of e.g. [Vol01].
Let us detail the verification for the Navier-Stokes system:

$$\begin{aligned} \dot{y} + (y \cdot \nabla) y - \nu \Delta y + \nabla p = Bu \qquad & \text{in } \Omega \times (0,T), \\ \operatorname{div} y = 0 \qquad & \text{in } \Omega \times (0,T), \\ y = 0 \qquad & \text{on } \partial\Omega \times (0,T), \\ y(0) = y_0 \qquad & \text{in } \Omega. \end{aligned}$$

In the system above, Ω is a bounded domain of $\mathbb{R}^2$, with smooth boundary, and $B \in \mathcal{L}(U,X)$ is a linear operator, for instance $B = \mathbb{1}_\omega$ where $\omega \subset \Omega$, and $U = [L^2(\omega)]^2$. We consider the solenoidal spaces

$$Y = \left\{ y \in [\mathrm{H}^1_0(\Omega)]^2 \mid \operatorname{div} y = 0 \right\}, \quad X = \left\{ y \in [\mathrm{L}^2(\Omega)]^2 \mid \operatorname{div} y = 0 \right\}, \quad Y' \supset [\mathrm{H}^{-1}(\Omega)]^2,$$

and $y_0 \in X$. In the variational formulation given below, the pressure p disappears:

Find $y \in W(0,T;Y)$ such that for all $\varphi \in \mathrm{L}^2(0,T;Y)$ we have almost everywhere in $(0,T)$:

$$\left\{ \begin{array}{l} \langle \dot{y} + (y \cdot \nabla) y ; \varphi \rangle_{Y';Y} + \nu \langle \nabla y ; \nabla \varphi \rangle_{[\mathrm{L}^2(\Omega)]^2} = \langle Bu ; \varphi \rangle_{Y';Y}, \\ \langle y(0) ; \varphi \rangle_X = \langle y_0 ; \varphi \rangle_X. \end{array} \right.$$

For details we refer to [Tem79]. Here we have $f(y,u) = \nu\Delta y - (y\cdot\nabla)y + Bu$. In order to verify assumption **A1**, a short consideration shows that first and second order directional differentiability and continuity of the derivatives (and hence Fréchet differentiability) of f will follow from the continuity of the Oseen–type term $(z_1, z_2, z_3) \mapsto (z_1\cdot\nabla)z_2 + (z_3\cdot\nabla)z_1$ from $[W(0,T;Y)]^3$ to $\mathrm{L}^2(0,T;Y')$, which will be given below. Since $\operatorname{div} z_1 = \operatorname{div} z_2 = \operatorname{div} z_3 = 0$, we have

$$\begin{aligned}
(z_1\cdot\nabla)z_2 + (z_3\cdot\nabla)z_1 &= \operatorname{div}(z_2\otimes z_1 + z_1\otimes z_3),\\
\|(z_1\cdot\nabla)z_2 + (z_3\cdot\nabla)z_1\|_{Y'} &\leq \|(z_1\cdot\nabla)z_2 + (z_3\cdot\nabla)z_1\|_{[\mathrm{H}^{-1}(\Omega)]^2}\\
&\leq \|z_1\otimes z_2 + z_3\otimes z_1\|_{[\mathrm{L}^2(\Omega)]^2} \leq \|z_1\otimes z_2\|_{[\mathrm{L}^2(\Omega)]^4} + \|z_3\otimes z_1\|_{[\mathrm{L}^2(\Omega)]^4}.
\end{aligned}$$

In view of the symmetric role played by z_1, z_2 and z_3, we only estimate the first term. From [GS91] (Appendix B, Proposition B.1), in dimension 2 there exists a constant $C > 0$ independent of z_1 and z_2 such that

$$\|z_1\otimes z_2\|_{[\mathrm{L}^2(\Omega)]^4} \leq C\|z_1\|_{[\mathrm{H}^{1/2}(\Omega)]^2}\|z_2\|_{[\mathrm{H}^{1/2}(\Omega)]^2}.$$

By interpolation we deduce

$$\|z_1\otimes z_2\|_{[\mathrm{L}^2(\Omega)]^4} \leq C\|z_1\|^{1/2}_{[\mathrm{L}^2(\Omega)]^2}\|z_1\|^{1/2}_{[\mathrm{H}^1(\Omega)]^2}\|z_2\|^{1/2}_{[\mathrm{L}^2(\Omega)]^2}\|z_2\|^{1/2}_{[\mathrm{H}^1(\Omega)]^2}.$$

By integrating in time, this yields

$$\begin{aligned}
\|z_1\otimes z_2\|_{\mathrm{L}^2(0,T;[\mathrm{L}^2(\Omega)]^4)} &\leq C\|z_1\|^{1/2}_{\mathrm{L}^\infty(0,T;X)}\|z_2\|^{1/2}_{\mathrm{L}^\infty(0,T;X)}\|z_1\|^{1/2}_{\mathrm{L}^2(0,T;Y)}\|z_2\|^{1/2}_{\mathrm{L}^2(0,T;Y)}\\
&\leq \tilde{C}\|z_1\|_{W(0,T;Y)}\|z_2\|_{W(0,T;Y)},
\end{aligned}$$

for some constant $\tilde{C} > 0$. Thus, assumption **A1** is satisfied. Assumptions **A2** and **A3** are due to [HK01] (Proposition 2.1 page 928, and Proposition 2.4 page 929, respectively).

3.2.2 Additional regularity

In other partial differential equations examples, the function space framework $W(0,T;Y)$ can be too restrictive. This is due to the fact that, in the linearized state equation given in assumption **A3**, the term $f_y(\bar{y},\bar{u})$ appears as a coefficient. Hence the solution of this linearized system may not be well-defined, unless f satisfies appropriate growth bounds. For this purpose an alternative functional framework can be appropriate. For instance, let $\hat{Y} \subset Y \subset X$ be three Hilbert spaces endowed with a chain of continuous embeddings. Duality is understood with respect to $X \equiv X'$. We set

$$\hat{W}(0,T;\hat{Y}) = \{y \in \mathrm{L}^2(0,T;\hat{Y}) \mid \dot{y} \in \mathrm{L}^2(0,T;X)\}.$$

We still have $\hat{W}(0,T;\hat{Y}) \hookrightarrow C([0,T];X)$, but in general we do not have $\hat{W}(0,T;\hat{Y}) \hookrightarrow C([0,T];Y)$, except for instance when we have the interpolation $Y = [X;\hat{Y}]_{1/2}$. When we do not have this embedding, we can add $y \in \mathcal{C}([0,T];Y)$ into the definition of $\hat{W}(0,T;\hat{Y})$ above. In applications, for a given smooth domain Ω, we may think of $X = \mathrm{L}^2(\Omega)$, and Y, $\hat{Y}$ subspaces of $\mathrm{H}^1(\Omega)$, $\mathrm{H}^2(\Omega)$, respectively. The mapping e introduced in the proof of Lemma 1 is then modified to be

$$e: \quad \hat{W}(0,2;\hat{Y}) \times \mathrm{L}^2(0,2;U) \times \mathbb{R} \quad\to\quad \mathrm{L}^2(0,2;X) \times Y.$$

The assumptions utilized in this proof are implied by **A1**–**A3**. In order to transpose the assumptions **A1**–**A3** and to derive differentiability in the framework considered here, we introduce the mapping $\hat{f}: \hat{Y} \times U \to X$ associated with f as a restriction. We would assume:

B1 The mapping $\hat{f}: W(0,T;\hat{Y}) \times \mathrm{L}^2(0,T;U) \times \mathbb{R} \to \mathrm{L}^2(0,T;X)$ is twice continuously Fréchet-differentiable.

B2 For all $(u,\tau) \in \mathrm{L}^2(0,T;U) \times \mathbb{R}$, system (5) admits a unique solution in $\hat{W}(0,T;\hat{Y})$.

B3 For all $\xi \in \mathrm{L}^2(0,T;X)$, $z_0 \in Y$, there exists a unique $z \in \hat{W}(0,T;\hat{Y})$ solution to the following system

$$\begin{cases} \dot{z} = \hat{f}_y(\bar{y},\bar{u}).z + \xi \quad \text{on } (0,T),\\ z(0) = z_0. \end{cases}$$

This framework, where strong regularity is considered, is needed when the nonlinearity of the mapping f cannot be handled in the context of weak solutions. For instance, polynomial nonlinearities, as those occurring in the Schlögel and FitzHugh-Nagumo systems (see [CRT13]), require the notion of strong solutions. In the context of parabolic equations, the time-dependent operator $\hat{f}_y(\bar{y}, \bar{u})$ can be studied with the approaches of [Bar71] or [Trö10] for instance.

For a sake of being specific, in the rest of the paper we will keep the framework of the function space $W(0,T;Y)$, with assumptions **A1**–**A3**. Analogous results as those obtained for $W(0,T;Y)$ also hold for $\hat{W}(0,T;\hat{Y})$.

3.3 Vectorial formalism

We define the functional space $\mathcal{Y}$ and its dual space as follows:

$$\mathcal{Y} = X \times X \times \mathrm{L}^2(0,2;Y), \qquad \mathcal{Y}' = X \times X \times \mathrm{L}^2(0,2;Y').$$

Next we introduce the mapping $\mathbf{S}$ as follows:

$$\mathbf{S} : (u,\tau) \in \mathrm{L}^2(0,2;U) \times (0,T) \quad \mapsto \quad (S(u,\tau)(1), S(u,\tau)(2), S(u,\tau)) \in \mathcal{Y}.$$

As a consequence of Lemma 1, the mapping $\mathbf{S}$ is twice differentiable. Its first-order derivatives are given by:

$$\mathbf{S}_u(u,\tau) = \big(S_u(u,\tau)(1), S_u(u,\tau)(2), S_u(u,\tau)\big), \qquad \mathbf{S}_\tau(u,\tau) = \big(S_\tau(u,\tau)(1), S_\tau(u,\tau)(2), S_\tau(u,\tau)\big). \tag{7}$$

Let us define the operator $\mathcal{K} \in \mathcal{L}\left(\mathrm{L}^2(0,2;Z);\mathcal{Y}\right)$ by

$$\mathcal{K}: \quad \xi \quad \mapsto \quad (z(1), z(2), z)$$

where $z \in W(0,2;Y)$ is defined – in virtue of assumption **A3** – as the solution of

$$\left\{ \begin{array}{l} \dot{z} = \dot{\pi}(\cdot,\bar{\tau}) f_y(\bar{y},\bar{u}).z + \xi \quad \text{on } (0,2), \\ z(0) = 0. \end{array} \right. \tag{8}$$

Lemma 2. *The adjoint $\mathcal{K}^* \in \mathcal{L}\left(\mathcal{Y}';\mathrm{L}^2(0,2;Z')\right)$ of $\mathcal{K}$ is given by $\mathcal{K}^*(a,b,w) = q$, where q is the solution of*

$$\left\{ \begin{array}{l} -\dot{q} = \dot{\pi}(\cdot,\bar{\tau}) f_y(\bar{y},\bar{u})^*.q + w \quad \text{on } (0,1) \cup (1,2), \\ q(2) = b, \\ q(1^+) - q(1^-) + a = 0. \end{array} \right. \tag{9}$$

Proof. Let $\xi \in \mathrm{L}^2(0,2;Z)$ and let z be the solution of system (8) corresponding to ξ. Let $(a,b,w) \in \mathcal{Y}'$ and denote by q the solution of system (9) corresponding to (a,b,w). We calculate by integration by parts

$$\begin{aligned} \langle (a,b,w); \mathcal{K}(\xi) \rangle_{\mathcal{Y}';\mathcal{Y}} &= \langle w; z \rangle_{\mathrm{L}^2(0,2;Y');\mathrm{L}^2(0,2;Y)} + \langle a; z(1) \rangle_X + \langle b; z(2) \rangle_X \\ &= \int_0^1 \langle -\dot{q} - \dot{\pi} f_y^*(\bar{y},\bar{u}).q; z \rangle_{Y';Y} \mathrm{d}s + \int_1^2 \langle -\dot{q} - \dot{\pi} f_y^*(\bar{y},\bar{u}).q; z \rangle_{Y';Y} \mathrm{d}s \\ &\quad + \langle a; z(1) \rangle_X + \langle b; z(2) \rangle_X \\ &= \int_0^1 \langle q; \dot{z} - \dot{\pi} f_y(\bar{y},\bar{u}).z \rangle_{Z';Z} \mathrm{d}s - \langle q(1^-); z(1) \rangle_X + \int_1^2 \langle q; \dot{z} - \dot{\pi} f_y(\bar{y},\bar{u}).z \rangle_{Z';Z} \mathrm{d}s \\ &\quad + \langle q(1^+); z(1) \rangle_X - \langle q(2); z(2) \rangle_X + \langle a; z(1) \rangle_X + \langle b; z(2) \rangle_X \\ &= \int_0^1 \langle q; \xi \rangle_{Z';Z} \mathrm{d}s + \int_1^2 \langle q; \xi \rangle_{Z';Z} \mathrm{d}s, \end{aligned}$$

which leads to $\langle (a,b,w); \mathcal{K}(\xi) \rangle_{\mathcal{Y}';\mathcal{Y}} = \langle q; \xi \rangle_{\mathrm{L}^2(0,2;Z');\mathrm{L}^2(0,2;Z)}$ and thus completes the proof. □

Lemma 2 enables us to conveniently express the adjoint operators of $\mathbf{S}_u(\bar{u},\bar{\tau})$ and $\mathbf{S}_\tau(\bar{u},\bar{\tau})$.

Corollary 1. *The adjoint operators $\mathbf{S}_u(\bar{u},\bar{\tau})^* \in \mathcal{L}\left(\mathcal{Y}';\mathrm{L}^2(0,2;U')\right)$ and $\mathbf{S}_\tau(\bar{u},\bar{\tau})^* \in \mathcal{L}(\mathcal{Y}';\mathbb{R})$ are given by*

$$\mathbf{S}_u(\bar{u},\bar{\tau})^*.(a,b,w) = \dot{\pi}(\cdot,\bar{\tau}) f_u^*(\bar{y},\bar{u}) \mathcal{K}^*(a,b,w), \qquad \mathbf{S}_\tau(\bar{u},\bar{\tau})^*.(a,b,w) = \int_0^2 \dot{\pi}_\tau \langle f(\bar{y},\bar{u}); \mathcal{K}^*(a,b,w) \rangle_{Y';Y} \mathrm{d}s.$$

Proof. As a consequence of Lemma 1 and (7), we have $\mathbf{S}_u(\bar{u},\bar{\tau}) = \dot{\pi}(\cdot,\bar{\tau}) \mathcal{K} \circ f_u(\bar{y},\bar{u})$ and $\mathbf{S}_\tau(\bar{u},\bar{\tau}) = \dot{\pi}_\tau \mathcal{K} \circ f(\bar{y},\bar{u})$. The result now follows from Lemma 2. □

3.4 Lagrangian formulation

We introduce the Hamiltonian:

$$\begin{array}{rrcl} H: & Y \times U \times Z' & \mapsto & \mathbb{R} \\ & (y,u,p) & \to & \ell(y,u) + \langle p; f(y,u)\rangle_{Z';Z}. \end{array}$$

Given, $(\bar{y},\bar{u},\bar{\tau}) \in W(0,2;Y) \times \mathrm{L}^2(0,2;U) \times (0,T)$, the adjoint state $\bar{p}$ is assumed to satisfy

$$\bar{p}_{|(0,1)} \in W(0,1;Z'), \qquad \bar{p}_{|(1,2)} \in W(1,2;Z')$$

(and thus $\bar{p} \in W(0,2;Z')$), by being defined as the solution of the following linear system:

$$\left\{ \begin{array}{l} -\dot{p} = \dot{\pi}(\cdot,\bar{\tau}) H_y(\bar{y},\bar{u},p) \quad \text{on } (0,1)\cup(1,2), \\ p(2) = D\phi_2(\bar{y}(2)), \\ p(1^+) - p(1^-) + D\phi_1(\bar{y}(1)) = 0. \end{array} \right. \tag{10}$$

Recall the continuous embeddings $W(I;Z') \hookrightarrow \mathcal{C}(\overline{I};X)$, for $I=(0,1)$ and $I=(1,2)$. In order to solve this backward system, we first consider $\bar{p}(2) = D\phi_2(\bar{y}(2))$ as the initial condition in X, next compute $\bar{p}$ on $(1,2)$ according to the first equation of (10), deduce $\bar{p}(1^-)$ from $\bar{p}(1^+)$ with the transmission condition in X, and finally compute $\bar{p}$ on $(0,1)$ as previously. From a more abstract point of view, since the affine mapping $p \mapsto H_y(\bar{y},\bar{u},p) = f_y(\bar{y},\bar{u})^*.p + \ell_y(\bar{y},\bar{u})$ is in the form of the right-hand-side in system (9), and thus Lemma 2 allows the existence and uniqueness of a solution to system (10).

We define the Lagrangian as follows:

$$\begin{array}{rl} L: & \big(X\times X\times W(0,2;Y)\big)\times \mathrm{L}^2(0,2;U)\times(0,T)\times W(0,2;Y) \to \mathbb{R} \\ & \big(\mathbf{y}=(a_1,a_2,y),u,\tau,p\big) \mapsto \phi_1(a_1)+\phi_2(a_2)+\displaystyle\int_0^2 \Big(\dot{\pi}(s,\tau)H(y,u,p)(s) - \langle p(s),\dot{y}(s)\rangle_{Z';Z}\Big)\mathrm{d}s \\ & \qquad -\langle p(0), y(0)-y_0\rangle_X + \langle p(2), y(2)-a_2\rangle_X - \langle [p]_1, y(1)-a_1\rangle_X, \end{array}$$

where we denote $[p]_1 = p(1^+) - p(1^-)$. Note also that the Lagrangian L is twice differentiable. The following lemma will enable us to calculate the first and second-order derivatives of the cost function J in a convenient way.

Lemma 3. *The following identity holds:*

$$J(u,\tau) = L(\mathbf{S}(u,\tau),u,\tau,p), \quad \forall (u,\tau,p) \in \mathrm{L}^2(0,2;U)\times(0,T)\times W(0,2;Y). \tag{11}$$

Moreover, setting $\bar{\mathbf{y}} = (\bar{y}(1),\bar{y}(2),\bar{y}) = \mathbf{S}(\bar{u},\bar{\tau}) \in \mathcal{Y}$ and $\bar{p}$ as the solution of the adjoint state equation (10) *corresponding to $(\bar{y},\bar{u},\bar{\tau})$, we have $L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = 0$ in $\mathcal{Y}'$.*

Proof. Identity (11) follows directly from the definitions of J, $\mathbf{S}$, and L. We decompose $L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \in \mathcal{Y}'$ into $L_{a_1}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \in X$, $L_{a_2}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \in X$ and $L_y(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \in Y'$. From the definition of the adjoint state, we obtain the following identities in X:

$$L_{a_1}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = D\phi_1(\bar{y}(1)) + [\bar{p}]_1 = 0, \qquad L_{a_2}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = D\phi_2(\bar{y}(2)) - \bar{p}(2) = 0.$$

Moreover, for all $\delta y \in \mathrm{W}(0,2;Y)$, we obtain by integration by parts

$$\begin{array}{rcl} \langle L_y(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p});\delta y)\rangle_{Y';Y} & = & \displaystyle\int_0^2 \dot{\pi}(s,\bar{\tau})\langle H_y(\bar{y},\bar{u},\bar{p})(s);\delta y(s)\rangle_{Y';Y}\mathrm{d}s - \int_0^2 \langle \bar{p}(s);\delta\dot{y}(s)\rangle_{Y;Y'}\mathrm{d}s \\ & & \quad - \langle \bar{p}(0),\delta y(0)\rangle_X + \langle \bar{p}(2),\delta y(2)\rangle_X - \langle [\bar{p}]_1,\delta y(1)\rangle_X \\ & = & 0, \end{array}$$

which concludes the proof. □

3.5 First and second-order optimality conditions

Throughout this subsection $\bar{p}$ denotes the adjoint state corresponding to the triplet $(\bar{y}, \bar{u}, \bar{\tau})$, with $\bar{y} = S(\bar{u}, \bar{\tau})$. We further denote by I the identity mapping on $\mathrm{L}^2(0,2;U')$.

Proposition 1. *The first-order derivatives of J are given by:*

$$J_u(\bar{u},\bar{\tau}).v = L_u(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}).v = \int_0^2 \dot{\pi}(s,\bar{\tau}) H_u(\bar{y},\bar{u},\bar{p})(s).v(s)\mathrm{d}s, \quad J_\tau(\bar{u},\bar{\tau}) = L_\tau(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = \int_0^2 \dot{\pi}_\tau H(\bar{y},\bar{u},\bar{p})(s)\mathrm{d}s.$$

If the pair $(\bar{u},\bar{\tau})$ is optimal, then $DJ(\bar{u},\bar{\tau}) = 0$.

Proof. The proposition follows directly from Lemma 3. Applying the chain rule to (11), we obtain:

$$DJ(\bar{u},\bar{\tau}) \quad = \quad \begin{pmatrix} L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p})\mathbf{S}_u(\bar{u},\bar{\tau}) + L_u(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \\ L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p})\mathbf{S}_\tau(\bar{u},\bar{\tau}) + L_\tau(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \end{pmatrix}.$$

Since from Lemma 3 we have $L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = 0$, the result follows. □

Remark 1. *Note that even in case where the Hamiltonian is strongly uniformly convex with respect to u, the optimal control will not be continuous at time 1 (in general), because of the jump of the adjoint state.*

In the following lemma, we calculate the Hessian of J easily, thanks to the Lagrangian formalism described above. The fact that $L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = 0$ is a key property here.

Proposition 2. *The second-order derivative of J is given by:*

$$D^2 J(\bar{u},\bar{\tau}) \quad = \quad \begin{pmatrix} \mathbf{S}_u^*(\bar{u},\bar{\tau}) & \mathrm{I} & 0 \\ \mathbf{S}_\tau^*(\bar{u},\bar{\tau}) & 0 & 1 \end{pmatrix} D^2 L(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \begin{pmatrix} \mathbf{S}_u(\bar{u},\bar{\tau}) & \mathbf{S}_\tau(\bar{u},\bar{\tau}) \\ \mathrm{I} & 0 \\ 0 & 1 \end{pmatrix}.$$

The second-order derivatives read, in a more explicit form:

$$\begin{aligned} D^2 J(\bar{u},\bar{\tau}).\big((v,\theta),(\hat{v},\hat{\theta})\big) \quad = \quad & D^2\phi_1(\bar{y}(1)).\big(z(1),\hat{z}(1)\big) + D^2\phi_2(\bar{y}(2)).\big(z(2),\hat{z}(2)\big) \\ & + \int_0^2 \dot{\pi}(s,\bar{\tau}) D^2 H(\bar{y},\bar{u},\bar{p}).\big((z,v),(\hat{z},\hat{v})\big)(s)\mathrm{d}s \\ & + \theta \int_0^2 \dot{\pi}_\tau(s) DH(\bar{y},\bar{u},\bar{p})\big(\hat{z},\hat{v}\big)(s)\mathrm{d}s + \hat{\theta}\int_0^2 \dot{\pi}_\tau(s) DH(\bar{y},\bar{u},\bar{p})\big(z,v\big)(s)\mathrm{d}s, \end{aligned}$$

where $z = S_u(\bar{u},\bar{\tau}).v + S_\tau(\bar{u},\bar{\tau}).\theta$ and $\hat{z} = S_u(\bar{u},\bar{\tau}).\hat{v} + S_\tau(\bar{u},\bar{\tau}).\hat{\theta}$.

Proof. Once again, the proposition follows directly from Lemma 3. Applying the chain rule to (11), we obtain:

$$D^2 J(\bar{u},\bar{\tau}) \quad = \quad \begin{pmatrix} \mathbf{S}_u^*(\bar{u},\bar{\tau}) & \mathrm{I} & 0 \\ \mathbf{S}_\tau^*(\bar{u},\bar{\tau}) & 0 & 1 \end{pmatrix} D^2 L(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) \begin{pmatrix} \mathbf{S}_u(\bar{u},\bar{\tau}) & \mathbf{S}_\tau(\bar{u},\bar{\tau}) \\ \mathrm{I} & 0 \\ 0 & 1 \end{pmatrix} + L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau}) D^2\mathbf{S}(\bar{u},\bar{\tau}).$$

The term involving $D^2\mathbf{S}(\bar{u},\bar{\tau})$ vanishes, since $L_{\mathbf{y}}(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p}) = 0$. The explicit form follows from the compact relation below, where the notation of the variable $(\bar{\mathbf{y}},\bar{u},\bar{\tau},\bar{p})$ has been omitted, for a sake of clarity:

$$D^2 L \quad = \quad \left(\begin{array}{cc|ccc} D^2\phi_1(\bar{y}(1)) & 0 & 0 & 0 & 0 \\ 0 & D^2\phi_2(\bar{y}(2)) & 0 & 0 & 0 \\ \hline 0 & 0 & L_{yy} & L_{yu} & L_{y\tau} \\ 0 & 0 & L_{uy} & L_{uu} & L_{u\tau} \\ 0 & 0 & L_{\tau y} & L_{\tau u} & 0 \end{array}\right).$$

Denoting $\mathbf{z} = (z(1), z(2), z)$ and $\hat{\mathbf{z}} = (\hat{z}(1),\hat{z}(2),\hat{z})$, the partial derivatives above are formally given by:

$$\begin{aligned} \left\langle \begin{pmatrix} L_{yy} & L_{yu} \\ L_{uy} & L_{uu} \end{pmatrix} \cdot \begin{pmatrix} z \\ v \end{pmatrix} ; \begin{pmatrix} \hat{z} \\ \hat{v} \end{pmatrix} \right\rangle_{\mathrm{L}^2(0,2;Y)';\mathrm{L}^2(0,2;Y)} \quad &= \quad \int_0^2 \dot{\pi}(s,\bar{\tau}) D^2 H(\bar{y},\bar{u},\bar{p})(s).\big((z,v),(\hat{z},\hat{v})\big)(s)\mathrm{d}s \\ \left\langle \begin{pmatrix} L_{\tau y} \\ L_{\tau u} \end{pmatrix} ; \begin{pmatrix} z \\ v \end{pmatrix} \right\rangle_{\mathrm{L}^2(0,2;Y)';\mathrm{L}^2(0,2;Y)} \quad &= \quad \int_0^2 \dot{\pi}_\tau DH(\bar{y},\bar{u},\bar{p})(s).(z,v)(s)\mathrm{d}s. \end{aligned}$$

So the proof is complete. □

Proposition 3. *If $(\bar{u}, \bar{\tau})$ is a solution to problem (6), then for all $(v, \theta) \in \mathrm{L}^2(0, 2; U) \times \mathbb{R}$,*

$$D^2 J(\bar{u}, \bar{\tau}).(v, \theta)^2 \quad \leq \quad 0.$$

Conversly, if $DJ(\bar{u}, \bar{\tau}) = 0$, and if there exists $\alpha > 0$ such that for all $(v, \theta) \in \mathrm{L}^2(0, 2; U) \times \mathbb{R}$

$$D^2 J(\bar{u}, \bar{\tau}).(v, \theta)^2 \quad \leq \quad -\alpha\big(\|v\|^2_{L^2(0,2;U)} + \theta^2\big), \tag{12}$$

then $(\bar{u}, \bar{\tau})$ is a local solution to problem (6). More precisely, for all $\beta \in (0, \alpha)$, there exists $\varepsilon > 0$, such that for all $(u, \tau) \in \mathrm{L}^2(0, 2; U) \times (0, T)$,

$$\|u - \bar{u}\|_{L^2(0,T;U)} + |\tau - \bar{\tau}| \leq \varepsilon \quad \Rightarrow \quad J(u, \tau) \leq J(\bar{u}, \bar{\tau}) - \frac{\beta}{2}\big(\|u - \bar{u}\|^2_{L^2(0,2;U)} + (\tau - \bar{\tau})^2\big). \tag{13}$$

Proof. If $(\bar{u}, \bar{\tau})$ is a solution to (6), then for $\varepsilon > 0$ small enough the pair $(\bar{u} + v, \bar{\tau} + \varepsilon\theta)$ is feasible and therefore

$$0 \geq \lim_{\varepsilon \downarrow 0} \frac{J(\bar{u} + \varepsilon v, \bar{\tau} + \varepsilon\theta) - J(\bar{u}, \bar{\tau})}{\varepsilon^2} = \frac{1}{2} D^2 J(\bar{u}, \bar{\tau})(v, \theta)^2,$$

since $DJ(\bar{u}, \bar{\tau}) = 0$. Conversly, assume that $DJ(\bar{u}, \bar{\tau}) = 0$ and that (12) holds. Let $\varepsilon > 0$ be such that for all $(u, \tau) \in \mathrm{L}^2(0, 2; U) \times (0, T)$ we have

$$\|u - \bar{u}\|_{\mathrm{L}^2(0,2;U)} + |\tau - \bar{\tau}| \leq \varepsilon \quad \Rightarrow \quad |(D^2 J(u, \tau) - D^2 J(\bar{u}, \bar{\tau})).(v, \theta)^2| \leq (\alpha - \beta)(\|v\|^2_{\mathrm{L}(0,2;Y)} + \theta^2). \tag{14}$$

By Taylor's Theorem, for all $(u, \tau) \in \mathrm{L}^2(0, 2; U) \times (0, T)$ such that $\|u - \bar{u}\|_{\mathrm{L}^2(0,2;U)} + |\tau - \bar{\tau}| \leq \varepsilon$, there exists $\gamma \in [0, 1]$ such that

$$J(u, \tau) \quad = \quad J(\bar{u}, \bar{\tau}) + \frac{1}{2} D^2 J(\bar{u} + \gamma v, \bar{\tau} + \gamma\theta).(v, \theta)^2,$$

where $v = u - \bar{u}$ and $\theta = \tau - \bar{\tau}$. Combined with (14), we obtain (13), which completes the proof. ☐

4 Numerical realization

4.1 Method

The numerical realization is based on a Newton method for the reduced formulation. In order to reach the attraction area for the Newton's method, first some Barzilai-Borwein gradient steps are performed (see [Ray97] for instance). In these gradient steps, only two inner products are computed for each step. Next, when the norm of the gradient is small enough, we switch to the full-step Newton's algorithm, which is faster (quadratic convergence), but demands one linear system solve at each iteration. Switching to the gradient step is monitored by the norm of the gradient given by

$$|||(J_u, J_\tau)||| := \|(J_u, J_\tau)\|^2_{\mathrm{L}^2(0,2;\mathbb{R}^m)\times\mathbb{R}} \quad = \quad \int_0^2 |J_u|^2_{\mathbb{R}^m}(s)\mathrm{d}s + |J_\tau|^2_{\mathbb{R}}.$$

The integral above is approximated by the trapezoidal rule. The algorithm then performed is the following:

Algorithm 1 Solving the first-order optimality conditions

Initialization: $u = 0$, $\tau_0 = T/2$, for $1 \leq i \leq N$, $s(i) = 2i/N$.

Gradient: Compute (J_u, J_τ).

Barzilai-Borwein steps: While $|||(J_u, J_\tau)||| > 1.e-4$, do gradient steps.

Newton steps: While $|||(J_u, J_\tau)||| > 1.e-12$, do:
- Compute $(\delta u, \delta\tau)$ by solving system (15).
- Update the unknowns: $u_{k+1} = u_k + \delta u$, $\tau_{k+1} = \tau_k + \delta\tau$.
- Update the gradient.

Post-processing: for $1 \leq i \leq N$, $t(i) := \pi(s(i), \tau)$.

Recall that J is defined in (6). The derivatives of J are provided by Proposition (1) and Proposition (2). For solving one Newton step, we use the Gmres algorithm, calling only the evaluation of the mapping

$$\begin{pmatrix} \delta u \\ \delta\tau \end{pmatrix} \quad \mapsto \quad \begin{pmatrix} J_{uu} & J_{u\tau} \\ J_{\tau u} & J_{\tau\tau} \end{pmatrix} \cdot \begin{pmatrix} \delta u \\ \delta\tau \end{pmatrix}, \tag{15}$$

which is in particular, for (u, τ) and $y = S(u, \tau)$ given, the evaluation of the following quantities:

$$\begin{aligned} J_{uu}.(\delta u, \cdot) &= \dot{\pi}(\cdot, \tau)\Big(S_u^* H_{yy} S_u.\delta u + H_{uy} S_u.\delta u + S_u^* H_{yu}.\delta u + H_{uu}.\delta u\Big) \\ &\quad + S_u^* D^2\phi_1(y(1)) S_u.\delta u + S_u^* D^2\phi_2(y(2)) S_u.\delta u, \\ J_{\tau u} &= \dot{\pi}(\cdot, \tau)\Big(S_u^* H_y + H_u + H_{uy} S_\tau + S_u^* H_{yy} S_\tau\Big) + S_u^* D^2\phi_1(y(1)) S_\tau + S_u^* D^2\phi_2(y(2)) S_\tau. \end{aligned}$$

Note, in particular, that we do not need any evaluation of the adjoint operator S_τ^*.

4.2 Illustrations

In all the tests below, for the cost function we choose

$$\ell(y, u) = -\frac{\alpha}{2}|u|^2_{\mathbb{R}^m},$$

for a cost parameter $\alpha > 0$. The examples dealing with ordinary differential systems, considered below, are inspired by [Tré05].

4.2.1 The Lotka-Volterra prey-predator system

Consider the following differential system:

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} \quad = \quad \begin{pmatrix} (y_1(a - by_2) + u_1 y_1)(1 - c_1 y_1) \\ (y_2(qy_1 - r) + u_2 y_2)(1 - c_2 y_2) \end{pmatrix}.$$

In this system the variables y_1 and y_2 represent the densities of population of preys and predators, respectively. The multiplicative terms of type $(1 - c_i y_i)$ are considered in order to limit the values of these densities to $1/c_i$. We assume that we can control the birth rates and death rates of both species, through the bilinear control made of u_1 and u_2. The numerical method given in section 4.1 is applied to this system, with

$$T = 30.0, \quad y_0 = (1.0, 2.0)^T, \quad \alpha = 10.0, \quad a = 0.3, \quad b = 0.1, \quad r = 0.2, \quad q = 0.1, \quad c_1 = c_2 = 0.05.$$

We do not consider any terminal cost, namely $\phi_2 \equiv 0$, and the functional we maximize at some time τ is $\phi_1(y) = y_2$. It means that we want to maximize the density of population of predators. The tests presented in Figures 1 and 2 are obtained with a Crank-Nicholson time-discretization, with $N = 3000$ time steps.

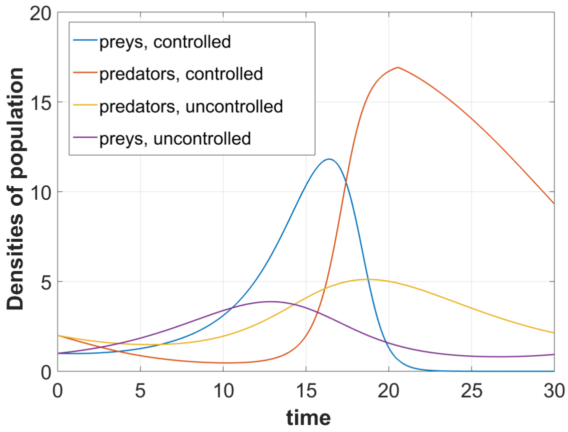

Figure 1: Comparison of the evolutions of states for the Lotka-Volterra system, with and without control.

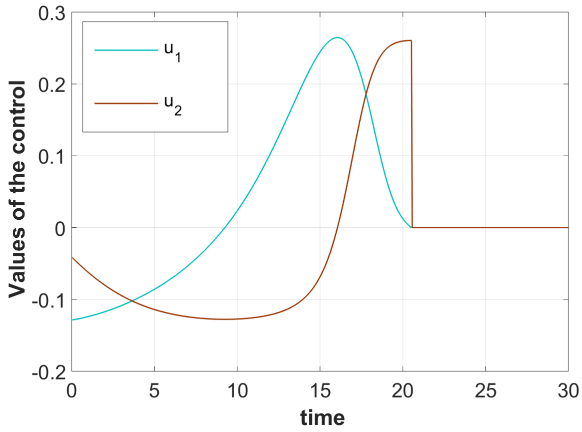

Figure 2: Values of the bilinear control through the time.

At the beginning, the action of the control leads to diminution of the populations of both preys and predators, then leads to introduction of preys in order to feed the predators, and then favor their reproduction. The maximum of predators is reached at $\tau \approx 20.57$. As expected, the time-derivative of the second-component of the state has a jump. Note that in this example the first-order optimality condition gives in particular the equalities

$$\alpha u_1 = y_1(1 - c_1 y_1)p_1, \qquad \alpha u_2 = y_2(1 - c_2 y_2)p_2.$$

Without any terminal cost, the control is indeed null for $t > \tau$, as expected in system (10) defining the adjoint-state $(p_1, p_2)^T$.

With terminal cost. In order to avoid the extinction of population of the preys after having maximized the population of predators, we consider the terminal cost functional

$$\phi_2(y) \quad = \quad -\beta \log\left(\left|\frac{y_1}{y_{\text{des}}}\right|\right)^2,$$

where $\beta > 0$ is a coefficient chosen large enough and y_{des} is the desired value for the density of preys at time $t = T$. The idea is to penalize the extinction of this population (the case $y_1(T) = 0$ is forbidden), and to force to reach the desired value by choosing β large enough. With the same coefficients chosen as previously, the same time-discretization, and with $\beta = 25.0$ and $y_{\text{des}} = 1.0$, we obtain the results presented in Figures 3 and 4.

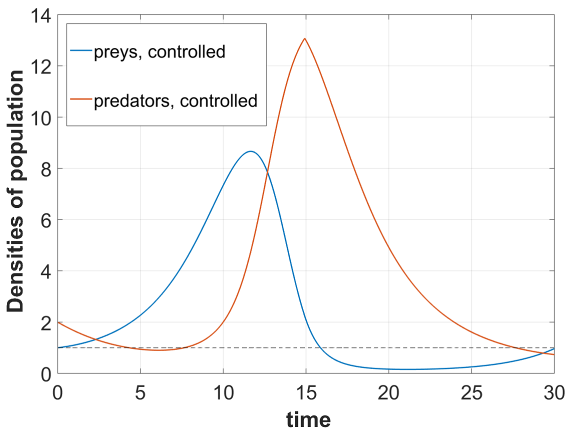

Figure 3: Evolutions of the state for the Lotka-Volterra system, with control and terminal cost.

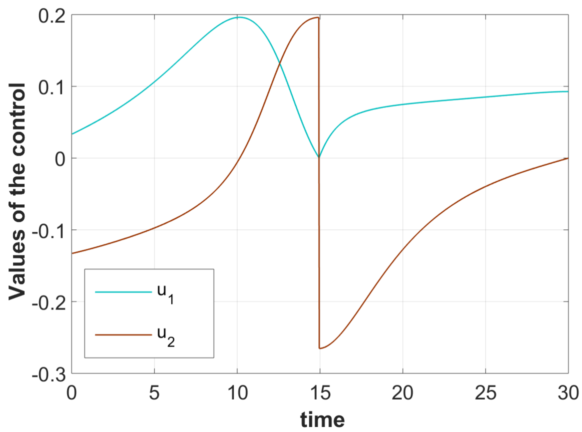

Figure 4: Values of the bilinear control through the time, with terminal cost.

The optimal time for the maximum of predators is $\tau \approx 14.87$. As expected, the maximum is smaller than the one reached without terminal cost, because the control has to be activated for $t > \tau$ in order to take into account the functional ϕ_2.

4.2.2 The simple damped pendulum

Consider the model of a simple pendulum, as described in Figure 5 below.

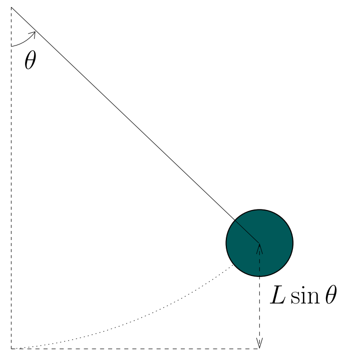

Figure 5: Simple pendulum.

The weight is assumed to satisfy the Newton's law, and so in particular the angle θ has to to satisfy the equation $\ddot{\theta} + \lambda\dot{\theta} + \mu \sin\theta = 0$, where $\lambda > 0$ is a damping term, and μ is a coefficient depending on the gravity field and the length of the taut rope. the corresponding differential system is

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} y_2 \\ -\lambda y_2 - \mu \sin y_1 \end{pmatrix} + \begin{pmatrix} 0 \\ u \end{pmatrix}.$$

where $y = (y_1, y_2)^T := (\theta, \dot{\theta})^T$, and where the control u represents some additional horizontal force in the Newton's law. The numerical method developed in section 4.1 is performed, with

$$T = 25.0, \quad y_0 = (-1.0, 0.0)^T, \quad \alpha = 10.0, \quad \lambda = 0.03, \quad \mu = 1.0.$$

Here again, we do not consider any terminal cost, namely $\phi_2 \equiv 0$. The functional we maximize at some time τ is $\phi_1(y) = y_1$, namely the angle and thus the height of the weight. The results presented in Figures 6 and 7 are obtained with a Crank-Nicholson time-discretization, with $N = 2500$ time steps.

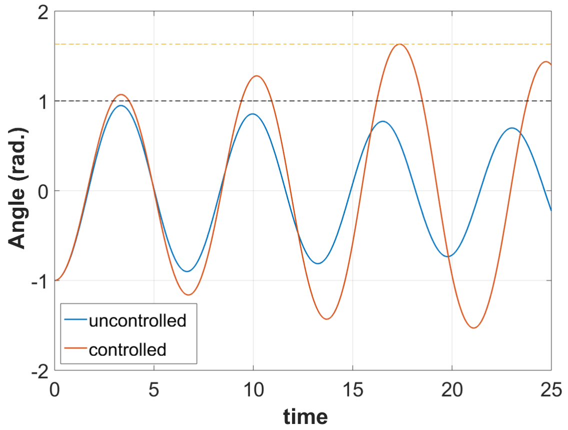

Figure 6: Comparison of the evolutions of angles for the damped simple pendulum, with and without control.

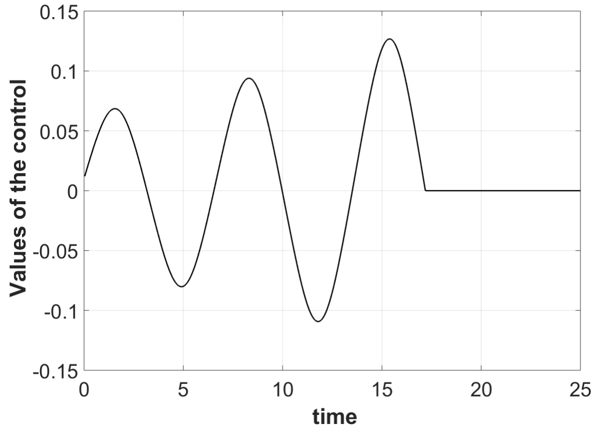

Figure 7: Values of the control through the time.

The maximum is reached at $\tau \approx 17.22$. As we can see, the control can be kept activated on several pseudo-periods, and it can compensate the damping effect. But numerically, the difficulty lies in considering an appropriate initialization for τ (which is not $T/2$ in that case). Indeed, our numerical approach enables us only to get a critical point, and thus without a correct initialization, we can also catch some local maximum or minimum, instead of the desired maximum.

4.2.3 A partial differential equation

Consider the following Burgers-type system

$$\left\{ \begin{array}{ll} \dot{y} = \nu y_{xx} - \beta y y_x + \mathbb{1}_\omega u, & (x,t) \in (0,1) \times (0,T), \\ y(0,t) = y(1,t) = 0, & t \in (0,T), \\ y(x,0) = 10.(1 - e^{-(1-x)})(e^{-(1-x)} - e^{-1}), & x \in (0,1), \end{array} \right.$$

where ν and β are positive constant. Here the unknown y is considered in the space $W(0,T;\mathrm{H}^1_0(0,1))$ (defined in section 2.1), corresponding to the Gelfand triplet $\mathrm{H}^1_0(0,1) \hookrightarrow \mathrm{L}^2(0,1) \hookrightarrow \mathrm{H}^{-1}(0,1)$. Recall that $\mathrm{H}^1(0,1) \hookrightarrow \mathcal{C}([0,1])$. The question of well-posedness for such a system is addressed in [Vol01]. The control u is considered in $\mathrm{L}^2(\omega)$, with $\omega = [0.00; 0.25]$, and the cost term is given by $\ell(y,u) = -\frac{\alpha}{2}\|u\|^2_{\mathrm{L}^2(\omega)}$. We want to maximize, at some optimal time $\tau \in (0,T)$, the following quantity

$$\phi_1(y(\cdot,\tau)) \quad = \quad \frac{1}{2}\int_D |y(x,\tau)|^2 \mathrm{d}x$$

with $D = [0.25; 0.30]$, and without considering any terminal cost: $\phi_2 \equiv 0$. The space discretization is done with finite P1-elements, with $n = 101$ degrees of freedom for the state variable, and hence $m = 26$ unknowns for the control variable. The time discretization is done with a Crank-Nicholson scheme, with $N = 1000$ time steps. We consider the following parameters

$$T = 10.0, \quad \alpha = 2.10^{-9}, \quad \nu = 2.10^{-4}, \quad \beta = 0.05.$$

The evolutions of the state and the control through the time are represented in Figure 8 below.

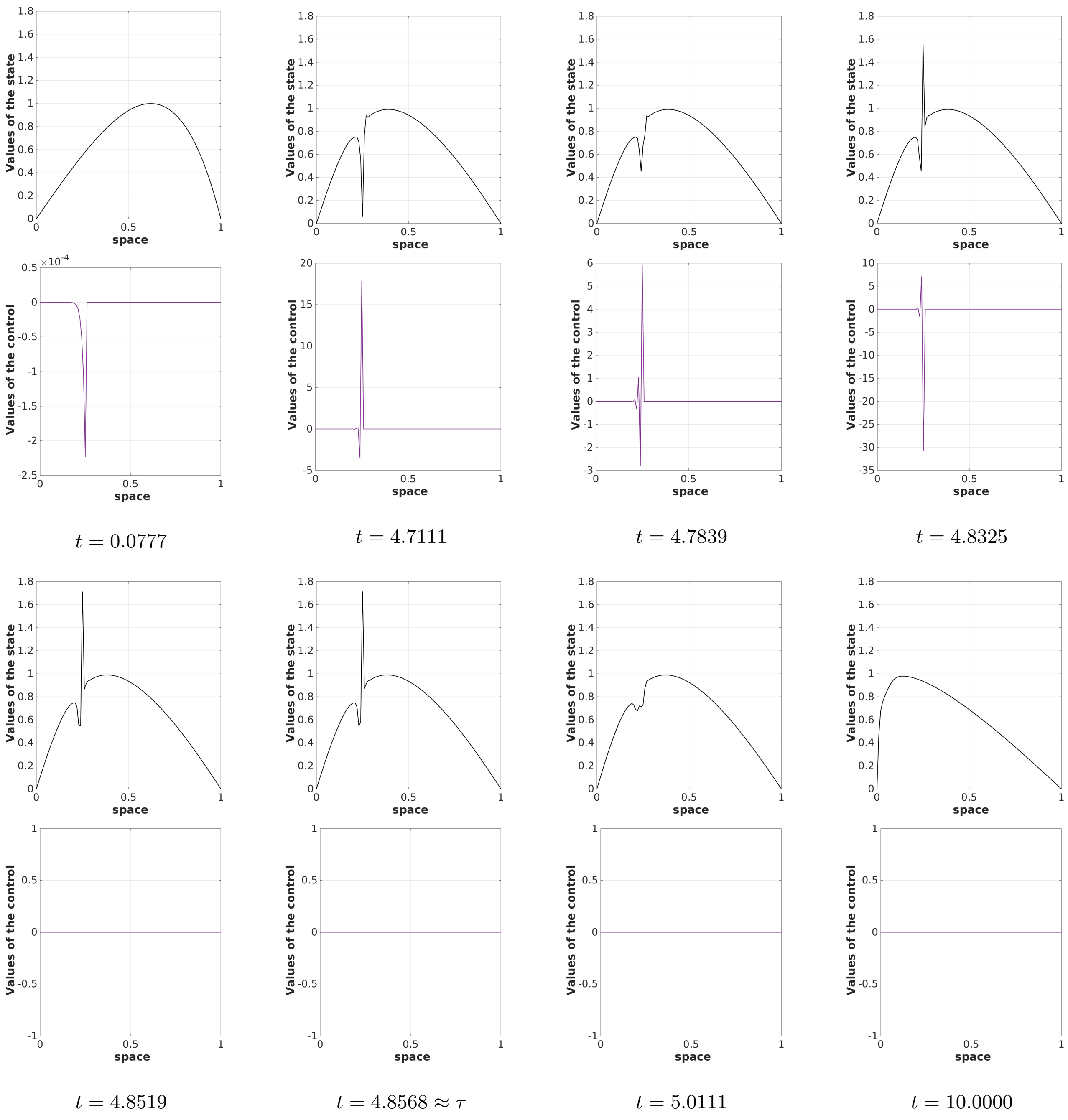

Figure 8: Values of the state and the control, for different values of the time.

The maximum is reached for $\tau \approx 4.86$. In view of the profile of the initial condition, without control the solution is transported to the left part of the domain. The simulation shows that the control seems to wait for the so transported energy, before being mainly active during a small period before $t = \tau$, operating a bumping effect. Its influence on the state leads to transport some energy from ω to D. For $t > \tau$, the energy obtained on D is diffused into the profile (the viscosity ν is chosen here very small, so that the diffusion due to the term νy_{xx} is almost not noticed). Note that some delay is encoded into the model, that is to say when the maximum is reached for the state, at time τ, and even a little bit before this moment, the control is no longer active.

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