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AN INSTANTANEOUS SEMI-LAGRANGIAN APPROACH FOR
BOUNDARY CONTROL OF A MELTING PROBLEM

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Abstract. In this paper, a sub-optimal boundary control strategy for a free boundary problem is investigated. The model is described by a non-smooth convection-diffusion equation. The control problem is addressed by an instantaneous strategy based on the characteristics method. The resulting time independent control problems are formulated as function space optimization problems with complementarity constraints. At each time step, the existence of an optimal solution is proved and first-order optimality conditions with regular Lagrange multipliers are derived for a penalized-regularized version. The performance of the overall approach is illustrated by numerical examples.

Keywords: free boundary problem; sub-optimal boundary control; characteristics method; complementarity constraint; penalization-regularization

MSC 2020: 35R35, 65M25, 49K20, 90C33

1. INTRODUCTION

Heat transfer processes involving phase change are relevant to many engineering disciplines including casting of metals, thermal storage, power systems, micro-electronics, etc., see [10]. Enhancing the thermal performance of systems using such processes requires a proper control of the temperature profile and the associated phase change interface.

Our motivation in this paper is to design an optimization strategy for a melting process that might be affected by a convection in the liquid phase. We focus on two-phase materials with sharp interface and we adopt a single domain approach, where the Stefan condition is automatically satisfied across the free boundary. More precisely, we consider a source-based method in which the total enthalpy is split into a specific heat and a latent heat acting as a source term in the energy equation [5]. Our goal is to control the temperature profile using the heat flux on a part of the

boundary. This task is, nevertheless, quite challenging even for simple geometries. In fact, the liquid-solid free boundary changes sharply with respect to the temperature. Furthermore, from a numerical point of view, solutions may exhibit non-physical oscillations for convection dominated flows. Finally, the related optimal control problem is very demanding in terms of computational time and storage.

Optimal control problems in the context of Stefan-like models have attracted a lot of attention since the eighties of the last century. We refer, in particular, to the monograph [13] and the references therein. However, most used models were generally based on simplified assumptions on the free boundary, and therefore describe roughly the phase-change process. Subsequent studies [16], [17], [7], [6] have considered two-phase Stefan problems with a focus on numerical aspects. Recently, some existence and differentiability results are established in [1], [2], [3] for one-dimensional problems.

To accommodate the problem, our strategy here exploits a semi-Lagrangian scheme [20] in the context of an instantaneous control approach [9], [8]. The time derivative and the convection terms are combined as a directional derivative along the characteristics. We show that the time-discrete state equation satisfies a maximum principle. Then, at each time step we cast the time-discrete optimal control problem—which only depends on the state at the previous time—as an optimization problem with a complementarity constraint between the temperature and solid fraction. However, due to the structure of the feasible set, standard numerical algorithms cannot be applied directly to solve such optimization problems (see for instance [14]). Here, we propose a regularization-penalization technique, where we first regularize the constraint on the temperature variable, then we incorporate the related complementarity into the objective functional via an ℓ_1 -penalty approach [15]. For the resulting regularized-penalized problems we show an existence and consistency result and further we derive first-order necessary optimality conditions that enjoy regular Lagrange multipliers. The overall approach leads, naturally, to sub-optimal solutions. Nevertheless, a good performance is achieved in the numerical experiments.

2. STATE EQUATION

Mathematical model. We consider the melting of a finite slab of a pure substance. The model is described by the non-dimensional source-based Stefan equation

$$\frac{\partial y}{\partial t} + \vec{v} \cdot \nabla y - \nabla \cdot (\kappa \nabla y) = \frac{\partial}{\partial t} \xi + \vec{v} \cdot \nabla \xi \quad \text{in } \Omega \times (t_0, t_f),$$

where $\kappa = \kappa(x, t)$ is the thermal conductivity and $\vec{v} = \vec{v}(x, t)$ is a convection velocity. The solid fraction $\xi = \xi(x, t)$ and temperature distribution $y = y(x, t)$ are related

through the relation

$$\xi \in \mathcal{H}(y) := \begin{cases} 0 & \text{if } y > 0, \\ [0, 1] & \text{if } y = 0, \\ 1 & \text{if } y < 0. \end{cases}$$

Here the phase-change processes are assumed to be isothermal. The model domain Ω is an open bounded subdomain of \mathbb{R}^d ($d = 1, 2$) with a smooth boundary Γ corresponding to both solid and liquid regions (see Fig. 1). On Γ we distinguish three parts: the system is insulated on Γ_N , a fixed temperature $y_D = 0$ is maintained on Γ_D and a non-negative heat flux control $u = u(x, t)$ is applied on Γ_C . The normal is denoted by ν . The substance is initially at the melting/freezing point

$$y(x, t_0) = 0, \quad \xi(x, t_0) = \xi_0(x) \in [0, 1] \quad \text{for } x \in \Omega.$$

The complete model equation reads

$$(\mathcal{M}^t) \quad \begin{cases} \frac{\partial y}{\partial t} + \vec{v} \cdot \nabla y - \nabla \cdot (\kappa \nabla y) = \frac{\partial}{\partial t} \xi + \vec{v} \cdot \nabla \xi & \text{in } \Omega \times (t_0, t_f), \\ \xi \in \mathcal{H}(y) & \text{in } \Omega \times (t_0, t_f), \\ \frac{\partial y}{\partial \nu} = 0 & \text{in } \Gamma_N \times (t_0, t_f), \\ \frac{\partial y}{\partial \nu} = u & \text{in } \Gamma_C \times (t_0, t_f), \\ y = 0 & \text{in } \Gamma_D \times (t_0, t_f), \\ y(t_0) = 0, \xi(t_0) = \xi_0 & \text{in } \Omega. \end{cases}$$

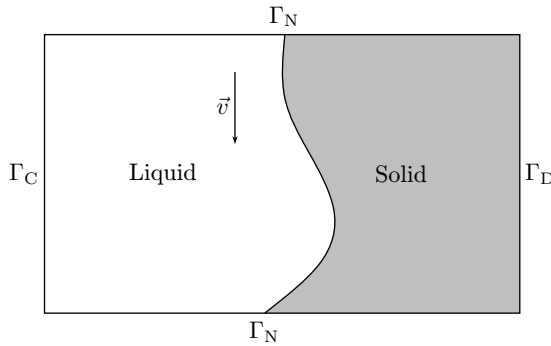


Figure 1. Problem configuration.

Time discretization. Due to the hyperbolic character of the state equation, the numerical solutions may exhibit undesired oscillations for dominated convection terms. One approach to deal with this issue consists in writing $\partial \varphi / \partial t + \vec{v} \cdot \nabla \varphi$

as $D\varphi/Dt$ the material derivative of a given function φ in the direction of \vec{v} . The corresponding characteristic curves are defined by

$$\begin{cases} \frac{dX(x, t; s)}{ds} = \vec{v}(x, t), \\ X(x, t; t) = x \end{cases}$$

with $X(x, t; s)$ being the position of a particle at time s , which was at x at time t .

Now for a given uniform time step size $\tau = (t_f - t_0)/N > 0$ we can get an approximate value of X at time $t^{n-1} = t_0 + (n-1)\tau$ by

$$X^n(x) := X(x, t^n; t^{n-1}) = x - \tau \vec{v}(x, t^n), \quad n = 1, \dots, N.$$

Using a fully-implicit scheme, we obtain the semi-discrete form of (\mathcal{M}^t)

$$(\mathcal{M}^\tau) \quad \begin{cases} y^n - \tau \nabla \cdot (\kappa^n \nabla y^n) = \xi^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \Omega, \\ \xi^n \in \mathcal{H}(y^n) & \text{in } \Omega, \\ \frac{\partial y^n}{\partial \nu} = 0 & \text{on } \Gamma_N, \\ \frac{\partial y^n}{\partial \nu} = u^n & \text{on } \Gamma_C, \\ y^n = 0 & \text{on } \Gamma_D, \\ \xi^0 = \xi_0, \quad y^0 = 0 & \text{in } \Omega, \end{cases}$$

where $n = 1, \dots, N$, $\varphi^n(\cdot) := \varphi(\cdot, t^n)$ and $\bar{\varphi}^{n-1} := \varphi^{n-1} \circ X^n$. To avoid technical difficulties, it is assumed that X^n maps Ω to itself. Formulation (\mathcal{M}^τ) has the advantage of not being restricted by a CFL condition and large time steps may be used [19].

Variational formulation. In the following, standard notations for Lebesgue and Sobolev spaces are employed (see e.g. [12], Chap. 5). The $L^2(\Omega)$ norm for either vector-valued or real-valued functions is denoted by $\|\cdot\|$. The $L^2(\Gamma_C)$ norm is specified by $\|\cdot\|_{\Gamma_C}$. To define a variational formulation for the semi-discrete problem we introduce the space

$$\mathcal{V} := \{\varphi \in H^1(\Omega); \varphi = 0 \text{ on } \Gamma_D\}$$

endowed with the $H^1(\Omega)$ norm $\|\cdot\|_{H^1(\Omega)}$.

At a specific time step t^n the variational formulation of the semi-discrete state equation consists in finding $(y^n, \xi^n) \in \mathcal{V} \times L^2(\Omega)$ such that

$$(\mathcal{WF}^n) \quad \begin{cases} Ay^n = \xi^n + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}', \\ \xi^n \in \mathcal{H}(y^n) & \text{a.e. in } \Omega \end{cases}$$

for given $u^n \in L^2(\Gamma_C)$, $\xi^{n-1} \in L^2(\Omega)$ and $y^{n-1} \in \mathcal{V}$. Here $B: L^2(\Gamma_C) \mapsto \mathcal{V}'$ and $A: \mathcal{V} \mapsto \mathcal{V}'$ standing for the linear bounded operator defined by

$$\begin{aligned} \langle Bv, \varphi \rangle &:= \tau(v, \gamma_0 \varphi)_{\Gamma_C} \quad \forall (v, \varphi) \in L^2(\Gamma_C) \times \mathcal{V}, \\ \langle A\psi, \varphi \rangle &:= (\psi, \varphi) + \tau(\kappa^n \nabla \psi, \nabla \varphi) \quad \forall (\psi, \varphi) \in \mathcal{V} \times \mathcal{V}, \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the pairing between \mathcal{V} and its dual \mathcal{V}' . The inner products in $L^2(\Omega)$ and $L^2(\Gamma_C)$ are indicated by (\cdot, \cdot) and $(\cdot, \cdot)_{\Gamma_C}$, respectively. Moreover, γ_0 is the trace operator in $H^1(\Omega)$ and $\kappa^n \in L^\infty(\Omega)$ is such that the operator A is uniformly coercive with a constant $\underline{\kappa}$.

Regarding the solvability of (\mathcal{WF}^n) we state the following theorem whose proof is deferred to Appendix A.

Theorem 2.1. *Let $u^n \in L^2(\Gamma_C)$, $y^{n-1} \in \mathcal{V}$ and $\xi^{n-1} \in L^2(\Omega)$ such that $u^n \geq 0$ a.e. in Γ_C , $y^{n-1} \geq 0$ a.e. in Ω and $0 \leq \xi^{n-1} \leq 1$ a.e. in Ω . Problem (\mathcal{WF}^n) has one and only one solution $(y^n, \xi^n) \in \mathcal{V} \times L^2(\Omega)$ that is given by the solution of*

$$(\mathcal{CS}^n) \quad \begin{cases} Ay^n = \xi^n + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}', \\ y^n \geq 0, \quad \xi^n \geq 0 & \text{a.e. in } \Omega, \\ (y^n, \xi^n) = 0. \end{cases}$$

3. SUB-OPTIMAL CONTROL PROBLEM

In the following we aim to steer the system to a desired configuration, by acting on the heat flux u at the boundary Γ_C . We adopt an instantaneous optimal control concept: at each time step t^n , given the previous temperature and solid fraction profiles y^{n-1} and ξ^{n-1} , we solve a time-independent optimal control problem. Regarding the previous theorem, we consider the following PDE-constrained optimization problems

$$(\mathcal{O}^n) \quad \begin{cases} \min & J(y^n, \xi^n, u^n) = \frac{1}{2} \|y^n - y_d^n\|_{H^1(\Omega)}^2 + \frac{1}{2} \|\xi^n - \xi_d^n\|^2 + \frac{\nu}{2} \|u^n\|_{\Gamma_C}^2, \\ \text{over} & (y^n, \xi^n, u^n) \in \mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C), \\ \text{s.t.} & Ay^n = \xi^n + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}', \\ & y^n \geq 0 \quad \text{a.e. in } \Omega, \\ & \xi^n \geq 0 \quad \text{a.e. in } \Omega, \\ & u^n \geq 0 \quad \text{a.e. on } \Gamma_C, \\ & (\xi^n, y^n) = 0, \end{cases}$$

where $y_d^n \in H^1(\Omega)$ and $\xi_d^n \in L^2(\Omega)$ correspond to a desired state at time t^n and ν is a regularization parameter.

The next lemma serves as a tool to establish some results of this paper. Its proof is straightforward.

Lemma 3.1. *Let $(y_k, \xi_k, u_k)_{k \in \mathbb{N}}$ be a sequence in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$ such that $(\xi_k, u_k)_{k \in \mathbb{N}}$ is bounded in $L^2(\Omega) \times L^2(\Gamma_C)$ and*

$$(3.1) \quad Ay_k = Bu_k + \xi_k + \bar{y}^{n-1} - \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}',$$

$$(3.2) \quad y_k \geq 0, \quad \xi_k \geq 0 \quad \text{a.e. in } \Omega,$$

$$(3.3) \quad u_k \geq 0 \quad \text{a.e. on } \Gamma_C.$$

Then there exists a sub-sequence still denoted by $(y_k, u_k, \xi_k)_{k \in \mathbb{N}}$ such that

$$(3.4) \quad u_k \rightharpoonup u \quad \text{in } L^2(\Gamma_C),$$

$$(3.5) \quad \xi_k \rightharpoonup \xi \quad \text{in } L^2(\Omega),$$

$$(3.6) \quad y_k \rightarrow y \quad \text{in } L^2(\Omega),$$

$$(3.7) \quad y_k \rightharpoonup y \quad \text{in } \mathcal{V}$$

with (y, ξ, u) being an element of $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$ satisfying

$$(3.8) \quad Ay = Bu + \xi + \bar{y}^{n-1} - \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}',$$

$$(3.9) \quad y \geq 0, \quad \xi \geq 0 \quad \text{a.e. in } \Omega,$$

$$(3.10) \quad u \geq 0 \quad \text{a.e. on } \Gamma_C.$$

Further,

$$(3.11) \quad \lim_{k \rightarrow \infty} (\xi_k, y_k) = (\xi, y).$$

In particular, if $(\xi_k, y_k) = 0$, then $(\xi, y) = 0$.

Theorem 3.1. *Problem (\mathcal{O}^n) has at least one solution.*

Proof. Let $(y_k^n, \xi_k^n, u_k^n)_{k \in \mathbb{N}} \in \mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$ be a minimizing sequence of J over the feasible set of (\mathcal{O}^n) . Then $(\xi_k^n, u_k^n)_{k \in \mathbb{N}}$ is bounded in $L^2(\Omega) \times L^2(\Gamma_C)$. From Lemma 3.1 there exists a feasible element (y^n, ξ^n, u^n) such that up to a sub-sequence, $(y_k^n, \xi_k^n, u_k^n)_{k \in \mathbb{N}}$ converges weakly to (y^n, ξ^n, u^n) in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$. It is immediate to verify that J is weakly lower semi-continuous, which proves that (y^n, ξ^n, u^n) is a solution of (\mathcal{O}^n) . \square

4. PENALIZED-REGULARIZED OPTIMAL CONTROL PROBLEM

In this section we propose a function space approach to solve the problem (\mathcal{O}^n) . Inspired by [15], we process a series of sub-problems $(\mathcal{O}_\gamma^n)_{\gamma>0}$ defined by

$$(\mathcal{O}_\gamma^n) \quad \left\{ \begin{array}{l} \min J_\gamma(y^n, \xi^n, u^n) := J(y^n, \xi^n, u^n) + \gamma(\xi^n, y^n + \varepsilon_\gamma \xi^n), \\ \text{over } (y^n, \xi^n, u^n) \in \mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C), \\ \text{s.t. } Ay^n = Bu^n + \xi^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}', \\ \quad y^n + \varepsilon_\gamma \xi^n \geq 0 \quad \text{a.e. in } \Omega, \\ \quad \xi^n \geq 0 \quad \text{a.e. in } \Omega, \\ \quad u^n \geq 0 \quad \text{a.e. on } \Gamma_C, \end{array} \right.$$

where γ and ε_γ are positive parameters such that $\gamma \rightarrow \infty$ and $\varepsilon_\gamma \rightarrow 0$. More precisely, we assume that

$$\varepsilon_\gamma \gamma \xrightarrow{\gamma \rightarrow \infty} 0.$$

The complementarity constraint will be increasingly satisfied by letting $\gamma \rightarrow \infty$, which provides a path-following method for the solution of the original control problems (\mathcal{O}^n) . Further we will show that Lagrange multipliers for (\mathcal{O}_γ^n) are regular functions, so that using, for instance, a conforming finite elements discretization in numerical experiments is justified.

Here and in the following, C is a generic constant not depending on γ .

Solvability and consistency of $(\mathcal{O}_\gamma^n)_{\gamma>0}$.

Theorem 4.1. *For every fixed $\gamma > 0$ the penalized-regularized problem (\mathcal{O}_γ^n) has at least one solution $(y_\gamma^n, \xi_\gamma^n, u_\gamma^n)$ in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$. Furthermore, there exist (y_*^n, ξ_*^n, u_*^n) in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$ and a sub-sequence $(y_\gamma^n, \xi_\gamma^n, u_\gamma^n)_{\gamma>0}$ such that*

$$(4.1) \quad u_\gamma^n \rightharpoonup u_* \quad \text{in } L^2(\Gamma_C),$$

$$(4.2) \quad \xi_\gamma^n \rightharpoonup \xi_* \quad \text{in } L^2(\Omega),$$

$$(4.3) \quad y_\gamma^n \rightarrow y_*^n \quad \text{in } L^2(\Omega),$$

$$(4.4) \quad y_\gamma^n \rightharpoonup y_*^n \quad \text{in } \mathcal{V},$$

and (y_*^n, ξ_*^n, u_*^n) is a solution of (\mathcal{O}^n) .

Proof. The existence of a solution $(y_\gamma^n, \xi_\gamma^n, u_\gamma^n)$ to (\mathcal{O}_γ^n) follows from Lemma 3.1 and J_γ weak lower semi-continuity applied to a minimizing sequence. We recall that

$$\begin{aligned} J_\gamma(y_\gamma^n, \xi_\gamma^n, u_\gamma^n) &:= J(y_\gamma^n, \xi_\gamma^n, u_\gamma^n) + \gamma(\xi_\gamma^n, y_\gamma^n + \varepsilon_\gamma \xi_\gamma^n), \\ &= J(y_\gamma^n, \xi_\gamma^n, u_\gamma^n) + \gamma(\xi_\gamma^n, y_\gamma^n) + \gamma \varepsilon_\gamma \|\xi_\gamma^n\|^2. \end{aligned}$$

On the other hand,

$$(4.5) \quad J_\gamma(y_\gamma^n, \xi_\gamma^n, u_\gamma^n) \leq J_\gamma(\tilde{y}, \tilde{\xi}, \tilde{u}) \leq J(\tilde{y}, \tilde{\xi}, \tilde{u}) + \gamma \varepsilon_\gamma \|\tilde{\xi}\|^2 \leq J(\tilde{y}, \tilde{\xi}, \tilde{u}) + C \|\tilde{\xi}\|^2$$

for all $(\tilde{y}, \tilde{\xi}, \tilde{u})$ in \mathcal{F}^n . Notice that $\mathcal{F}^n \subseteq \mathcal{F}_\gamma^n$ for all $\gamma > 0$ with \mathcal{F}^n and \mathcal{F}_γ^n being the feasible sets of (\mathcal{O}^n) and (\mathcal{O}_γ^n) , respectively.

Therefore, there exists a constant C not depending on γ such that

$$(4.6) \quad \|\xi_\gamma^n\| \leq C, \quad \|u_\gamma^n\| \leq C, \quad 0 \leq (\xi_\gamma^n, y_\gamma^n + \varepsilon_\gamma \xi_\gamma^n) \leq \frac{C}{\gamma} \quad \forall \gamma > 0.$$

Then, by Lemma 3.1, there exist sub-sequences still denoted by $(y_\gamma, \xi_\gamma, u_\gamma) \in \mathcal{F}_\gamma$ and (y_*^n, ξ_*^n, u_*^n) in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C)$ such that (4.1)–(4.4) hold and

$$\begin{aligned} Ay_*^n &= Bu_*^n + \xi_*^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} && \text{in } \mathcal{V}', \\ y_*^n &\geq 0 && \text{a.e. in } \Omega, \\ \xi_*^n &\geq 0 && \text{a.e. in } \Omega, \\ u_*^n &\geq 0 && \text{a.e. on } \Gamma_C. \end{aligned}$$

From (4.2), (4.3), (4.6) and $\lim_{\gamma \rightarrow \infty} \varepsilon_\gamma = 0$ we have

$$\lim_{\gamma \rightarrow \infty} (\xi_\gamma^n, y_\gamma^n + \varepsilon_\gamma \xi_\gamma^n) = \lim_{\gamma \rightarrow \infty} \varepsilon_\gamma \|\xi_\gamma^n\|^2 + \lim_{\gamma \rightarrow \infty} (\xi_\gamma^n, y_\gamma^n) = (\xi_*^n, y_*^n)$$

additionally, (4.6) yields that

$$\lim_{\gamma \rightarrow \infty} (\xi_\gamma^n, y_\gamma^n + \varepsilon_\gamma \xi_\gamma^n) = 0.$$

Hence, $(\xi_*^n, y_*^n) = 0$ and $(y_*^n, \xi_*^n, u_*^n) \in \mathcal{F}^n$.

Now from the weak lower semi-continuity of J we have

$$J(y_*^n, \xi_*^n, u_*^n) \leq \liminf_{\gamma \rightarrow \infty} J(y_\gamma^n, \xi_\gamma^n, u_\gamma^n).$$

Since $J \leq J_\gamma$, $\mathcal{F}^n \subseteq \mathcal{F}_\gamma^n$ and $\varepsilon_\gamma \gamma \xrightarrow{\gamma \rightarrow \infty} 0$, it follows that

$$\begin{aligned} J(y_*^n, \xi_*^n, u_*^n) &\leq \liminf_{\gamma \rightarrow \infty} J_\gamma(y_\gamma^n, \xi_\gamma^n, u_\gamma^n) \leq \liminf_{\gamma \rightarrow \infty} J_\gamma(\tilde{y}, \tilde{\xi}, \tilde{u}) \\ &\leq J(\tilde{y}, \tilde{\xi}, \tilde{u}) + \lim_{\gamma \rightarrow \infty} \gamma \varepsilon_\gamma \|\tilde{\xi}\|^2 \leq J(\tilde{y}, \tilde{\xi}, \tilde{u}) \end{aligned}$$

for any $(\tilde{y}, \tilde{\xi}, \tilde{u})$ in \mathcal{F} . Consequently, (y_*^n, ξ_*^n, u_*^n) is a solution to the limit optimal control problem (\mathcal{O}^n) . \square

First order optimality conditions for $(\mathcal{O}_\gamma^n)_{\gamma>0}$. In order to derive the first order optimality system for the regularized-penalized problems $(\mathcal{O}_\gamma^n)_{\gamma>0}$ we check the Zowe-Kurcyusz constraints qualification [22], [21] which we recall in Appendix B. In our context it requires the existence of $(c_y, c_\xi, c_u, \zeta, \lambda)$ in $\mathcal{V} \times L^2(\Omega) \times L^2(\Gamma_C) \times L^2(\Omega) \times \mathbb{R}$ such that the following system holds:

$$(CQ) \quad \begin{cases} Ac_y = Bc_u + c_\xi + z' & \text{in } \mathcal{V}', \\ c_y + \varepsilon_\gamma c_\xi - \zeta + \lambda(y_\gamma^n + \varepsilon_\gamma \xi_\gamma^n) = z & \text{a.e. in } L^2(\Omega), \\ c_\xi \geq 0, \quad \zeta \geq 0 & \text{a.e. in } L^2(\Omega), \\ c_u \geq 0 & \text{a.e. in } L^2(\Gamma_C), \\ \lambda \geq 0 \end{cases}$$

for a given $(z', z) \in \mathcal{V}' \times L^2(\Omega)$. First, we pose

$$\lambda = 0, \quad c_u = 0, \quad c_\xi = c_{\xi,1} + c_{\xi,2}, \quad \zeta = \zeta_1 + \zeta_2$$

with

$$c_{\xi,2} = \frac{1}{\varepsilon_\gamma} \max(0, z), \quad \zeta_2 = \max(0, -z).$$

Then, we choose $\zeta_1 \in \mathcal{V}$ such that the system

$$(4.7) \quad A\zeta_1 = c_{\xi,2} + z' + \Lambda \quad \text{in } \mathcal{V}',$$

$$(4.8) \quad \Lambda \geq 0, \quad \zeta_1 \geq 0, \quad \langle \Lambda, \zeta_1 \rangle = 0,$$

holds for some $\Lambda \in \mathcal{V}'$. We mention that (4.7)–(4.8) is well-posed by the theory of variational inequalities [18]. Finally, we assign to $c_{\xi,1}$ the solution of the following elliptic partial differential equation

$$(4.9) \quad \varepsilon_\gamma Ac_{\xi,1} + c_{\xi,1} = \Lambda \quad \text{in } \mathcal{V}'.$$

Observe that $c_{\xi,1} \geq 0$ by a standard maximum principle [12], p. 327. Now for

$$c_y = \zeta_1 - \varepsilon_\gamma c_{\xi,1}$$

we obtain

$$\begin{aligned} c_y + \varepsilon_\gamma c_\xi - \zeta &= c_y + \varepsilon_\gamma c_{\xi,1} - \zeta_1 + \varepsilon_\gamma c_{\xi,2} - \zeta_2 \\ &= \varepsilon_\gamma c_{\xi,2} - \zeta_2 = \max(0, z) - \max(0, -z) = z \end{aligned}$$

and

$$Ac_y = A\zeta_1 - \varepsilon_\gamma Ac_{\xi,1} = c_{\xi,2} + z' + \Lambda - \varepsilon_\gamma Ac_{\xi,1} = c_{\xi,2} + z' + c_{\xi,1} = c_\xi + z'.$$

Here we have used (4.7)–(4.8) and (4.9). Therefore, problem (\mathcal{O}_γ^n) constraints are qualified and the next proposition holds true.

Proposition 4.1. *Let $(y_\gamma^n, \xi_\gamma^n, u_\gamma^n)$ be a solution for the problem (\mathcal{O}_γ^n) . Then there exists a Lagrange multiplier vector $(p_\gamma^n, \lambda_\gamma^n)$ in $\mathcal{V} \times L^2(\Gamma_C)$ such that the following first order optimality system holds*

$$(4.10) \quad Ay_\gamma^n - Bu_\gamma^n - \xi_\gamma^n - \bar{y}_\gamma^{n-1} + \bar{\xi}_\gamma^{n-1} = 0 \quad \text{in } \mathcal{V}',$$

$$(4.11) \quad Ap_\gamma^n + y_\gamma^n - y_d^n + \gamma\xi_\gamma^n - \lambda_\gamma^n = 0 \quad \text{in } \mathcal{V}',$$

$$(4.12) \quad y_\gamma^n + \varepsilon_\gamma\xi_\gamma^n \geq 0, \quad \lambda_\gamma^n \geq 0, \quad (y_\gamma^n + \varepsilon_\gamma\xi_\gamma^n, \lambda_\gamma^n) = 0,$$

$$(4.13) \quad \xi_\gamma^n \geq 0, \quad (\xi_\gamma^n - \xi_d^n + 2\gamma\varepsilon_\gamma\xi_\gamma^n + \gamma y_\gamma^n - p_\gamma^n - \varepsilon_\gamma\lambda_\gamma^n, \tau - \xi_\gamma^n) \geq 0,$$

$$(4.14) \quad u_\gamma^n \geq 0, \quad (\alpha u_\gamma^n - \tau B^* p_\gamma^n, v - u_\gamma^n)_{\Gamma_C} \geq 0,$$

where τ and v are two non-negative arbitrary functions in $L^2(\Omega)$ and $L^2(\Gamma_C)$, respectively, and B^* is the adjoint operator of B .

Remark 4.1. (i) Conditions (4.13) and (4.14) correspond to the projection of $(1 + 2\gamma\varepsilon_\gamma)^{-1}(\xi_d^n + \lambda_\gamma^n)$ and $\tau\alpha^{-1}B^*p_\gamma^n$ over the non-negative cones in $L^2(\Omega)$ and $L^2(\Gamma_C)$, respectively:

$$u_\gamma^n = \max\left(0, \frac{\tau}{\alpha}B^*p_\gamma^n\right), \quad \xi_\gamma^n = \max\left(0, \frac{1}{1 + 2\gamma\varepsilon_\gamma}(p_\gamma^n + \xi_d^n + \varepsilon_\gamma\lambda_\gamma^n - \gamma y_\gamma^n)\right).$$

(ii) The step function u_γ^τ , which is equal to the time discrete controls u_γ^n on each interval $[(n-1)\tau, n\tau]$ for $n = 1, \dots, N$, comprises a sub-optimal solution to a time-continuous optimal control problem related to (\mathcal{M}^t) . A convergence analysis—with respect to time step size τ —of u_γ^τ and the corresponding state and Lagrange multipliers is of interest. In this respect one may investigate adapting the arguments presented in [4] and the references therein. This analysis will be discussed in some upcoming work.

5. NUMERICAL EXPERIMENTS

In this section we present two preliminary numerical experiments to assess the validity of the above developed theoretical procedure. At each time step $t^n = n\tau$ we solve a discrete version of the optimization problem $(\mathcal{O}^n)_{\gamma_k}$ for a sequence of penalty parameters $(\gamma_k)_{k \in \mathbb{N}}$ with $\gamma_k = 10^{-3} \times 1.5^k$ and $k = 1, \dots, 40$. We select a regularization parameter $\varepsilon_{\gamma_k} = (10^3 + \gamma_k^4)^{-1}$. The parameter for the cost of the control is taken $\nu = 10^{-4}$. The thermal conductivity is set to 1 in the two examples. All functions are discretized by continuous piecewise linear finite elements. The fully discretized penalized-regularized control problems corresponding to $(\mathcal{O}^n)_{\gamma_k}$ are then solved numerically using the `fmincon` Matlab function.

Example 5.1. We consider a one-dimensional free convection problem with a known analytical solution [11]:

$$y_{\text{ex}}(x, t) = \begin{cases} \exp(t - x) - 1 & \text{if } 0 \leq x \leq t, \\ 0 & \text{if } t \leq x \leq x_{\text{max}}, \end{cases} \quad \xi_{\text{ex}}(x, t) = \begin{cases} 0 & \text{if } 0 \leq x \leq t, \\ 1 & \text{if } t \leq x \leq x_{\text{max}}. \end{cases}$$

Our aim here is to apply a heat flux on the left boundary, $\Gamma_C = \{0\}$, to get temperature and solid fraction profiles as close as possible to the exact solution. For the instantaneous boundary control problem we choose a fixed time step $\tau = 0.01$ and we set

$$y_d^n = y_{\text{ex}}(x, n\tau), \quad \xi_d^n = \xi_{\text{ex}}(x, n\tau) \quad \text{for } n = 1, \dots, N = 300.$$

For the computational domain we choose a uniform grid of size $h = 0.01$ with $x_{\text{max}} = 4$. The analytical control $u_{\text{ex}}(t) = \exp(t)$ is very well reconstructed up to the first few iterations as shown in Fig. 2. An excellent agreement has been found between the analytical and controlled temperature profiles as depicted in Fig. 3. The complementarity condition between the temperature and solid fraction are respected, as shown in Fig. 4 for the sample instant $t = 3$, which emphasizes the relevance of the developed regularization-penalization approach.

Example 5.2. Here we consider a two-dimensional problem where the computational domain $\Omega = (0, 2) \times (0, 4)$ is discretized using a 50×100 uniform grid. The time step is taken $\tau = 0.1$ and a constant convection velocity $\vec{v} = \begin{pmatrix} -\frac{1}{2} \\ 0 \end{pmatrix}$ is used. No-heat flux condition is applied on the right boundary and temperature $y = 0$ is held at the top and bottom. We apply the heat flux control on $\Gamma_C := \{x \in \Omega; x_1 = 0\}$ to govern the system toward the following time-independent desired state:

$$y_d^n(x) = y_d(x) = \begin{cases} \exp(\frac{1}{4}(4 - x_2)x_2 - x_1) - 1 & \text{if } x_1 < \frac{1}{4}(4 - x_2)x_2, \\ 0 & \text{if } x_1 \geq \frac{1}{4}(4 - x_2)x_2, \end{cases}$$

$$\xi_d^n(x) = \xi_d(x) = \begin{cases} 0 & \text{if } x_1 < \frac{1}{4}(4 - x_2)x_2, \\ 1 & \text{if } x_1 \geq \frac{1}{4}(4 - x_2)x_2. \end{cases}$$

Figs. 5–6 show the evolution of temperature y and solid fraction ξ driven by the sub-optimal controls towards the desired state. A fairly good approximation is obtained. The significant reduction of the cost functional value is achieved during the first five time steps and almost stagnates up to $t \approx 1$ as shown in Fig. 7. In Fig. 8 we present the computed sub-optimal control at sample instances. We observe a strong control at the first time step getting inactive near the boundaries. The controls shape is consistent with the desired state one.

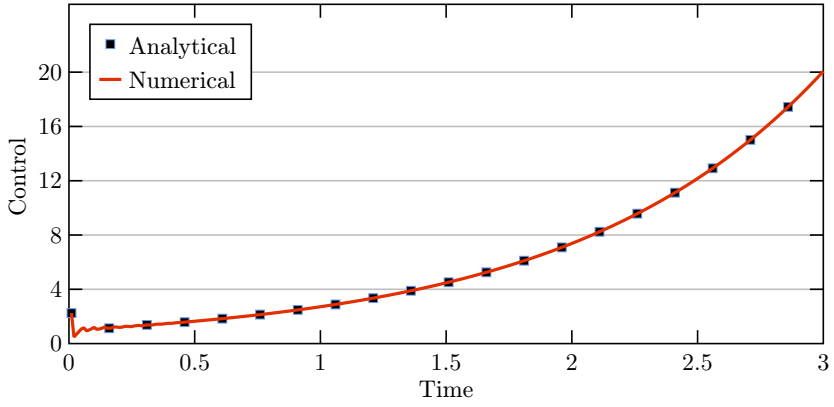


Figure 2. Analytical and computed sub-optimal controls.

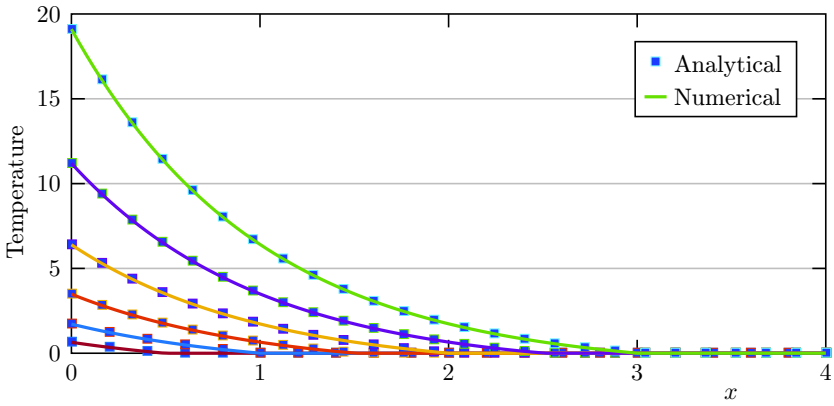


Figure 3. Analytical and computed temperature profiles at different instants.

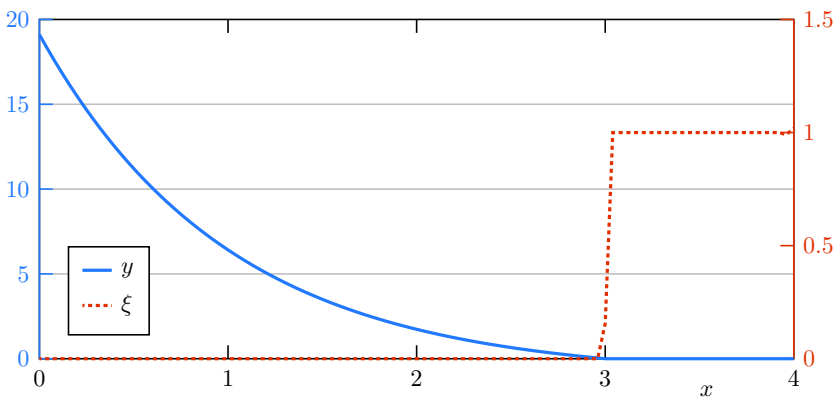


Figure 4. Computed temperature and solid fraction profiles at time $t = t_f = 3$.

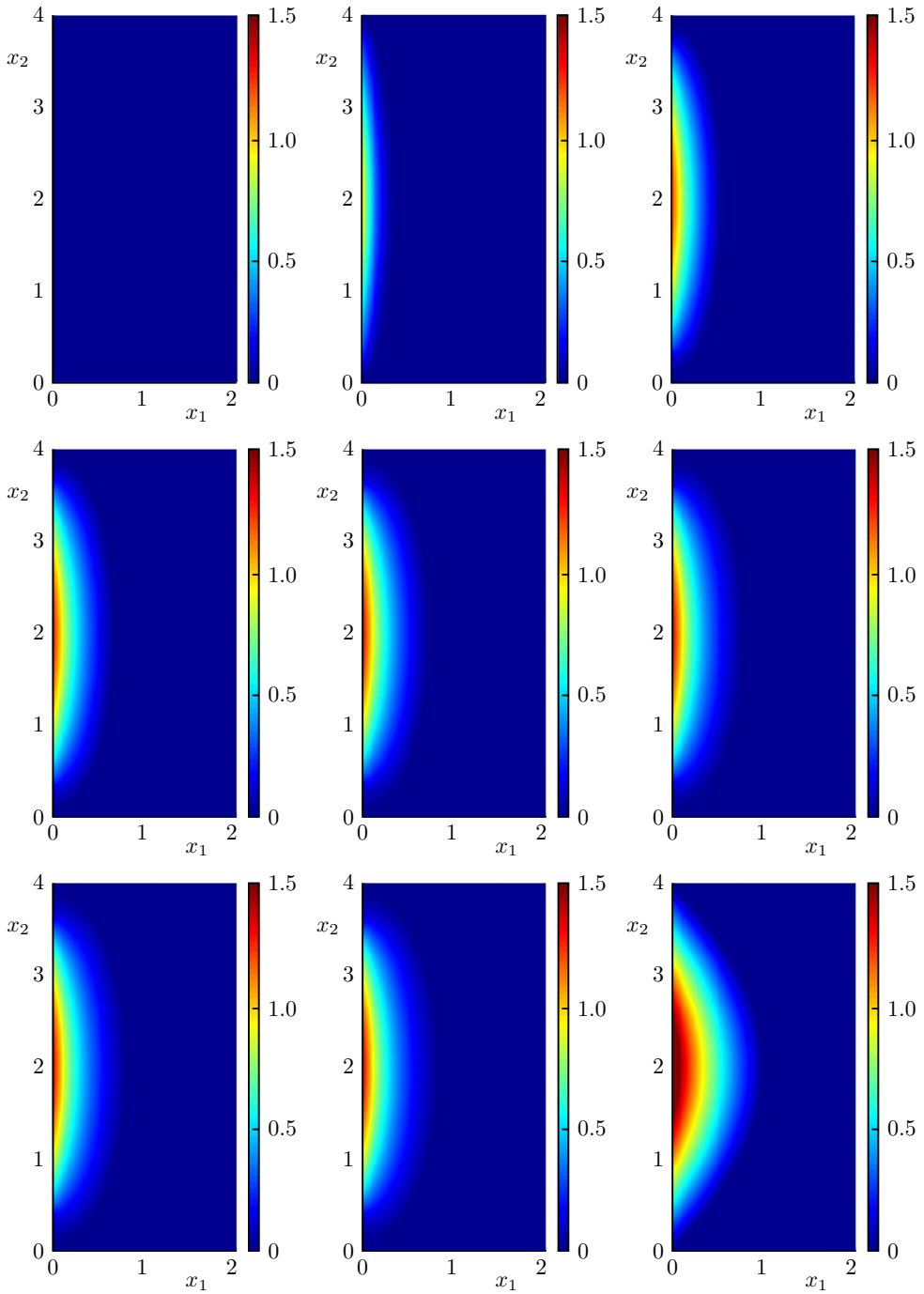


Figure 5. Computed temperatures at $t = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.1, 1.4$ and the desired temperature profile.

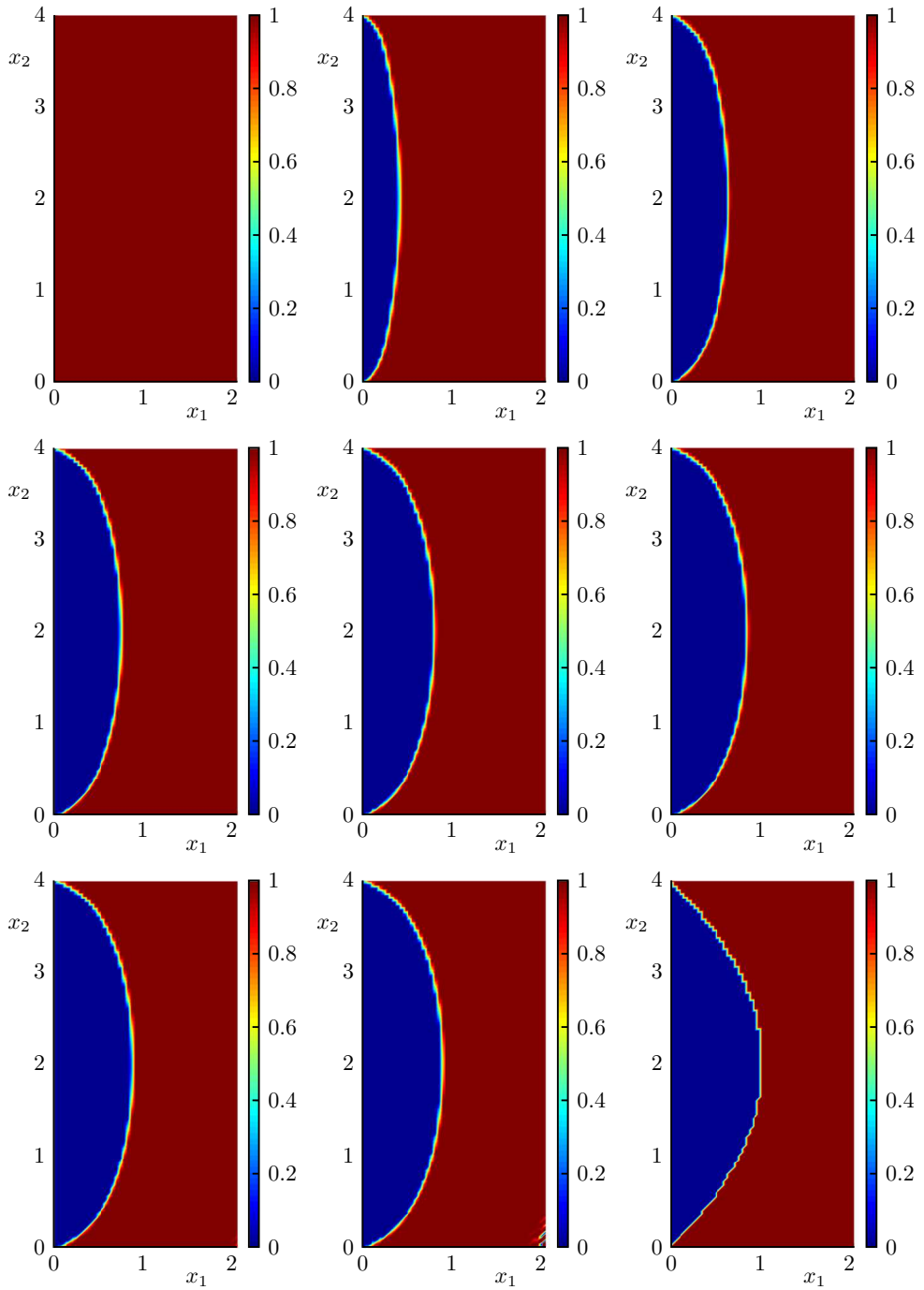


Figure 6. Computed solid fraction at $t = 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.1, 1.4$ and the desired solid fraction profile.

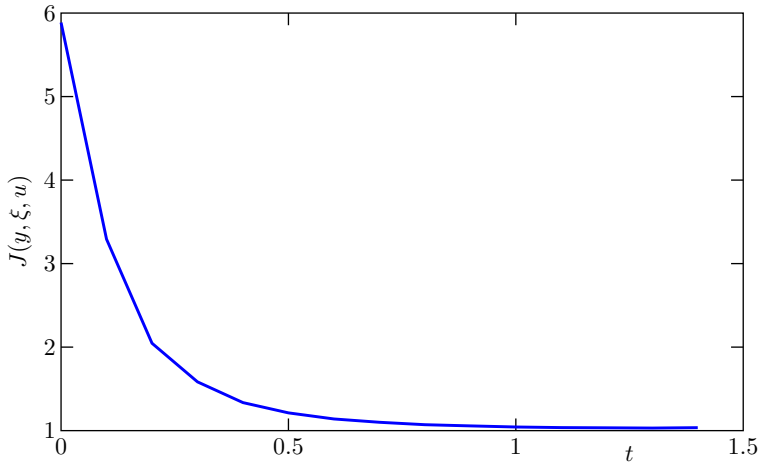


Figure 7. Reduction of the cost functional.

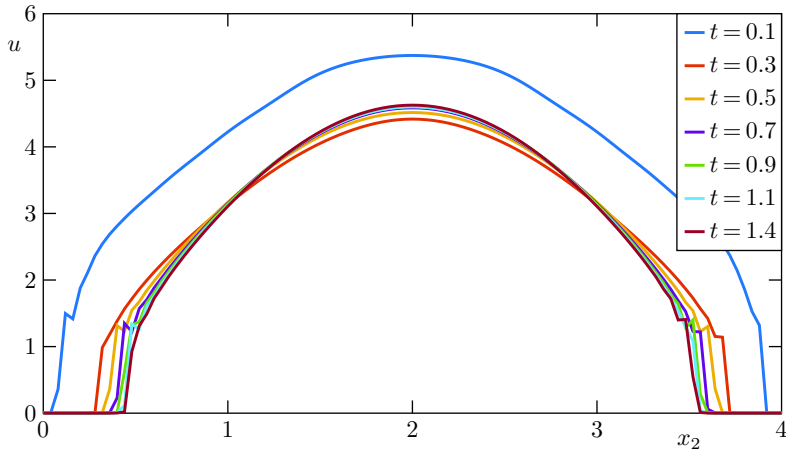


Figure 8. Computed sub-optimal controls at different time steps.

Remark 5.1. To apply the developed approach on more realistic benchmarks, a coupling with momentum and mass conservation equations is required. However, many discretization and algorithmic aspects have to be developed first. Questions related to adaptive mesh refinement, selection of the optimization parameters, solution algorithm and preconditioning will be addressed in a forthcoming study.

APPENDIX A: PROOF OF THEOREM 2.1

To show that the problem

$$\begin{cases} Ay^n = \xi^n + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}', \\ \xi^n \in \mathcal{H}(y^n), & \text{a.e. in } \Omega \end{cases}$$

has a solution, let \mathcal{H}_ε be a regularization of the Heaviside operator \mathcal{H} given by

$$\mathcal{H}_\varepsilon(x) = \begin{cases} 0 & \text{if } x \geq \varepsilon, \\ 1 - x/\varepsilon & \text{if } 0 \leq x \leq \varepsilon, \\ 1 & \text{if } x \leq 0. \end{cases}$$

Correspondingly, we consider the following regularized problem:

$$(\mathcal{WF}_\varepsilon^n) \quad \begin{cases} \text{Find } y_\varepsilon^n \in \mathcal{V} \text{ such that } y_\varepsilon^n \geq 0 & \text{a.e. in } \Omega, \\ Ay_\varepsilon^n = \mathcal{H}_\varepsilon(y_\varepsilon^n) + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}'. \end{cases}$$

Lemma 5.1. *The regularized problem $(\mathcal{WF}_\varepsilon^n)$ has a unique solution y_ε^n . Moreover, there exists a constant C not depending on ε such that*

$$(5.1) \quad \|y_\varepsilon^n\|_{H^1(\Omega)} \leq C.$$

Proof. Consider the mapping T which, for any $y_\varepsilon^n \in L^2(\Omega)$, associates $\widetilde{y}_\varepsilon^n = T(y_\varepsilon^n)$ to the solution of the elliptic problem

$$(5.2) \quad A\widetilde{y}_\varepsilon^n = \mathcal{H}_\varepsilon(y_\varepsilon^n) + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}'.$$

Problem (5.2) has a unique solution by Lax-Milgram theorem. Moreover, there exists a constant Const not depending on ε such that

$$(5.3) \quad \|\widetilde{y}_\varepsilon^n\|_{H^1(\Omega)} \leq \text{Const}.$$

Here, we have used the fact that $(\mathcal{H}_\varepsilon(y_\varepsilon^n))_\varepsilon$ is bounded in $L^\infty(\Omega)$ independently of ε .

The mapping T is then bounded from $L^2(\Omega)$ to $H^1(\Omega)$. From the compact embedding of $H^1(\Omega)$ into $L^2(\Omega)$, it follows that T is completely continuous from \mathcal{V} to $L^2(\Omega)$. Moreover, estimate (5.3) shows that $T(B_{\text{Const}}) \subset B_{\text{Const}}$ with B_{Const} being the $H^1(\Omega)$ -ball of radius Const . Schauder's fixed-point theorem yields the existence of a function y_ε^n such that $T(y_\varepsilon^n) = y_\varepsilon^n$ satisfying (5.1) with $C = \text{Const}$.

Next, we claim that $y_\varepsilon^n \geq 0$ a.e. in Ω . Let $(y_\varepsilon^n)^- = \min(0, y_\varepsilon^n)$. It is clear that $(y_\varepsilon^n)^- \in \mathcal{V}$. By choosing $\varphi = (y_\varepsilon^n)^-$ in (5.2), we arrive at

$$\langle Ay_\varepsilon^n, (y_\varepsilon^n)^- \rangle = \langle Bu^n, (y_\varepsilon^n)^- \rangle + (\bar{y}^{n-1} + \mathcal{H}(y_\varepsilon^n) - \bar{\xi}^{n-1}, (y_\varepsilon^n)^-).$$

Since $u^n \geq 0$ a.e. in Γ_C , $y^{n-1} \geq 0$ a.e. in Ω and $0 \leq \xi^{n-1} \leq 1$ a.e. in Ω and using the fact that $\mathcal{H}_\varepsilon(x) = 1$ for $x \leq 0$, we obtain

$$\langle A(y_\varepsilon^n)^-, (y_\varepsilon^n)^- \rangle = \langle Bu^n, (y_\varepsilon^n)^- \rangle + (\bar{y}^{n-1} + 1 - \bar{\xi}^{n-1}, (y_\varepsilon^n)^-) \leq 0.$$

The coercivity of A leads to $(y_\varepsilon^n)^- = 0$ a.e. in Ω and then $y_\varepsilon^n \geq 0$ a.e. in Ω . Consequently, the solution y_ε^n is a solution of $(\mathcal{WF}_\varepsilon^n)$. \square

Now for any $\varepsilon > 0$, let y_ε^n be the solution of the regularized problem $(\mathcal{WF}_\varepsilon^n)$. From (5.1) we can find a subsequence, also denoted $(y_\varepsilon^n)_{\varepsilon>0}$, such that

$$\begin{aligned} y_\varepsilon^n &\rightharpoonup y^n && \text{in } H^1(\Omega), \\ y_\varepsilon^n &\rightarrow y^n && \text{in } L^2(\Omega), \\ \mathcal{H}_\varepsilon(y_\varepsilon^n) &\overset{*}{\rightharpoonup} \xi^n && \text{in } L^\infty(\Omega). \end{aligned}$$

By passing to the limit, we deduce that

$$(5.4) \quad \begin{cases} y^n \geq 0 & \text{a.e. in } \Omega, \\ 0 \leq \xi^n \leq 1 & \text{a.e. in } \Omega, \\ Ay^n = \xi^n + Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}'. \end{cases}$$

Further, observe that

$$(5.5) \quad y^n \geq 0, \quad \xi^n \in \mathcal{H}(y^n) \Leftrightarrow y^n \geq 0, \quad 0 \leq \xi^n \leq 1, \quad (y^n, \xi^n) = 0.$$

Therefore, to complete the proof of existence of a solution for the initial problem, it remains to prove that $(y^n, \xi^n) = 0$. One has

$$(5.6) \quad (y_\varepsilon^n, \mathcal{H}_\varepsilon(y_\varepsilon^n)) \rightarrow (y^n, \xi^n)$$

from the $L^2(\Omega)$ strong convergence of y_ε^n to y^n and the $L^\infty(\Omega)$ weak-* convergence of $\mathcal{H}_\varepsilon(y_\varepsilon^n)$ to ξ^n .

On the other hand, from \mathcal{H}_ε expression we have

$$(y_\varepsilon^n, \mathcal{H}_\varepsilon(y_\varepsilon^n)) \leq \varepsilon \text{meas}(\Omega) \rightarrow 0.$$

Consequently $(y^n, \xi^n) = 0$.

Now, notice that if $(y^n, \xi^n) \in \mathcal{V} \times L^2(\Omega)$ is a solution to the complementarity problem

$$(CS^n) \quad \begin{cases} \xi^n + Ay^n = Bu^n + \bar{y}^{n-1} - \bar{\xi}^{n-1} & \text{in } \mathcal{V}', \\ y^n \geq 0, \quad \xi^n \geq 0, \quad (y^n, \xi^n) = 0 & \text{a.e. in } \Omega, \end{cases}$$

then y^n is a solution to the variational inequality

$$(VI^n) \quad \begin{cases} y^n \in \mathcal{K} := \{q \in \mathcal{V}; q \geq 0 \text{ a.e. in } \Omega\}, \\ \langle Ay^n, q - y^n \rangle \geq \langle Bu^n, q - y^n \rangle + \langle \bar{y}^{n-1} - \bar{\xi}^{n-1}, q - y^n \rangle \quad \forall q \in \mathcal{K}. \end{cases}$$

Since (VI^n) possesses a unique solution in \mathcal{V} by virtue of Stampacchia-Rodriguez, we deduce that y^n is unique.

Finally, the uniqueness of ξ^n follows from the uniqueness of y^n . More precisely, if $(y^n, \xi_1^n) \in \mathcal{V} \times L^2(\Omega)$ and $(y^n, \xi_2^n) \in \mathcal{V} \times L^2(\Omega)$ are two solutions to (CS^n) , then

$$\xi_1^n = \xi_2^n = Ay^n - Bu^n - \bar{y}^{n-1} + \bar{\xi}^{n-1} \quad \text{in } \mathcal{V}'.$$

Therefore, $\xi_1^n - \xi_2^n = 0$ in \mathcal{V}' . By the density of $\mathcal{V} \supset H_0^1(\Omega)$ in $L^2(\Omega)$ we conclude that $\xi_1^n = \xi_2^n$ in $L^2(\Omega)$.

APPENDIX B: MATHEMATICAL OPTIMIZATION IN BANACH SPACES

Let \mathcal{X} and \mathcal{Y} be real Banach spaces. For

$$\begin{aligned} F: \mathcal{X} &\rightarrow \mathbb{R} && \text{Fréchet-differentiable functional,} \\ g: \mathcal{X} &\rightarrow \mathcal{Y} && \text{continuously Fréchet-differentiable,} \end{aligned}$$

we consider the following mathematical program:

$$(5.7) \quad \min\{F(x); g(x) \in M, x \in C\},$$

where C is a closed convex subset of \mathcal{X} and M a closed cone in \mathcal{Y} with vertex at 0.

We suppose that problem (5.7) has an optimal solution \hat{x} , and we introduce the conical hulls of $C - \{\hat{x}\}$ and $M - \{y\}$, respectively, by

$$\begin{aligned} C(\hat{x}) &= \{x \in \mathcal{X}; \exists \beta \geq 0, \exists c \in C, x = \beta(c - \hat{x})\}, \\ M(y) &= \{z \in \mathcal{Y}; \exists \lambda \geq 0, \exists \zeta \in M, z = \zeta - \lambda y\}. \end{aligned}$$

The main result concerning the existence of a Lagrange multiplier for (5.7) is given in the next theorem.

Theorem 5.1 ([22]). *Let \hat{x} be an optimal solution of problem (5.7) satisfying the following constraints qualification:*

$$(5.8) \quad g'(\hat{x}) \cdot C(\hat{x}) - M(g(\hat{x})) = \mathcal{Y}.$$

Then there exists a Lagrange multiplier $\mu^ \in \mathcal{Y}^*$ such that*

$$(5.9) \quad \langle \mu^*, z \rangle_{\mathcal{Y}^*, \mathcal{Y}} \geq 0 \quad \forall z \in M,$$

$$(5.10) \quad \langle \mu^*, g(\hat{x}) \rangle_{\mathcal{Y}^*, \mathcal{Y}} = 0,$$

$$(5.11) \quad F'(\hat{x}) - \mu^* \circ g'(\hat{x}) \in C(\hat{x})_+,$$

where $A_+ = \{x^* \in \mathcal{X}^*; \langle x^*, a \rangle_{\mathcal{X}^*, \mathcal{X}} \geq 0 \text{ for all } a \in A\}$, \mathcal{Y}^* and \mathcal{X}^* are the topological dual spaces of \mathcal{Y} and \mathcal{X} , respectively, and $(\mu^* \circ g'(\hat{x}))d = \langle \mu^*, g'(\hat{x})d \rangle_{\mathcal{Y}^*, \mathcal{Y}}$ for all $d \in \mathcal{X}$.

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