Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 2198-5855

Sparse optimal control of a phase field system with singular potentials arising in the modeling of tumor growth

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submitted: May 12, 2020

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No. 2721
Berlin 2020

2010 *Mathematics Subject Classification.* 49J20, 49K20, 49K40, 35K57, 37N25.

Key words and phrases. Sparse optimal control, tumor growth models, singular potentials, optimality conditions.

Edited by
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Sparse optimal control of a phase field system with singular potentials arising in the modeling of tumor growth

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Abstract

In this paper, we study an optimal control problem for a nonlinear system of reaction-diffusion equations that constitutes a simplified and relaxed version of a thermodynamically consistent phase field model for tumor growth originally introduced in [13]. The model takes the effect of chemotaxis into account but neglects velocity contributions. The unknown quantities of the governing state equations are the chemical potential, the (normalized) tumor fraction, and the nutrient extra-cellular water concentration. The equation governing the evolution of the tumor fraction is dominated by the variational derivative of a double-well potential which may be of singular (e.g., logarithmic) type. In contrast to the recent paper [10] on the same system, we consider in this paper sparsity effects, which means that the cost functional contains a nondifferentiable (but convex) contribution like the L^1-norm. For such problems, we derive first-order necessary optimality conditions and conditions for directional sparsity, both with respect to space and time, where the latter case is of particular interest for practical medical applications in which the control variables are given by the administration of cytotoxic drugs or by the supply of nutrients. In addition to these results, we prove that the corresponding control-to-state operator is twice continuously differentiable between suitable Banach spaces, using the implicit function theorem. This result, which complements and sharpens a differentiability result derived in [10], constitutes a prerequisite for a future derivation of second-order sufficient optimality conditions.

1 Introduction

Let $\Omega \subset \mathbb{R}^3$ denote some open, bounded and connected set having a smooth boundary $\Gamma = \partial\Omega$ and unit outward normal $\mathbf{n}$. We denote by $\partial_{\mathbf{n}}$ the outward normal derivative to Γ. Moreover, we fix some final time $T > 0$ and introduce for every $t \in (0, T]$ the sets $Q_t := \Omega \times (0, t)$ and $\Sigma_t := \Gamma \times (0, t)$, where we put, for the sake of brevity, $Q := Q_T$ and $\Sigma := \Sigma_T$. We then consider the following optimal control problem:

($\mathcal{CP}$) Minimize the cost functional

$$\mathcal{J}((\mu, \varphi, \sigma), \mathbf{u}) := \frac{\beta_1}{2} \int_Q |\varphi - \widehat{\varphi}_Q|^2 + \frac{\beta_2}{2} \int_\Omega |\varphi(T) - \widehat{\varphi}_\Omega|^2 + \frac{\nu}{2} \int_Q |\mathbf{u}|^2 \, + \, \kappa \, g(\mathbf{u}) \, , \qquad (1.1)$$

DOI 10.20347/WIAS.PREPRINT.2721

subject to the state system

$$\alpha\partial_t\mu + \partial_t\varphi - \Delta\mu = (P\sigma - A - u_1)h(\varphi) \quad \text{in } Q\,, \tag{1.2}$$

$$\beta\partial_t\varphi - \Delta\varphi + F'(\varphi) = \mu + \chi\,\sigma \quad \text{in } Q\,, \tag{1.3}$$

$$\partial_t\sigma - \Delta\sigma = -\chi\Delta\varphi + B(\sigma_s - \sigma) - E\,\sigma h(\varphi) + u_2 \quad \text{in } Q\,, \tag{1.4}$$

$$\partial_{\mathbf{n}}\mu = \partial_{\mathbf{n}}\varphi = \partial_{\mathbf{n}}\sigma = 0 \quad \text{on } \Sigma\,, \tag{1.5}$$

$$\mu(0) = \mu_0, \quad \varphi(0) = \varphi_0, \quad \sigma(0) = \sigma_0 \quad \text{in } \Omega\,, \tag{1.6}$$

and to the control constraint

$$\mathbf{u} = (u_1, u_2) \in \mathcal{U}_{\rm ad}\,. \tag{1.7}$$

Here, the constants β_1, β_2 are nonnegative, while ν and κ are positive. Moreover, $\widehat{\varphi}_Q$ and $\widehat{\varphi}_\Omega$ are given target functions, and $g : \mathcal{U} \to [0, +\infty)$ is a nonnegative and convex, but not necessarily differentiable, functional on the control space

$$\mathcal{U} := L^\infty(Q)^2. \tag{1.8}$$

Moreover, $\mathcal{U}_{\rm ad}$ is a suitable bounded, closed and convex subset of $\mathcal{U}$. Since we are interested in sparse controls in this note, typical (nondifferentiable) examples for the functional g are given by

$$g(\mathbf{u}) = \|\mathbf{u}\|_{L^1(Q)} = \int_Q |\mathbf{u}(x,t)|\,dx\,dt, \tag{1.9}$$

$$g(\mathbf{u}) = \int_0^T \Big(\int_\Omega |\mathbf{u}(x,t)|^2\,dx\Big)^{1/2} dt, \tag{1.10}$$

$$g(\mathbf{u}) = \int_\Omega \Big(\int_0^T |\mathbf{u}(x,t)|^2\,dt\Big)^{1/2} dx. \tag{1.11}$$

The functionals in (1.10) and (1.11) are associated with the notion of *directional sparsity* (with respect to t and to x, respectively). Since we have two control variables in our system, we could "mix" the sparsity directions by taking different ones for u_1 and u_2; also, different weights could be given to the directions. For the sake of avoiding unnecessary technicalities, we restrict ourselves to the simplest case here.

The state system (1.2)–(1.6) constitutes a simplified and relaxed version of a thermodynamically consistent phase field model for tumor growth that includes the effect of chemotaxis and was originally introduced in [13]. Indeed, the velocity contributions in [13] were neglected, and the two relaxation terms $\alpha\partial_t\mu$ are $\beta\partial_t\varphi$ have been added. We note that a different thermodynamically consistent model was introduced in [14] and studied mathematically in [5–8], where [8] focused on optimal control problems. In this connection, we also refer to [9].

In all of the abovementioned models, the unknowns μ, φ, σ stand for the chemical potential, the normalized tumor fraction, and the nutrient extra-cellular water concentration, in this order. The quantity σ is usually normalized between 0 and 1, where these values model nutrient-poor and nutrient-rich cases. The variable φ plays the role of an order parameter and is usually taken between the values -1 and $+1$, which represent the healthy cell case and the tumor phase, respectively. The capital letters A, B, E, P, χ denote positive coefficients that stand for the apoptosis rate, nutrient supply rate, nutrient consumption rate, and chemotaxis coefficient, in this order. In addition, let us point out that the contributions $\chi\,\sigma$ and $\chi\,\Delta\varphi$ model pure chemotaxis. Furthermore, the nonlinear function h

has been considered in [13] as an interpolation function satisfying $h(-1) = 0$ and $h(1) = 1$, so that the mechanisms modeled by the terms $(P\sigma - A - u_1)h(\varphi)$ and $E\sigma h(\varphi)$ are switched off in the healthy tissue (which corresponds to $\varphi = -1$) and are fully active in the tumorous case $\varphi = 1$. Moreover, the term σ_s is a nonnegative constant that models the nutrient concentration in a pre-existing vasculature.

Very important for the evolution of the state system is the nonlinearity F, which is assumed to be a double-well potential. Typical examples are given by the regular and logarithmic potentials, which are given, in this order, by

$$F_{\text{reg}}(r) = \frac{1}{4}\left(1 - r^2\right)^2 \quad \text{for } r \in \mathbb{R}, \tag{1.12}$$

$$F_{\log}(r) = (1 + r)\,\ln(1 + r) + (1 - r)\,\ln(1 - r) - kr^2 \quad \text{for } r \in (-1, 1), \tag{1.13}$$

where $k > 1$ so that $F_{\log}$ is nonconvex. Observe that $F_{\log}$ is very relevant in the applications, where $F'_{\log}(r)$ becomes unbounded as $r \to \pm 1$.

In this paper, we work with two source controls that act in the phase equation and in the nutrient equation, respectively. The control variable u_1 in the phase equation models the application of a cytotoxic drug into the system; it is multiplied by $h(\varphi)$ in order to have the action only in the spatial region where the tumor cells are located. On the other hand, the control u_2 can model either an external medication or some nutrient supply. In this connection, sparsity of the control is highly desirable: indeed, if a distributed cytotoxic drug is to be administered, this should be done only where it does not harm healthy tissue, which calls for directional sparsity with respect to space; on the other hand, and even more importantly, cytotoxic drugs should only be applied for very short periods of time, in order to prevent the tumor cells from developing a resistance against the drug. This, of course, calls for a directional sparsity with respect to time.

Optimal control problems for the system (1.2)–(1.6) have recently been studied in [10], where the cost functional, while containing some additional quadratic terms, did not have a nondifferentiable contribution, i. e., we had $g \equiv 0$. However, besides existence of optimal controls, it was shown in [10] that the control-to-state operator is Fréchet differentiable between suitable function spaces, and first-order necessary optimality conditions in terms of the adjoint state variables were derived. The Fréchet differentiability was shown "directly" without using the implicit function theorem, and therefore the existence of higher-order derivatives was not proved. Note that the existence of second-order derivatives forms a prerequisite for deriving second-order sufficient optimality conditions and efficient numerical techniques. To pave the way for such an analysis (which shall not be given in this paper), we have decided to include a proof of the Fréchet differentiability of the control-to-state operator via the implicit function theorem.

Another novelty of this paper is the discussion of optimal controls that are sparse with respect to the time. Since the seminal paper [21], sparse optimal controls have been discussed extensively in the literature. Directional sparsity was introduced in [16, 17] and extended to semilinear parabolic optimal control problems in [2]. Sparse optimal controls for reaction-diffusion equations were investigated in [3, 4].

Although the main techniques of the analysis for sparse controls are known from the abovementioned papers, a discussion of sparsity for the control of the system of reaction-diffusion equations (1.2)–(1.6) seems to be worth investigating in view of its medical background. In this connection, temporal sparsity is particularly interesting. It means that drugs are not needed in certain time periods. For the control of the class of reaction-diffusion equations (1.2)–(1.6), the investigation of sparse controls is new.

The paper is organized as follows: in the subsequent Section 2, we give the general setting of the problem, and recall known well-posedness results for the state system (1.2)–(1.6). Moreover, we employ the implicit function theorem to show that the control-to-state is twice continuously Fréchet differentiable between suitable Banach spaces, thereby sharpening the differentiability result of [10]. Section 3 then deals with first-order necessary optimality conditions for the problem $(\mathcal{CP})$, and the final Section 4 brings a discussion of the sparsity of optimal controls.

Throughout this paper, we make repeated use of Hölder's inequality, of the elementary Young's inequality

$$a\,b \,\le\, \gamma|a|^2 \,+\, \frac{1}{4\gamma}\,|b|^2 \quad \forall\, a,b\in\mathbb{R}, \quad \forall\,\gamma>0, \tag{1.14}$$

as well as the continuity of the embeddings $H^1(\Omega)\subset L^p(\Omega)$ for $1\le p\le 6$ and $H^2(\Omega)\subset C^0(\overline{\Omega})$. Notice that the latter embedding is also compact, while this holds true for the former embeddings only if $p<6$. Moreover, throughout the paper, for a Banach space X we denote by $\|\cdot\|_X$ the norm in the space X or in a power of it, and by X^* its dual space. The only exemption from this rule applies to the norms of the L^p spaces and of their powers, which we often denote by $\|\cdot\|_p$, for $1\le p\le+\infty$. As usual, for Banach spaces X and Y we introduce the linear space $X\cap Y$ which becomes a Banach space when equipped with its natural norm $\|u\|_{X\cap Y} := \|u\|_X \,+\, \|u\|_Y$, for $u\in X\cap Y$.

2 General setting and properties of the state system

In this section, we introduce the general setting of our control problem and state some results on the state system (1.2)–(1.6). To begin with, we recall the definition (1.8) of $\mathcal{U}$ and introduce the spaces

$$H := L^2(\Omega)\,, \quad V := H^1(\Omega)\,, \quad W_0 := \{v\in H^2(\Omega) : \partial_{\mathbf{n}}v = 0 \text{ on } \Gamma\}. \tag{2.1}$$

By $(\,\cdot\,,\,\cdot\,)$ we denote the standard inner product in H.

For the potential F, we generally assume:

(F1) $F=F_1+F_2$, where $F_1:\mathbb{R}\to[0,+\infty]$ is convex and lower semicontinuous with $F_1(0)=0$.

(F2) There exists an interval (r_-,r_+) with $-\infty\le r_-<0<r_+\le+\infty$ such that the restriction of F_1 to (r_-,r_+) belongs to $C^4(r_-,r_+)$.

(F3) $F_2\in C^4(\mathbb{R})$, and F_2' is globally Lipschitz continuous on $\mathbb{R}$.

(F4) It holds $\lim_{r\to r_\pm} F'(r)=\pm\infty$.

It is worth noting that both (1.12) and (1.13) fit into this framework with the choices $(r_-,r_+)=\mathbb{R}$ and $(r_-,r_+)=(-1,1)$, respectively, where in the latter case we extend $F_{\log}$ by $F_{\log}(\pm1)=2\ln(2)-k$ and $F_{\log}(r)=+\infty$ for $r\notin[-1,1]$.

For the initial data, we make the following assumptions:

(A1) $\varphi_0,\mu_0,\sigma_0\in W_0$, and $r_-<\min_{x\in\overline{\Omega}}\varphi_0(x)\le\max_{x\in\overline{\Omega}}\varphi_0(x)<r_+$.

Notice that **(A1)** entails that $F(\varphi_0),F'(\varphi_0),F''(\varphi_0)\in C^0(\overline{\Omega})$. This condition can be restrictive for the case of singular potentials; for instance, in the case of the logarithmic potential $F_{\log}$ we have $r_\pm=\pm1$, so that **(A1)** excludes the pure phases (tumor and healthy tissue) as initial data.

For the other data and the target functions, we postulate:

(A2) $h \in C^3(\mathbb{R}) \cap W^{3,\infty}(\mathbb{R})$, and h is positive on (r_-, r_+).

(A3) α, β, χ are positive constants, while P, A, B, E, σ_s are nonnegative constants.

(A4) β_1, β_2 are nonnegative, and ν, κ are positive.

(A5) $\varphi_Q \in L^2(Q)$ and $\varphi_\Omega \in L^2(\Omega)$.

Observe that **(A2)** entails that h, h', h'' are Lipschitz continuous on $\mathbb{R}$. We now assume for the set of admissible controls:

(A6) $\mathcal{U}_{\rm ad} = \{\mathbf{u} = (u_1, u_2) \in \mathcal{U} : \underline{u}_i \le u_i \le \widehat{u}_i \text{ a.e. in } Q, \ \ i = 1,2\}$,
where $\underline{u}_i, \widehat{u}_i \in L^\infty(Q)$ satisfy $\underline{u}_i \le \widehat{u}_i$ a.e. in Q, $i = 1, 2$.

Notice that $\mathcal{U}_{\rm ad}$ is a nonempty, closed and convex subset of $\mathcal{U} = L^\infty(Q)^2$. In the following, it will sometimes be convenient to work with a bounded open superset of $\mathcal{U}_{\rm ad}$. We therefore once and for all fix some $R > 0$ such that

$$\mathcal{U}_R := \left\{ \mathbf{u} = (u_1, u_2) \in L^\infty(Q)^2 : \ \|\mathbf{u}\|_\infty < R \right\} \supset \mathcal{U}_{\rm ad}. \tag{2.2}$$

The following result concerning the wellposedness of the state system has been shown in [10, Thm. 2.2].

Theorem 2.1. *Suppose that the conditions* **(F1)–(F4)***,* **(A1)–(A3)***,* **(A6)***, and* (2.2) *are fulfilled. Then the state system* (1.2)–(1.6) *has for every* $\mathbf{u} = (u_1, u_2) \in \mathcal{U}_R$ *a unique solution* (μ, φ, σ) *with the regularity*

$$\mu \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W_0) \cap C^0(\overline{Q}), \tag{2.3}$$

$$\varphi \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W_0) \cap C^0(\overline{Q}), \tag{2.4}$$

$$\sigma \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W_0) \cap C^0(\overline{Q}). \tag{2.5}$$

Moreover, there exists a constant $K_1 > 0$*, which depends on* $\Omega, T, R, \alpha, \beta$ *and the data of the system, but not on the choice of* $\mathbf{u} \in \mathcal{U}_R$*, such that*

$$\begin{aligned} &\|\varphi\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)\cap L^2(0,T;W_0)\cap C^0(\overline{Q})} \\ &+ \|\mu\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W_0)\cap C^0(\overline{Q})} \\ &+ \|\sigma\|_{H^1(0,T;H)\cap C^0([0,T];V)\cap L^2(0,T;W_0)\cap C^0(\overline{Q})} \le K_1 . \end{aligned} \tag{2.6}$$

In addition, there are constants r_*, r^**, which depend on* $\Omega, T, R, \alpha, \beta$ *and the data of the system, but not on the choice of* $\mathbf{u} \in \mathcal{U}_R$*, such that*

$$r_- < r_* \le \varphi(x,t) \le r^* < r_+ \quad \textit{for all } (x,t) \in \overline{Q}. \tag{2.7}$$

Finally, there is some constant $K_2 > 0$*, which depends on* $\Omega, T, R, \alpha, \beta$ *and the data of the system, but not on the choice of* $\mathbf{u} \in \mathcal{U}_R$*, such that*

$$\max_{i=0,1,2,3} \left\|h^{(i)}(\varphi)\right\|_{C^0(\overline{Q})} + \max_{i=0,1,2,3,4} \left\|F^{(i)}(\varphi)\right\|_{C^0(\overline{Q})} \le K_2 . \tag{2.8}$$

Remark 2.2. If the initial data $\mu_0, \varphi_0, \sigma_0 \in W_0$ also belong to the Sobolev–Slobodeckii space $W^{5/3,6}(\Omega)$, then the solution enjoys additional regularity.

Indeed, by the above bounds, we have $\mu + \chi\,\sigma - F'(\varphi) \in L^6(Q)$, in particular. We thus may employ the maximal regularity result from [11, Thm. 2.1] with $p = 6$ to the parabolic initial-boundary value problem satisfied by φ, which shows that $\varphi \in W^{1,6}(0,T;L^6(\Omega)) \cap L^6(0,T;W^{2,6}(\Omega))$. But then $(P\sigma - A - u_1)h(\varphi) - \partial_t\varphi \in L^6(Q)$, and [11, Thm. 2.1] implies that also $\mu \in W^{1,6}(0,T;L^6(\Omega)) \cap L^6(0,T;W^{2,6}(\Omega))$. Finally, we also have that $u_2 + B(\sigma_s - \sigma) - E\sigma h(\varphi) - \chi\Delta\varphi \in L^6(Q)$, and thus $\sigma \in W^{1,6}(0,T;L^6(\Omega)) \cap L^6(0,T;W^{2,6}(\Omega))$, again by virtue of [11, Thm. 2.1].

Remark 2.3. The *separation condition* (2.7) is particularly important for the case of singular potentials such as $F_{\log}$. Indeed, it guarantees that the phase variable always stays away from the critical values r_-, r_+ that usually correspond to the pure phases. In this way, the singularity is no longer an obstacle for the analysis; however, the case of pure phases is then excluded, which is not desirable from the viewpoint of medical applications.

Owing to Theorem 2.1, the control-to-state operator $\mathcal{S} : \mathbf{u} = (u_1, u_2) \mapsto (\mu, \varphi, \sigma)$ is well defined as a mapping between $\mathcal{U} = L^\infty(Q)^2$ and the Banach space specified by the regularity results (2.3)–(2.5).

We now discuss the Fréchet differentiability of $\mathcal{S}$, considered as a mapping between suitable Banach spaces. We remark that in [10, Thm. 2.6] Fréchet differentiability was established between $L^2(Q)^2$ and $(C^0([0,T];H) \cap L^2(0,T;V)) \times (H^1(0,T;H) \cap L^\infty(0,T;V)) \times (C^0([0,T];H) \cap L^2(0,T;V))$. The proof was a direct one that did not use the implicit function theorem. The result was strong enough to derive meaningful first-order necessary conditions, but it did not admit the derivation of second-order sufficient conditions, since these require the control-to-state operator to be twice continuously Fréchet differentiable. To show such a result, it is more favorable to employ the implicit function theorem, because, if applicable, it yields that the control-to-state operator automatically inherits the differentiability order from that of the involved nonlinearities. For this, some functional analytic preparations are in order. We first define the linear spaces

$$\begin{aligned} \mathcal{X} &:= X \times X \times X, \quad \text{where} \\ X &:= H^1(0,T;H) \cap C([0,T];V) \cap L^2(0,T;W_0) \cap C^0(\overline{Q}), \end{aligned} \tag{2.9}$$

which are Banach spaces when endowed with their natural norms. Next, we introduce the linear space

$$\begin{aligned} \mathcal{Y} := \big\{ &(\mu,\varphi,\sigma) \in \mathcal{X} : \ \alpha\partial_t\mu + \partial_t\varphi - \Delta\mu \in L^\infty(Q), \ \ \beta\partial_t\varphi - \Delta\varphi - \mu \in L^\infty(Q), \\ &\partial_t\sigma - \Delta\sigma + \chi\Delta\varphi \in L^\infty(Q) \big\}, \end{aligned} \tag{2.10}$$

which becomes a Banach space when endowed with the norm

$$\begin{aligned} \|(\mu,\varphi,\sigma)\|_{\mathcal{Y}} := &\|(\mu,\varphi,\sigma)\|_{\mathcal{X}} + \|\alpha\partial_t\mu + \partial_t\varphi - \Delta\mu\|_{L^\infty(Q)} + \|\beta\partial_t\varphi - \Delta\varphi - \mu\|_{L^\infty(Q)} \\ &+ \|\partial_t\sigma - \Delta\sigma + \chi\Delta\varphi\|_{L^\infty(Q)}\,. \end{aligned} \tag{2.11}$$

Finally, we fix constants $\tilde r_-, \tilde r_+$ such that

$$r_- < \tilde r_- < r_* \le r^* < \tilde r_+ < r_+, \tag{2.12}$$

with the constants introduced in **(F2)** and (2.7). We then consider the set

$$\Phi := \big\{ \varphi, \mu, \sigma) \in \mathcal{Y} : \tilde r_- < \varphi(x,t) < \tilde r_+ \ \text{for all} \ (x,t) \in \overline{Q} \big\}, \tag{2.13}$$

which is obviously an open subset of the space $\mathcal{Y}$.

We first prove an auxiliary result for the linear initial-boundary value problem

$$\alpha\partial_t\mu + \partial_t\varphi - \Delta\mu \,=\, \lambda_1\,[P\sigma h(\overline{\varphi}) + (P\overline{\sigma} - A - \overline{u}_1)h'(\overline{\varphi})\varphi] - \lambda_2 k_1 h(\overline{\varphi}) + \lambda_3 f_1 \quad \text{in } Q, \tag{2.14}$$

$$\beta\partial_t\varphi - \Delta\varphi - \mu \,=\, \lambda_1\,[\chi\,\sigma - F''(\overline{\varphi})\varphi] + \lambda_3 f_2 \quad \text{in } Q, \tag{2.15}$$

$$\partial_t\sigma - \Delta\sigma + \chi\Delta\varphi \,=\, \lambda_1\,[-B\sigma - E\sigma h(\overline{\varphi}) - E\overline{\sigma}h'(\overline{\varphi})\varphi] + \lambda_2 k_2 + \lambda_3 f_3 \quad \text{in } Q, \tag{2.16}$$

$$\partial_{\mathbf{n}}\mu \,=\, \partial_{\mathbf{n}}\varphi \,=\, \partial_{\mathbf{n}}\sigma \,=\, 0 \quad \text{on } \Sigma, \tag{2.17}$$

$$\mu(0) \,=\, \lambda_4\mu_0, \quad \varphi(0) \,=\, \lambda_4\varphi_0, \quad \sigma(0) \,=\, \lambda_4\sigma_0, \quad \text{in } \Omega, \tag{2.18}$$

which for $\lambda_1 = \lambda_2 = 1$ and $\lambda_3 = \lambda_4 = 0$ coincides with the linearization of the state equation at $((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma}))$. We will need this slightly more general version later for the application of the implicit function theorem.

Lemma 2.4. *Suppose that $\lambda_1, \lambda_2, \lambda_3, \lambda_4 \in \{0, 1\}$ are given and that the assumptions* **(F1)–(F4)**, **(A1)–(A3)**, **(A6)**, *and* (2.2) *are fulfilled. Moreover, let $((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma})) \in \mathcal{U}_R \times \Phi$ be arbitrary. Then the linear initial-boundary value problem* (2.14)–(2.18) *has for every $(k_1, k_2) \in L^\infty(Q)^2$ and every $(f_1, f_2, f_3) \in L^\infty(Q) \times (H^1(0,T;H) \cap L^\infty(Q)) \times L^\infty(Q)$ a unique solution $(\mu, \varphi, \sigma) \in \mathcal{Y}$. Moreover, the linear mapping*

$$((k_1, k_2), (f_1, f_2, f_3), (\mu_0, \varphi_0, \sigma_0)) \mapsto (\mu, \varphi, \sigma)$$

is continuous from $L^\infty(Q)^2 \times \big(L^\infty(Q) \times (H^1(0,T;H) \cap L^\infty(Q)) \times L^\infty(Q)\big) \times W_0^3$ into $\mathcal{Y}$.

Proof. We use a standard Faedo–Galerkin approximation. To this end, let $\{\lambda_k\}_{k\in\mathbb{N}}$ and $\{e_k\}_{k\in\mathbb{N}}$ denote the eigenvalues and associated eigenfunctions of the eigenvalue problem

$$-\Delta y + y = \lambda y \quad \text{in } \Omega, \quad \partial_{\mathbf{n}} y = 0 \quad \text{on } \Gamma,$$

where the latter are normalized by $\|e_k\|_2 = 1$. Then $\{e_k\}_{k\in\mathbb{N}}$ forms a complete orthonormal system in H which is also dense in V. We put $V_n := \operatorname{span}\{e_1, \ldots, e_n\}$, $n \in \mathbb{N}$, noting that $\bigcup_{n\in\mathbb{N}} V_n$ is dense in V. We look for functions of the form

$$\mu_n(x,t) = \sum_{k=1}^n u_k^{(n)}(t)e_k(x), \quad \varphi_n(x,t) = \sum_{k=1}^n v_k^{(n)}(t)e_k(x), \quad \sigma_n(x,t) = \sum_{k=1}^n w_k^{(n)}(t)e_k(x),$$

that satisfy the system

$$(\alpha\partial_t\mu_n(t), v) + (\partial_t\varphi_n(t), v) + (\nabla\mu_n(t), \nabla v) \,=\, (z_{n1}(t), v) \quad \forall\, v \in V_n, \ \text{for a.e. } t \in (0,T), \tag{2.19}$$

$$(\beta\partial_t\varphi_n(t), v) + (\nabla\varphi_n(t), \nabla v) - (\mu_n(t), v) \,=\, (z_{n2}(t), v) \quad \forall\, v \in V_n, \ \text{for a.e. } t \in (0,T), \tag{2.20}$$

$$(\partial_t\sigma_n(t), v) + (\nabla\sigma_n(t), \nabla v) - \chi(\nabla\varphi_n(t), \nabla v) \,=\, (z_{n3}(t), v) \quad \forall\, v \in V_n, \ \text{for a.e. } t \in (0,T), \tag{2.21}$$

$$\mu_n(0) = \lambda_4 P_n\mu_0, \quad \varphi_n(0) = \lambda_4 P_n\varphi_0, \quad \sigma_n(0) = \lambda_4 P_n\sigma_0, \tag{2.22}$$

where P_n denotes the $H^1(\Omega)$–orthogonal projection onto V_n, and where

$$z_{n1} \,=\, \lambda_1\,[P\sigma_n h(\overline{\varphi}) + (P\overline{\sigma} - A - \overline{u}_1)h'(\overline{\varphi})\varphi_n] - \lambda_2 k_1 h(\overline{\varphi}) + \lambda_3 f_1, \tag{2.23}$$

$$z_{n2} \,=\, \lambda_1\,[\chi\,\sigma_n - F''(\overline{\varphi})\varphi_n] + \lambda_3 f_2, \tag{2.24}$$

$$z_{n3} \,=\, \lambda_1\,[-B\sigma_n - E\sigma_n h(\overline{\varphi}) - E\overline{\sigma}h'(\overline{\varphi})\varphi_n] + \lambda_2 k_2 + \lambda_3 f_3\,. \tag{2.25}$$

Insertion of $v = e_k$, for $k \in \mathbb{N}$, in (2.19)–(2.21), and substitution for the second summand in (2.19) by means of (2.20), then lead to an initial value problem for an explicit linear system of ordinary differential equations for the unknowns $u_1^{(n)}, \ldots, u_n^{(n)}, v_1^{(n)}, \ldots, v_n^{(n)}, w_1^{(n)}, \ldots, w_n^{(n)}$, in which all of the coefficient functions belong to $L^\infty(0,T)$. Hence, by virtue of Carathéodory's theorem, there exists a unique solution in $W^{1,\infty}(0,T;\mathbb{R}^{3n})$ that specifies the unique solution $(\mu_n, \varphi_n, \sigma_n) \in W^{1,\infty}(0,T;H^2(\Omega))^3$ to the system (2.19)–(2.22), for $n \in \mathbb{N}$.

We now derive some a priori estimates for the Faedo–Galerkin approximations. In this procedure, $C_i > 0,\ i \in \mathbb{N}$, will denote constants that are independent of $n \in \mathbb{N}$ and the data $((f_1, f_2, f_3), (\mu_0, \varphi_0, \sigma_0))$, while the constant $M > 0$ is given by

$$
\begin{aligned}
M :=& \lambda_2 \,\|(k_1,k_2)\|_{L^\infty(Q)^2} \,+\, \lambda_3 \,\|(f_1,f_2,f_3)\|_{L^\infty(Q)\times(H^1(0,T;H)\cap L^\infty(Q))\times L^\infty(Q)} \\
&+\, \lambda_4 \,\|(\mu_0,\varphi_0,\sigma_0)\|_{H^2(\Omega)^3}.
\end{aligned} \tag{2.26}
$$

Moreover, $(\overline{\mu}, \overline{\varphi}, \overline{\sigma}) \in \Phi$, and thus it follows that $\overline{\sigma}, h(\overline{\varphi}), h'(\overline{\varphi}), F''(\overline{\varphi}) \in C^0(\overline{Q})$. Hence, there is some constant $C_1 > 0$ such that, for a.e. $(x,t) \in Q$ and for all $n \in \mathbb{N}$,

$$
\begin{aligned}
\big(|z_{n1}| + |z_{n2}| + |z_{n3}|\big)(x,t) \,&\le\, C_1 \left(\lambda_1(|\varphi_n| + |\sigma_n|)(x,t) + \lambda_2(|k_1| + |k_2|)(x,t) \right. && (2.27)\\
&\qquad \left. + \lambda_3(|f_1| + |f_2| + |f_3|)(x,t)\right) \\
&\le\, C_1 \left(\lambda_1(|\varphi_n| + |\sigma_n|)(x,t) \,+\, M\right). && (2.28)
\end{aligned}
$$

First estimate. We insert $v = \mu_n(t)$ in (2.19), $v = \partial_t\varphi_n(t)$ in (2.20), and $v = \sigma_n(t)$ in (2.21), and add the resulting equations, whence a cancellation of two terms occurs. Then, in order to recover the full $H^1(\Omega)-$norm below, we add to both sides of the resulting equation the same term $\frac{1}{2}\frac{d}{dt}\|\varphi_n(t)\|_2^2 = (\varphi_n(t), \partial_t\varphi_n(t))$. Integration over $[0,\tau]$, where $\tau \in (0,T]$, then yields the identity

$$
\begin{aligned}
&\frac{1}{2}\left(\alpha\|\mu_n(\tau)\|_2^2 \,+\, \|\varphi_n(\tau)\|_V^2 + \|\sigma_n(\tau)\|_2^2\right) \,+\, \int_0^\tau\!\!\int_\Omega \left(|\nabla\mu_n|^2 + |\nabla\sigma_n|^2\right) \,+\, \beta\int_0^\tau\!\!\int_\Omega |\partial_t\varphi_n|^2 \\
&= \frac{\lambda_4^2}{2}\left(\alpha\|P_n\mu_0\|_2^2 + \|P_n\varphi_0\|_V^2 + \|P_n\sigma_0\|_2^2\right) \,+\, \int_0^\tau (\mu_n(t), z_{n1}(t))\,dt \,+\, \int_0^\tau (\sigma_n(t), z_{n3}(t))\,dt \\
&\quad + \int_0^\tau (\partial_t\varphi_n(t), z_{n2}(t) + \varphi_n(t))\,dt \,+ \chi\int_0^\tau (\nabla\varphi_n(t), \nabla\sigma_n(t))\,dt \,=:\, \sum_{i=1}^5 J_i,
\end{aligned} \tag{2.29}
$$

with obvious notation. We estimate the terms on the right-hand side individually. First observe that $\|y\|_V \le \|y\|_{H^2(\Omega)}$ for all $y \in H^2(\Omega)$, and thus, for all $n \in \mathbb{N}$,

$$
|J_1| \,\le\, C_2\,\lambda_4^2\,\|(P_n\mu_0, P_n\varphi_0, P_n\sigma_0)\|_{V\times V\times V}^2 \,\le\, C_2\,\lambda_4^2\,\|(\mu_0,\varphi_0,\sigma_0)\|_{V\times V\times V}^2 \,\le\, C_2\,M^2. \tag{2.30}
$$

Moreover, by virtue of (2.28) and Young's inequality,

$$
|J_2| + |J_3| \,\le\, C_3\,M^2 \,+\, C_4\int_0^\tau\!\!\int_\Omega \left(|\mu_n|^2 + |\varphi_n|^2 + |\sigma_n|^2\right). \tag{2.31}
$$

Likewise,

$$
|J_4| \,\le\, \frac{\beta}{2}\int_0^\tau\!\!\int_\Omega |\partial_t\varphi_n|^2 \,+\, \frac{C_5}{\beta}\,M^2 \,+\, \frac{C_6}{\beta}\int_0^\tau\!\!\int_\Omega \left(|\mu_n|^2 + |\varphi_n|^2 + |\sigma_n|^2\right). \tag{2.32}
$$

Finally, we have that

$$|J_5| \le \frac{1}{2}\int_0^\tau\!\!\int_\Omega |\nabla\sigma_n|^2 + \frac{\chi^2}{2}\int_0^\tau\!\!\int_\Omega |\nabla\varphi_n|^2. \tag{2.33}$$

Combining the estimates (2.29)–(2.33), where we subtract the first integral in (2.32) from the associated term on the left-hand side of (2.29), we have shown that

$$\frac{1}{2}\big(\alpha\|\mu_n(\tau)\|_2^2 + \|\varphi_n(\tau)\|_V^2 + \|\sigma_n(\tau)\|_2^2\big) + \int_0^\tau\!\!\int_\Omega \big(|\nabla\mu_n|^2 + \frac{1}{2}|\nabla\sigma_n|^2\big) + \frac{\beta}{2}\int_0^\tau\!\!\int_\Omega |\partial_t\varphi_n|^2$$
$$\le C_7 M^2 + C_8\int_0^\tau \big(\|\mu_n(t)\|_2^2 + \|\varphi_n(t)\|_V^2 + \|\sigma_n(t)\|_2^2\big)\,dt\,.$$

Therefore, invoking Gronwall's lemma, we conclude that, for all $n\in\mathbb{N}$,

$$\|\mu_n\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|\varphi_n\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\sigma_n\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \le C_9 M. \tag{2.34}$$

SECOND ESTIMATE. Next, we insert $v = \partial_t\mu_n(t)$ in (2.19) and integrate over $[0,\tau]$, where $\tau\in(0,T]$, to obtain the identity

$$\frac{1}{2}\|\nabla\mu_n(\tau)\|_2^2 + \alpha\int_0^\tau \|\partial_t\mu_n(t)\|_2^2\,dt$$
$$= \frac{\lambda_4^2}{2}\|\nabla P_n\mu_0\|_2^2 + \int_0^\tau (\partial_t\mu_n(t), z_{n1}(t))\,dt - \int_0^\tau (\partial_t\mu_n(t), \partial_t\varphi_n(t))\,dt.$$

Applying Young's inequality appropriately, where we make use of (2.28) and (2.34), we conclude the estimate

$$\|\mu_n\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} \le C_{10}\,M. \tag{2.35}$$

THIRD ESTIMATE. At this point, we insert $v = -\Delta\mu_n(t)$ in (2.19) and $v = -\Delta\varphi_n(t)$ in (2.20), add, and integrate over $[0,\tau]$ where $\tau\in(0,T]$. We then obtain that

$$\frac{\alpha}{2}\|\nabla\mu_n(\tau)\|_2^2 + \frac{\beta}{2}\|\nabla\varphi_n(\tau)\|_2^2 + \int_0^\tau \|\Delta\mu_n(t)\|_2^2\,dt + \int_0^\tau \|\Delta\varphi_n(t)\|_2^2\,dt$$
$$= \frac{\alpha\lambda_4^2}{2}\|\nabla P_n\mu_0\|_2^2 + \frac{\beta\lambda_4^2}{2}\|\nabla P_n\varphi_0\|_2^2 - \int_0^\tau (\Delta\mu_n(t), z_{n1}(t))\,dt$$
$$- \int_0^\tau (\Delta\varphi_n(t), \mu_n(t) + z_{n2}(t))\,dt\,,$$

whence, using (2.28)–(2.35) and Young's inequality,

$$\int_0^T \big(\|\Delta\mu_n(t)\|_2^2 + \|\Delta\varphi_n(t)\|_2^2\big)\,dt \le C_{11}M^2 \quad \forall\, n\in\mathbb{N}. \tag{2.36}$$

At this point, we invoke a classical elliptic estimate (see, e.g., [20, Chap. 2, Thm. 5.1]): there is a constant $C_\Omega > 0$, which only depends on Ω, such that, for every $v\in H^2(\Omega)$,

$$\|v\|_{H^2(\Omega)} \le C_\Omega\big(\|\Delta v\|_{L^2(\Omega)} + \|v\|_{H^1(\Omega)} + \|\partial_{\mathbf{n}} v\|_{H^{1/2}(\Gamma)}\big)\,. \tag{2.37}$$

In view of the zero Neumann boundary condition satisfied by μ_n and φ_n, we thus conclude from (2.34), (2.35), and (2.36), that

$$\|\mu_n\|_{L^2(0,T;H^2(\Omega))} + \|\varphi_n\|_{L^2(0,T;H^2(\Omega))} \le C_{12}M \quad \forall\, n \in \mathbb{N}. \tag{2.38}$$

With the estimate (2.38) at hand, we may (by first taking $v = \partial_t\sigma_n(t)$ in (2.21) and then $v = -\Delta\sigma_n(t)$) infer by similar reasoning that also

$$\|\sigma_n\|_{H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;H^2(\Omega))} \le C_{13}M \quad \forall\, n \in \mathbb{N}. \tag{2.39}$$

At this point, we can conclude from standard weak and weak-star compactness arguments the existence of a triple (μ, φ, σ) such that, possibly only on a subsequence which is again indexed by n,

$$\begin{aligned} &\mu_n \to \mu, \quad \varphi_n \to \varphi, \quad \sigma_n \to \sigma, \\ &\text{all weakly-star in } H^1(0,T;H) \cap L^\infty(0,T;V) \cap L^2(0,T;H^2(\Omega)). \end{aligned}$$

Standard arguments, which need no repetition here, then show that (μ, φ, σ) is a strong solution to the system (2.14)–(2.18). Moreover, recalling (2.34)–(2.39), and invoking the weak sequential lower semicontinuity of norms, we conclude that there is some $C_{13} > 0$ such that

$$\|(\mu, \varphi, \sigma)\|_{(H^1(0,T;H)\cap L^\infty(0,T;V)\cap L^2(0,T;H^2(\Omega)))^3} \le C_{13}M. \tag{2.40}$$

Next, we claim that $(\mu, \varphi, \sigma) \in C^0(\overline{Q})^3$ and that, with a suitable $C_{14} > 0$,

$$\|(\mu, \varphi, \sigma)\|_{C^0(\overline{Q})^3} \le C_{14}M. \tag{2.41}$$

It is easy to argue for the solution component φ. Indeed, we have (cf. (2.15))

$$\beta\partial_t\varphi - \Delta\varphi = \mu + \lambda_1(\chi\sigma - F''(\overline{\varphi})\varphi) + \lambda_3 f_2 =: g,$$

that is, φ solves a linear parabolic equation with zero Neumann boundary condition and with a right-hand side g which, by virtue of the estimates shown above, is known to be bounded in $L^\infty(0,T;H)$ by an expression of the form $C_{15}M$. Moreover, we have $\varphi_0 \in W_0$. Therefore, we may invoke the classical results from [19, Chap. 7] to conclude the validity of the claim for φ.

For the other solution components μ and σ, a similar argument is not yet possible, since the expressions $\partial_t\varphi$ and $\Delta\varphi$ occurring in (2.14) and (2.16), respectively, are so far merely known to be bounded in $L^2(Q)$. In order to prove the claim by the above argument also for μ and σ, we are now going to show corresponding bounds for $\partial_t\varphi$ and $\Delta\varphi$ in $L^\infty(0,T;H)$.

To this end, notice that

$$\partial_t g = \partial_t\mu + \lambda_1\big(\chi\partial_t\sigma - F''(\overline{\varphi})\partial_t\varphi - F'''(\overline{\varphi})\partial_t\overline{\varphi}\,\varphi\big) + \lambda_3\partial_t f_2, \tag{2.42}$$

where, owing to Hölder's inequality, (2.8), and the continuity of the embedding $V \subset L^4(\Omega)$,

$$\int_0^T\!\!\int_\Omega |F'''(\overline{\varphi})\partial_t\overline{\varphi}\,\varphi|^2 \le K_2^2 \int_0^T \|\partial_t\overline{\varphi}(t)\|_4^2\,\|\varphi(t)\|_4^2\,dt \le K_2^2\,\|\partial_t\overline{\varphi}\|^2_{L^2(0,T;V)}\,\|\varphi\|^2_{L^\infty(0,T;V)}.$$

Therefore, invoking (2.6) and (2.40),

$$\|\partial_t g\|_{L^2(Q)} \,\le\, C_{16} M. \tag{2.43}$$

At this point, we consider the linear parabolic initial-boundary value problem

$$\beta \partial_t z - \Delta z = \partial_t g \quad \text{in } Q, \tag{2.44}$$

$$\partial_{\mathbf{n}} z = 0 \quad \text{on } \Sigma, \tag{2.45}$$

$$z(0) = \beta^{-1}(\Delta \varphi_0 + g(0)) \quad \text{in } \Omega, \tag{2.46}$$

where $g(0) = \mu_0 + \lambda_1(\chi\sigma_0 - F''(\varphi_0)\varphi_0) + \lambda_3 f_2(0) \in L^2(\Omega)$. Since also $\partial_t g \in L^2(Q)$, it follows from a classical argument that the above system admits a unique weak solution $z \in H^1(0,T;V^*) \cap C([0,T];H) \cap L^2(0,T;V)$, and since $\partial_{\mathbf{n}}\varphi_0 = 0$, it is easily checked that the function

$$w(x,t) := \varphi_0(x) + \int_0^t z(x,s)\,ds \quad \text{for a.e. } (x,t) \in Q$$

coincides with φ, that is, in particular, we have $z = \partial_t \varphi$. Moreover, standard estimates and (2.40), (2.43) show that

$$\|\partial_t \varphi\|_{H^1(0,T;V^*)\cap C([0,T];H)\cap L^2(0,T;V)} \,\le\, C_{17}\big(\|\Delta\varphi_0 + g(0)\|_2 \,+\, \|\partial_t g\|_{L^2(Q)}\big) \,\le\, C_{18} M. \tag{2.47}$$

By comparison in (2.15), we then readily see that also

$$\|\Delta \varphi\|_{L^\infty(0,T;H)} \,\le\, C_{19} M, \tag{2.48}$$

and the elliptic estimate (2.37) shows that also

$$\|\varphi\|_{L^\infty(0,T;H^2(\Omega))} \,\le\, C_{20} M. \tag{2.49}$$

Since we now have available the $L^\infty(0,T;H)-$bounds for $\partial_t\varphi$ and $\Delta\varphi$, we can apply the classical results from [19, Chap. 7] to the equations (2.14) and (2.16) to infer that $\mu, \sigma \in C^0(\overline{Q})$ and that (2.41) actually holds true. The above claim is thus shown.

It then immediately follows that $(\mu,\varphi,\sigma) \in \mathcal{Y}$, as well as

$$\|(\mu,\varphi,\sigma)\|_{\mathcal{Y}} \,\le\, C_{21} M.$$

With this, the existence of a solution with the asserted properties is shown. It remains to prove the uniqueness. To this end, let $(\mu_i,\varphi_i,\sigma_i) \in \mathcal{Y}$, $i = 1,2$, be two solutions to the system. Then $(\mu,\varphi,\sigma) := (\mu_1,\varphi_1,\sigma_1) - (\mu_2,\varphi_2,\sigma_2)$ solves the system (2.14)–(2.18) with zero initial data, where the terms $\lambda_2 k_i$, $i = 1,2$, and $\lambda_3 f_i$, $i = 1,2,3$, on the right-hand sides do not occur. By the definition of $\mathcal{Y}$ (recall (2.9) and (2.10)), and since $(\mu,\varphi,\sigma) \in \mathcal{Y}$, all of the generalized partial derivatives occurring in (2.14)–(2.16) belong to $L^2(Q)$. Therefore, we may repeat – now for the continuous problem – the a priori estimates performed for the Faedo–Galerkin approximations that led us to the estimate (2.34). We then find analogous estimates for (μ,φ,σ), where this time the constant M from (2.26) equals zero. Thus, $(\mu,\varphi,\sigma) = (0,0,0)$. With this, the uniqueness is shown, which finishes the proof of the assertion. □

Remark 2.5. As it follows from the above proof, the solution component φ enjoys the additional regularity $\varphi \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W_0)$.

With Lemma 2.4 shown, we are in a position to prepare for the application of the implicit function theorem. For this purpose, let us consider two auxiliary linear initial-boundary value problems. The first,

$$\alpha\partial_t\mu + \partial_t\varphi - \Delta\mu \,=\, f_1 \quad \text{in } Q, \tag{2.50}$$

$$\beta\partial_t\varphi - \Delta\varphi - \mu \,=\, f_2 \quad \text{in } Q, \tag{2.51}$$

$$\partial_t\sigma - \Delta\sigma + \chi\Delta\varphi \,=\, f_3 \quad \text{in } Q, \tag{2.52}$$

$$\partial_{\mathbf{n}}\mu \,=\, \partial_{\mathbf{n}}\varphi \,=\, \partial_{\mathbf{n}}\sigma \,=\, 0 \quad \text{on } \Sigma, \tag{2.53}$$

$$\mu(0) \,=\, \varphi(0) \,=\, \sigma(0) \,=0, \quad \text{in } \Omega, \tag{2.54}$$

is obtained from (2.14)–(2.18) for $\lambda_1 = \lambda_2 = \lambda_4 = 0,\ \lambda_3 = 1$. Thanks to Lemma 2.4, this system has for each $(f_1, f_2, f_3) \in L^\infty(Q)\times\big(H^1(0,T;H)\cap L^\infty(Q)\big)\times L^\infty(Q)$ a unique solution $(\mu,\varphi,\sigma) \in \mathcal{Y}$, and the associated linear mapping

$$\mathcal{G}_1 : \big(L^\infty(Q) \times \big(H^1(0,T;H) \cap L^\infty(Q)\big) \times L^\infty(Q)\big) \to \mathcal{Y};\ (f_1,f_2,f_3) \mapsto (\mu,\varphi,\sigma), \tag{2.55}$$

is continuous. The second system reads

$$\alpha\partial_t\mu + \partial_t\varphi - \Delta\mu \,=\, 0 \quad \text{in } Q, \tag{2.56}$$

$$\beta\partial_t\varphi - \Delta\varphi - \mu \,=\, 0 \quad \text{in } Q, \tag{2.57}$$

$$\partial_t\sigma - \Delta\sigma + \chi\Delta\varphi \,=\, 0 \quad \text{in } Q, \tag{2.58}$$

$$\partial_{\mathbf{n}}\mu \,=\, \partial_{\mathbf{n}}\varphi \,=\, \partial_{\mathbf{n}}\sigma \,=\, 0 \quad \text{on } \Sigma, \tag{2.59}$$

$$\mu(0) \,=\, \mu_0, \quad \varphi(0) \,=\, \varphi_0, \quad \sigma(0) \,=\, \sigma_0, \quad \text{in } \Omega. \tag{2.60}$$

For each $(\mu_0,\varphi_0,\sigma_0) \in W_0^3$, it also enjoys a unique solution $(\mu,\varphi,\sigma) \in \mathcal{Y}$, and the associated mapping

$$\mathcal{G}_2 : W_0^3 \to \mathcal{Y};\ (\mu_0,\varphi_0,\sigma_0) \mapsto (\mu,\varphi,\sigma), \tag{2.61}$$

is linear and continuous as well.

In addition, we define on the open set $\mathcal{A} := (\mathcal{U}_R \times \Phi) \subset (\mathcal{U} \times \mathcal{Y})$ the nonlinear mapping

$$\begin{aligned}
&\mathcal{G}_3 : \mathcal{U}_R \times \Phi \to \big(L^\infty(Q) \times \big(H^1(0,T;H) \cap L^\infty(Q)\big) \times L^\infty(Q)\big);\\
&((u_1,u_2),(\mu,\varphi,\sigma)) \mapsto (f_1,f_2,f_3), \quad \text{where}\\
&(f_1,f_2,f_3) = ((P\sigma - A - u_1)h(\varphi), \chi\,\sigma - F'(\varphi), B(\sigma_s - \sigma) - E\sigma h(\varphi) + u_2)\,.
\end{aligned} \tag{2.62}$$

The solution (μ,φ,σ) to the nonlinear state equation (1.2)–(1.6) is the sum of the solution to the system (2.50)–(2.54), where (f_1,f_2,f_3) is chosen as above (with (μ,φ,σ) considered as known), and of the solution to the system (2.56)–(2.60). Therefore, the state vector (μ,φ,σ) associated with the control vector (u_1,u_2) is the unique solution to the nonlinear equation

$$(\mu,\varphi,\sigma) = \mathcal{G}_1\big(\mathcal{G}_3((u_1,u_2),(\mu,\varphi,\sigma)\big) + \mathcal{G}_2(\mu_0,\varphi_0,\sigma_0). \tag{2.63}$$

Let us now define the nonlinear mapping $\mathcal{F} : \mathcal{A} \to \mathcal{Y}$,

$$\mathcal{F}((u_1,u_2),(\mu,\varphi,\sigma)) \,=\, \mathcal{G}_1(\mathcal{G}_3((u_1,u_2),(\mu,\varphi,\sigma)) + \mathcal{G}_2(\mu_0,\varphi_0,\sigma_0) - (\mu,\varphi,\sigma). \tag{2.64}$$

With $\mathcal{F}$, the state equation can be shortly written as

$$\mathcal{F}((u_1, u_2)(\mu, \varphi, \sigma)) = (0, 0, 0). \tag{2.65}$$

This equation just means that (μ, φ, σ) is a solution to the state system (1.2)–(1.6) such that $((u_1, u_2), (\mu, \varphi, \sigma)) \in \mathcal{A}$. From Theorem 2.1 we know that such a solution exists for every $(u_1, u_2) \in \mathcal{U}_R$. A fortiori, any such solution automatically enjoys the separation property (2.7) and is uniquely determined.

We are going to apply the implicit function theorem to the equation (2.65). To this end, we need the differentiability of the involved mappings.

Observe that, owing to the differentiability properties of the involved Nemytskii operators (see, e.g., [22, Thm. 4.22]), the mapping $\mathcal{G}_3$ is twice continuously Fréchet differentiable, and for the first partial derivatives at any point $((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma})) \in \mathcal{A}$, and for all $(u_1, u_2) \in \mathcal{U}$ and $(\mu, \varphi, \sigma) \in \mathcal{Y}$, we have the identities

$$D_{(u_1,u_2)}\mathcal{G}_3((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma}))(u_1, u_2) = (-u_1 h(\overline{\varphi}), 0, u_2), \tag{2.66}$$

$$\begin{aligned} D_{(\mu,\varphi,\sigma)}\mathcal{G}_3((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma}))(\mu, \varphi, \sigma) &= ((P\overline{\sigma} - A - \overline{u}_1)h'(\overline{\varphi})\varphi + P\sigma h(\overline{\varphi}), \chi\sigma - F''(\overline{\varphi})\varphi, \\ &\quad - B\sigma - E\sigma h(\overline{\varphi}) - E\overline{\sigma} h'(\overline{\varphi})\varphi). \end{aligned} \tag{2.67}$$

It follows from the that $\mathcal{F}$ is twice continuously Fréchet differentiable from $\mathcal{U}_R \times \Phi$ into $\mathcal{Y}$, with the first-order partial derivatives

$$D_{(u_1,u_2)}\mathcal{F}((\overline{u}_1, \overline{u}_2)(\overline{\mu}, \overline{\varphi}, \overline{\sigma})) = \mathcal{G}_1 \circ D_{(u_1,u_2)}\mathcal{G}_3((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma})), \tag{2.68}$$

$$D_{(\mu,\varphi,\sigma)}\mathcal{F}((\overline{u}_1, \overline{u}_2)(\overline{\mu}, \overline{\varphi}, \overline{\sigma})) = \mathcal{G}_1 \circ D_{(\mu,\varphi,\sigma)}\mathcal{G}_3((\overline{u}_1, \overline{u}_2), (\overline{\mu}, \overline{\varphi}, \overline{\sigma})) - I_{\mathcal{Y}}, \tag{2.69}$$

where $I_{\mathcal{Y}}$ denotes the identity mapping on $\mathcal{Y}$.

At this point, we introduce for convenience abbreviating denotations, namely,

$$\begin{aligned} &\mathbf{u} := (u_1, u_2), \quad \overline{\mathbf{u}} := (\overline{u}_1, \overline{u}_2), \quad \mathbf{y} := (\mu, \varphi, \sigma), \quad \overline{\mathbf{y}} := (\overline{\mu}, \overline{\varphi}, \overline{\sigma}), \\ &\mathbf{y}_0 := (\mu_0, \varphi_0, \sigma_0), \quad \mathbf{0} := (0, 0, 0). \end{aligned} \tag{2.70}$$

With these denotations, we want to prove the differentiability of the control-to-state mapping $\mathbf{u} \mapsto \mathbf{y}$ defined implicitly by the equation $\mathcal{F}(\mathbf{u}, \mathbf{y}) = \mathbf{0}$, using the implicit function theorem. Now let $\overline{\mathbf{u}} \in \mathcal{U}_R$ be given and $\overline{\mathbf{y}} = \mathcal{S}(\overline{\mathbf{u}})$. We need to show that the linear and continuous operator $D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}}, \overline{\mathbf{y}})$ is a topological isomorphism from $\mathcal{Y}$ into itself.

To this end, let $\mathbf{v} \in \mathcal{Y}$ be arbitrary. Then the identity $D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{y}) = \mathbf{v}$ just means that $\mathcal{G}_1 \left(D_{\mathbf{y}}\mathcal{G}_3(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{y})\right) - \mathbf{y} = \mathbf{v}$, which is equivalent to saying that

$$\mathbf{w} := \mathbf{y} + \mathbf{v} = \mathcal{G}_1 \left(D_{\mathbf{y}}\mathcal{G}_3(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{w})\right) - \mathcal{G}_1 \left(D_{\mathbf{y}}\mathcal{G}_3(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{v})\right).$$

The latter identity means that $\mathbf{w}$ is a solution to the system (2.14)–(2.18) for $\lambda_1 = \lambda_3 = 1, \lambda_2 = \lambda_4 = 0$, with the specification $(f_1, f_2, f_3) = -\mathcal{G}_1 \left(D_{\mathbf{y}}\mathcal{G}_3(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{v})\right) \in \mathcal{Y}$. By Lemma 2.4, such a solution $\mathbf{w} \in \mathcal{Y}$ exists and is uniquely determined. We thus can infer that $D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}}, \overline{\mathbf{y}})$ is surjective. At the same time, taking $\mathbf{v} = \mathbf{0}$, we see that the equation $D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}}, \overline{\mathbf{y}})(\mathbf{y}) = \mathbf{0}$ means that $\mathbf{y}$ is the unique solution to (2.14)–(2.18) for $\lambda_1 = 1, \lambda_2 = \lambda_3 = \lambda_4 = 0$. Obviously, $\mathbf{y} = \mathbf{0}$, which implies that $D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}}, \overline{\mathbf{y}})$ is also injective and thus, by the open mapping principle, a topological isomorphism from $\mathcal{Y}$ into itself.

At this point, we may employ the implicit function theorem (cf., e.g., [1, Thms. 4.7.1 and 5.4.5] or [12, 10.2.1]) to conclude that the mapping $\mathcal{S}$ is twice continuously Fréchet differentiable from $\mathcal{U}_R$ into $\mathcal{Y}$ and that the first Fréchet derivative $D\mathcal{S}(\overline{\mathbf{u}})$ of $\mathcal{S}$ at $\overline{\mathbf{u}} \in \mathcal{U}_R$ is given by the formula

$$D\mathcal{S}(\overline{\mathbf{u}}) \;=\; -D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}},\overline{\mathbf{y}})^{-1} \circ D_{\mathbf{u}}\mathcal{F}(\overline{\mathbf{u}},\overline{\mathbf{y}}). \tag{2.71}$$

Now let $\mathbf{k}=(k_1,k_2)\in\mathcal{U}$ be arbitrary and $\mathbf{y}=(\mu,\varphi,\sigma)=D\mathcal{S}(\overline{\mathbf{u}})(\mathbf{k})$. Then,

$$D_{\mathbf{y}}\mathcal{F}(\overline{\mathbf{u}},\overline{\mathbf{y}})(\mathbf{y}) = -\mathbf{D}_{\mathbf{u}}\mathcal{F}(\overline{\mathbf{u}},\overline{\mathbf{y}})(\mathbf{k}),$$

which is obviously equivalent to saying that

$$\mathbf{y} = \mathcal{G}_1\left(D_{\mathbf{y}}\mathcal{G}_3(\overline{\mathbf{u}},\overline{\mathbf{y}})(\mathbf{y})\right) + \mathcal{G}_1(-k_1 h(\overline{\varphi}),0,k_2).$$

This, in turn, means that $\mathbf{y}$ is the unique solution to the problem (2.14)–(2.18) for $\lambda_1=\lambda_2=1, \lambda_3=\lambda_4=0$.

In summary, we have shown the following result.

Theorem 2.6. *Suppose that the conditions* **(F1)–(F4)**, **(A1)–(A3)**, **(A6)** *and* (2.2) *are fulfilled, let* $\overline{\mathbf{u}}=(\overline{u}_1,\overline{u}_2)\in\mathcal{U}_R$ *be arbitrary and* $(\overline{\mu},\overline{\varphi},\overline{\sigma})=\mathcal{S}(\overline{\mathbf{u}})$*. Then the control-to-state operator* $\mathcal{S}$ *is twice continuously Fréchet differentiable at* $\overline{\mathbf{u}}$ *as a mapping from* $\mathcal{U}$ *into* $\mathcal{Y}$*. Moreover, for every* $(k_1,k_2)\in\mathcal{U}$*, the Fréchet derivative* $D\mathcal{S}(\overline{\mathbf{u}})\in\mathcal{L}(\mathcal{U},\mathcal{Y})$ *of* $\mathcal{S}$ *at* $\overline{\mathbf{u}}$ *is given by the identity* $D\mathcal{S}(\overline{\mathbf{u}})(k_1,k_2)=(\mu,\varphi,\sigma)$*, where* (μ,φ,σ) *is the unique solution to the linear system* (2.14)–(2.18) *with* $\lambda_1=\lambda_2=1,\lambda_3=\lambda_4=0$*.*

3 First-order necessary optimality conditions

In this section, we aim at deriving associated first-order necessary optimality conditions. To this end, we define the (control) reduced objective functional $\widetilde{\mathcal{J}}$ by

$$\widetilde{\mathcal{J}}(\mathbf{u}) = \mathcal{J}(\mathcal{S}(\mathbf{u}),\mathbf{u}), \tag{3.1}$$

where we recall that $\mathcal{S}(\mathbf{u})=(\mu,\varphi,\sigma)$ is the unique solution to the state system associated with $\mathbf{u}$. The functional $\widetilde{\mathcal{J}}$ is the sum of a nonconvex functional $\mathcal{J}_1$ and the convex functional $\kappa\, g$, namely

$$\widetilde{\mathcal{J}} = \mathcal{J}_1 + \kappa g,$$

where

$$\mathcal{J}_1(\mathbf{u}) = \frac{\beta_1}{2}\int_Q |\varphi_{\mathbf{u}}-\widehat{\varphi}_Q|^2 + \frac{\beta_2}{2}\int_\Omega |\varphi_{\mathbf{u}}(T)-\widehat{\varphi}_\Omega|^2 + \frac{\nu}{2}\int_Q |\mathbf{u}|^2. \tag{3.2}$$

Here, g is one of the functionals (1.9)–(1.11), and we denote by $\varphi_{\mathbf{u}}$ the second component of $\mathcal{S}(\mathbf{u})$.

Since, owing to [10, Thm. 2.6], the control-to-state mapping is Fréchet differentiable from $L^2(Q)^2$ into $L^2(Q)\times C^0([0,T];L^2(\Omega))\times L^2(Q)$, in particular, the functional $\mathcal{J}_1$ is a Fréchet differentiable mapping from $L^2(Q)^2$ into $\mathbb{R}$. Therefore, the chain rule shows that, for every $\overline{\mathbf{u}}=(\overline{u}_1,\overline{u}_2)\in L^2(Q)^2$ and $\mathbf{k}=(k_1,k_2)\in L^2(Q)^2$, it holds that

$$D\mathcal{J}_1(\overline{\mathbf{u}})(\mathbf{k}) = \beta_1\int_Q(\varphi_{\overline{\mathbf{u}}}-\widehat{\varphi}_Q)\,\varphi \;+\; \beta_2\int_\Omega(\varphi_{\overline{\mathbf{u}}}(T)-\widehat{\varphi}_\Omega)\,\varphi(T) \;+\; \nu\int_Q \overline{\mathbf{u}}\cdot\mathbf{k}, \tag{3.3}$$

DOI 10.20347/WIAS.PREPRINT.2721

where φ is the second component of the solution (μ, φ, σ) to the linearized system (2.14)–(2.18) with $\lambda_1 = \lambda_2 = 1, \lambda_3 = \lambda_4 = 0$, and where " $\cdot$ " stands for the euclidean inner product in $\mathbb{R}^2$.

Now assume that $\overline{\mathbf{u}} = (\overline{u}_1, \overline{u}_2)$ is a locally optimal control for $(\mathcal{CP})$. Then it is easily seen that the variational inequality

$$D\mathcal{J}_1(\overline{\mathbf{u}})(\mathbf{u} - \overline{\mathbf{u}}) + \kappa(g(\mathbf{u}) - g(\overline{\mathbf{u}})) \geq 0 \quad \forall\, \mathbf{u} \in \mathcal{U}_{\rm ad} \tag{3.4}$$

is satisfied. Indeed, if $\mathbf{u} \in \mathcal{U}_{\rm ad}$ and $t \in (0,1)$ are given, then we can infer from the convexity of g that

$$\begin{aligned} 0 \leq\, & \mathcal{J}_1(\overline{\mathbf{u}} + t(\mathbf{u} - \overline{\mathbf{u}})) + \kappa g(\overline{\mathbf{u}} + t(\mathbf{u} - \overline{\mathbf{u}})) - \mathcal{J}_1(\overline{\mathbf{u}}) - \kappa g(\overline{\mathbf{u}}) \\ \leq\, & \mathcal{J}_1(\overline{\mathbf{u}} + t(\mathbf{u} - \overline{\mathbf{u}})) - \mathcal{J}_1(\overline{\mathbf{u}}) + \kappa\, t(g(\mathbf{u}) - g(\overline{\mathbf{u}})), \end{aligned}$$

whence, dividing by $t > 0$ and then taking the limit as $t \searrow 0$, (3.4) follows. But (3.4) implies that $\overline{\mathbf{u}}$ solves the convex minimization problem

$$\min_{\mathbf{u} \in L^2(Q)^2} \big(\Phi(\mathbf{u}) + \kappa g(\mathbf{u}) + I_{\mathcal{U}_{\rm ad}}(\mathbf{u})\big),$$

with $\Phi(\mathbf{u}) = D\mathcal{J}_1(\overline{\mathbf{u}})\mathbf{u}$, and where $I_{\mathcal{U}_{\rm ad}}$ denotes the indicator function of $\mathcal{U}_{\rm ad}$. Hence, denoting by the symbol ∂ the subdifferential mapping in $L^2(Q)^2$, we have that

$$\mathbf{0} \in \partial\big(\Phi + \kappa g + I_{\mathcal{U}_{\rm ad}}\big)(\overline{\mathbf{u}}).$$

At this point, we anticipate that we shall see in the next section that $\partial g(\mathbf{u}) \subset L^2(Q)^2$ for all of our choices of g. Therefore, we may infer from the well-known rules for subdifferentials of convex functionals that

$$\mathbf{0} \in \{D\mathcal{J}_1(\overline{\mathbf{u}})\} + \kappa \partial g(\overline{\mathbf{u}}) + \partial I_{\mathcal{U}_{\rm ad}}(\overline{\mathbf{u}}).$$

In other words, there are $\overline{\boldsymbol{\lambda}} \in \partial g(\overline{\mathbf{u}})$ and $\widehat{\boldsymbol{\lambda}} \in \partial I_{\mathcal{U}_{\rm ad}}(\overline{\mathbf{u}})$ such that

$$\mathbf{0} = D\mathcal{J}_1(\overline{\mathbf{u}}) + \kappa\overline{\boldsymbol{\lambda}} + \widehat{\boldsymbol{\lambda}}. \tag{3.5}$$

But, by the definition of $\partial I_{\mathcal{U}_{\rm ad}}(\overline{\mathbf{u}})$, we have $\widehat{\boldsymbol{\lambda}}(\mathbf{u} - \overline{\mathbf{u}}) \leq 0$ for every $\mathbf{u} \in \mathcal{U}_{\rm ad}$. Hence, thanks to (3.5),

$$0 \leq D\mathcal{J}(\overline{\mathbf{u}})(\mathbf{u} - \overline{\mathbf{u}}) + \kappa\overline{\boldsymbol{\lambda}}(\mathbf{u} - \overline{\mathbf{u}}) \quad \forall\, \mathbf{u} \in \mathcal{U}_{\rm ad}.$$

We have thus shown the following result (where we identify $\overline{\boldsymbol{\lambda}}$ with the corresponding element of $L^2(Q)^2$ according to the Riesz isomorphism).

Lemma 3.1. *If $\overline{\mathbf{u}} \in \mathcal{U}_{\rm ad}$ is a locally optimal control for $(\mathcal{CP})$, then there is some $\overline{\boldsymbol{\lambda}} \in \partial g(\mathbf{u}) \subset L^2(Q)^2$ such that*

$$D\mathcal{J}_1(\overline{\mathbf{u}})(\mathbf{u} - \overline{\mathbf{u}}) + \kappa \int_Q \overline{\boldsymbol{\lambda}}(x,t) \cdot (\mathbf{u}(x,t) - \overline{\mathbf{u}}(x,t))\, dx\, dt \geq 0 \quad \forall\, \mathbf{u} \in \mathcal{U}_{\rm ad}. \tag{3.6}$$

Remark 3.2. The idea for the proof of the above lemma goes back to [15] and to the papers [3, 4], where it has been worked out for control problems with semilinear reaction-diffusion equations. The concrete form of ∂g depends on the particular choice of g and will be presented below.

Next, we aim to simplify the expression $D\mathcal{J}_1(\overline{\mathbf{u}})(\mathbf{u}-\overline{\mathbf{u}})$ in (3.6) by introducing an adjoint state. To this end, we consider the following adjoint system:

$$-\alpha\partial_t\psi_1 - \Delta\psi_1 \,=\, \psi_2 \quad \text{in } Q, \tag{3.7}$$

$$\begin{aligned}-\partial_t(\psi_1+\beta\psi_2) - \Delta(\psi_2 - \chi\psi_3) \,=\, &\beta_1(\overline{\varphi}-\varphi_Q) + (P\overline{\sigma} - A - \overline{u}_1)h'(\overline{\varphi})\psi_1 \\ &- F''(\overline{\varphi})\psi_2 - E\overline{\sigma}h'(\overline{\varphi})\psi_3 \quad \text{in } Q,\end{aligned} \tag{3.8}$$

$$-\partial_t\psi_3 - \Delta\psi_3 \,=\, Ph(\overline{\varphi})\psi_1 + \chi\psi_2 - B\psi_3 - Eh(\overline{\varphi})\psi_3 \quad \text{in } Q, \tag{3.9}$$

$$\partial_n\psi_1 = \partial_n\psi_2 = \partial_n\psi_3 = 0 \quad \text{on } \Sigma, \tag{3.10}$$

$$\psi_1(T) = \psi_3(T) = 0, \quad \beta\psi_2(T) = \beta_2(\overline{\varphi}(T) - \varphi_\Omega), \quad \text{in } \Omega. \tag{3.11}$$

According to [10, Thm. 2.8], the adjoint system (3.7)–(3.11) has under the general assumptions **(F1)**–**(F4)** and **(A1)**–**(A6)** a unique weak solution $\boldsymbol{\psi} = (\psi_1, \psi_2, \psi_3)$ with the regularity

$$\psi_1 \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W_0), \tag{3.12}$$

$$\psi_2, \psi_3 \in H^1(0,T;V^*) \cap C^0([0,T];H) \cap L^2(0,T;V). \tag{3.13}$$

We have the following result.

Theorem 3.3. (Necessary optimality condition) *Suppose that* **(F1)**–**(F4)** *and* **(A1)**–**(A6)** *are fulfilled, and let* $\overline{\mathbf{u}} \in \mathcal{U}_{\rm ad}$ *be a locally optimal control of* $(\mathcal{CP})$ *with associated state* $(\overline{\mu}, \overline{\varphi}, \overline{\sigma}) = \mathcal{S}(\overline{\mathbf{u}})$ *and adjoint state* $\overline{\boldsymbol{\psi}} = (\overline{\psi}_1, \overline{\psi}_2, \overline{\psi}_3)$. *Then, there exists some* $\overline{\boldsymbol{\lambda}} = (\lambda_1, \lambda_2)^\top \in \partial g(\overline{\mathbf{u}})$ *such that*

$$\int_Q \big(\overline{\mathbf{d}}(x,t) + \kappa\overline{\boldsymbol{\lambda}}(x,t) + \nu\overline{\mathbf{u}}(x,t)\big)\cdot(\mathbf{u}(x,t) - \overline{\mathbf{u}}(x,t))\,dxdt \ge 0 \quad \forall \mathbf{u} \in \mathcal{U}_{\rm ad}, \tag{3.14}$$

where $\overline{\mathbf{d}} \in L^2(Q)^2$ *is defined by*

$$\overline{\mathbf{d}}(x,t) = \begin{pmatrix} -\overline{\psi}_1(x,t)h(\overline{\varphi}(x,t)) \\ \overline{\psi}_3(x,t) \end{pmatrix} \quad \textit{for a.e. } (x,t) \in Q.$$

Proof. Using the adjoint state $\overline{\boldsymbol{\psi}}$, we obtain the representation

$$D\mathcal{J}_1(\overline{\mathbf{u}})(\mathbf{u}-\overline{\mathbf{u}}) = \int_Q \big(\overline{\mathbf{d}} + \nu\overline{\mathbf{u}}\big)\cdot(\mathbf{u}-\overline{\mathbf{u}})\,dx\,dt.$$

This follows from the proof of [10, Thm. 2.9], where the notation $\boldsymbol{\psi} = (p,q,r)$ and $\mathbf{u} = (u,w)$ is used. The claim is now an immediate consequence of (3.6). ☐

4 Sparsity of optimal controls

The convex function g in the objective functional accounts for the sparsity of optimal controls, i.e., the optimal control can vanish in some region of the space-time cylinder Q. The form of this region depends on the particular choice of the functional g, while its size depends on the sparsity parameter κ. These sparsity properties can be deduced from the variational inequality (3.14) and the particular form of the subdifferential ∂g.

Therefore, we first provide known results on the subdifferential and apply them to the analysis of an auxiliary variational inequality.

4.1 Preliminaries

Let us begin with the subdifferential of the L^2-norm,

$$\gamma(v) = \|v\|_{L^2(\Omega)} = \left(\int_\Omega |v(x)|^2\,dx\right)^{1/2},$$

which is given by (see, e.g., [18])

$$\partial\gamma(v) = \begin{cases} \{z \in L^2(\Omega) : \|z\|_L^2(\Omega) \le 1\} & \text{if } v = 0 \\ v/\|v\|_{L^2(\Omega)} & \text{if } v \neq 0 \end{cases} \tag{4.1}$$

In order to have directional sparsity with respect to time, we use the functional

$$\begin{aligned} &g_T : L^1(0,T;L^2(\Omega)) \to \mathbb{R}, \\ &g_T(u) = \int_0^T \left(\int_\Omega |u(x,t)|^2\,dx\right)^{1/2} dt = \int_0^T \gamma(u(t))\,dt. \end{aligned} \tag{4.2}$$

The associated subdifferential is given by (cf., [17])

$$\partial g_T(u) = \{\lambda \in L^\infty(0,T;L^2(\Omega)) : \lambda(\cdot,t) \in \partial\gamma(u(\cdot,t)) \text{ for a.a. } t \in (0,T)\},$$

that is,

$$\partial g_T(u) = \left\{\lambda \in L^\infty(0,T;L^2(\Omega)) : \begin{cases} \|\lambda(\cdot,t)\|_{L^2(\Omega)} \le 1 & \text{if } u(\cdot,t) = 0 \\ \lambda(\cdot,t) \ = u(\cdot,t)/\|u(\cdot,t)\|_{L^2(\Omega)} & \text{if } u(\cdot,t) \neq 0 \end{cases}\right\}, \tag{4.3}$$

where the properties above are satisfied for a.a. $t \in (0,T)$.

Directional sparsity with respect to space is obtained from the functional

$$\begin{aligned} &g_\Omega : L^1(\Omega;L^2(0,T)) \to \mathbb{R}, \\ &g_\Omega(u) = \int_\Omega \left(\int_0^T |u(x,t)|^2\,dt\right)^{1/2} dx = \int_\Omega \|u(x,\cdot)\|_{L^2(0,T)}\,dx\,. \end{aligned} \tag{4.4}$$

Interchanging the roles of t and x, we get

$$\partial g_\Omega(u) = \left\{\lambda \in L^\infty(\Omega;L^2(0,T)) : \begin{cases} \|\lambda(x,\cdot)\|_{L^2(0,T)} \le 1 & \text{if } u(x,\cdot) = 0 \\ \lambda(x,\cdot) = u(x,\cdot)/\|u(x,\cdot)\|_{L^2(0,T)} & \text{if } u(x,\cdot) \neq 0 \end{cases}\right\} \tag{4.5}$$

where the properties above have to be fulfilled for a.a. $x \in \Omega$.

In the case of full sparsity, i.e., for

$$g_Q : L^1(Q) \to \mathbb{R}, \quad g_Q(u) = \int_Q |u(x,t)|\,dx\,dt, \tag{4.6}$$

the subdifferential is classical. We have (see [18])

$$\partial g_Q(u) = \left\{\lambda \in L^\infty(Q) : \ \lambda(x,t) \in \begin{cases} \{1\} & \text{if } u(x,t) > 0 \\ [-1,1] & \text{if } u(x,t) = 0 \\ \{-1\} & \text{if } u(x,t) < 0 \end{cases} \text{ for a.e. } (x,t) \in Q\right\}. \tag{4.7}$$

Here, we will concentrate on directional sparsity in time, since this seems to be the most important sparsity for medical applications. In this case, if an application to medication is considered, directional sparsity will allow to stop the administration of drugs in certain intervals of time. To this end, we now discuss the following auxiliary variational inequality:

$$\int_Q (d(x,t) + \kappa\lambda(x,t) + \nu u(x,t))(v(x,t) - u(x,t))\,dx\,dt \ge 0 \quad \forall\, v \in C, \tag{4.8}$$

where $\lambda \in \partial g_T(u)$ and

$$C = \{v \in L^\infty(Q) : \underline{u} \le v(x,t) \le \widehat{u} \text{ a.e. in } Q\} \tag{4.9}$$

with given real numbers $\underline{u} < 0 < \widehat{u}$, $\kappa > 0$, $\nu > 0$, and a given function $d \in L^2(Q)$. Obviously, (4.8) just means that u is the $L^2(Q)-$orthogonal projection of $-\frac{1}{\nu}(d+\kappa\lambda)$ onto the closed and convex subset C of $L^2(Q)$, which is well known to be given by the formula

$$u(x,t) = \mathbb{P}_{[\underline{u},\widehat{u}]}(-\nu^{-1}(d(x,t) + \kappa\lambda(x,t))) \quad \text{for a.e. } (x,t) \in Q, \tag{4.10}$$

where we denote by $\mathbb{P}_{[\underline{u},\widehat{u}]} : \mathbb{R} \to [\underline{u},\widehat{u}]$ the pointwise projection function

$$\mathbb{P}_{[\underline{u},\widehat{u}]}(s) = \min\{\widehat{u}, \max\{\underline{u}, s\}\}. \tag{4.11}$$

Moreover, it is well known that the following pointwise relations hold true for almost all $(x,t) \in Q$:

$$\begin{aligned} d(x,t) + \kappa\lambda(x,t) + \nu u(x,t) > 0 \quad &\Longrightarrow \quad u(x,t) = \underline{u} \\ d(x,t) + \kappa\lambda(x,t) + \nu u(x,t) < 0 \quad &\Longrightarrow \quad u(x,t) = \widehat{u}. \end{aligned} \tag{4.12}$$

The next result is already known from [2,17]. Nevertheless, we present a proof for the readers' convenience.

Lemma 4.1. (Sparsity) *Let $u \in C$ be a solution to the variational inequality* (4.8)*. Then, for a.e. $t \in (0,T)$,*

$$u(\cdot,t) = 0 \quad \Longleftrightarrow \quad \|d(\cdot,t)\|_{L^2(\Omega)} \le \kappa, \tag{4.13}$$

as well as

$$\lambda(\cdot,t) \begin{cases} \in B(0,1) & \text{if } \|u(\cdot,t)\|_{L^2(\Omega)} = 0 \\ = \dfrac{u(\cdot,t)}{\|u(\cdot,t)\|_{L^2(\Omega)}} & \text{if } \|u(\cdot,t)\|_{L^2(\Omega)} \ne 0 \end{cases}, \tag{4.14}$$

where $B(0,1) = \{v \in L^2(\Omega) : \|v\|_{L^2(\Omega)} \le 1\}$.

Proof. (i) We first show that, for a.e. $t \in (0,T)$, the condition $\|u(\cdot,t)\|_{L^2(\Omega)} = 0$ implies that $\|d(\cdot,t)\|_{L^2(\Omega)} \le \kappa$. So consider the set $E = \{t \in (0,T) : \|u(\cdot,t)\|_{L^2(\Omega)} = 0\}$. Then (4.12) yields that

$$d(\cdot,t) + \kappa\lambda(\cdot,t) + 0 = 0,$$

for a.e. $t \in E$, since otherwise the set of points $x \in \Omega$, where $u(x,t) = \underline{u}$ or $u(x,t) = \widehat{u}$, would have positive measure, which contradicts the assumption that $\|u(\cdot,t)\|_{L^2(\Omega)} = 0$.

From the equation above, we deduce that $d(\cdot,t) = -\kappa\lambda(\cdot,t)$, and thus

$$\|d(\cdot,t)\|_{L^2(\Omega)} = \kappa\|\lambda(\cdot,t)\|_{L^2(\Omega)} \le \kappa,$$

thanks to the form of $\partial g_T(u)$.

(ii) Next, we confirm that the reverse implication

$$\|d(\cdot,t)\|_{L^2(\Omega)} \le \kappa \implies \|u(\cdot,t)\|_{L^2(\Omega)} = 0$$

holds true for almost every $t \in (0,T)$. To this end, let

$$E = \{t \in (0,T) : \ \|d(\cdot,t)\|_{L^2(\Omega)} \le \kappa \ \text{and} \ \|u(\cdot,t)\|_{L^2(\Omega)} \ne 0\}.$$

We have to show that the Lebesgue measure $|E|$ of E is zero. We denote by $\Omega_+(t)$ and $\Omega_-(t)$ the sets of points $x \in \Omega$ where $u(x,t) > 0$ and $u(x,t) < 0$, respectively. Now recall that the implications (4.12) must be satisfied. Since, by assumption, $\underline{u} < 0 < \widehat{u}$, we readily deduce that

$$\begin{aligned} d(x,t) + \kappa\lambda(x,t) + \nu u(x,t) \le 0 \quad &\text{for a.e. } x \in \Omega_+(t), \\ d(x,t) + \kappa\lambda(x,t) + \nu u(x,t) \ge 0 \quad &\text{for a.e. } x \in \Omega_-(t). \end{aligned} \tag{4.15}$$

In E, we have $\|u(\cdot,t)\|_{L^2(\Omega)} \ne 0$, and therefore, by (4.1), $\lambda(\cdot,t) = u(\cdot,t)/\|u(\cdot,t)\|_{L^2(\Omega)}$. Now the upper inequality in (4.15) implies that

$$d(x,t) \le -\kappa \frac{u(x,t)}{\|u(\cdot,t)\|_{L^2(\Omega)}} - \nu u(x,t) \quad \text{for a.e. } x \in \Omega_+(t).$$

Since both summands on the right-hand side are negative, we have

$$|d(x,t)| > \kappa \frac{u(x,t)}{\|u(\cdot,t)\|_{L^2(\Omega)}} \quad \text{for a.e. } x \in \Omega_+(t).$$

In the same way, we deduce from the lower inequality in (4.15) that

$$d(x,t) \ge -\kappa \frac{u(x,t)}{\|u(\cdot,t)\|_{L^2(\Omega)}} - \nu u(x,t) \quad \text{for a.e. } x \in \Omega_-(t),$$

where both summands on the right-hand side are positive. This, in turn, yields that

$$|d(x,t)| > \kappa \frac{|u(x,t)|}{\|u(\cdot,t)\|_{L^2(\Omega)}} \quad \text{for a.e. } x \in \Omega_-(t).$$

Since $u(\cdot,t)$ vanishes on $\Omega \setminus (\Omega_+(t) \cup \Omega_-(t))$, we thus can infer that

$$\begin{aligned} \|d(\cdot,t)\|_{L^2(\Omega)} &\ge \left(\int_{\Omega_+(t)\cup\Omega_-(t)} |d(x,t)|^2 \, dx \right)^{\frac{1}{2}} > \kappa \left(\int_{\Omega_+(t)\cup\Omega_-(t)} \frac{|u(x,t)|^2}{\|u(\cdot,t)\|^2_{L^2(\Omega)}} \, dx \right)^{\frac{1}{2}} \\ &= \kappa \left(\int_\Omega \frac{|u(x,t)|^2}{\|u(\cdot,t)\|^2_{L^2(\Omega)}} \, dx \right)^{\frac{1}{2}} = \kappa. \end{aligned}$$

The last inequality contradicts the assumption that $\|d(\cdot,t)\|_{L^2(\Omega)} \le \kappa$ in E unless $|\Omega_+(t) \cup \Omega_-(t)| = 0$ for almost every $t \in E$. This proves that $\|u(\cdot,t)\|_{L^2(\Omega)} = 0$ almost everywhere in E. With (i) and (ii) proved, the equivalence relation (4.13) is shown.

The representation (4.14) for λ follows immediately from the formula for the subdifferential of g_T. □

4.2 Directional sparsity in time for the optimal control problem

The results of the last subsection will now be applied to derive sparsity properties of optimal controls from the variational inequality (3.14). For directional sparsity in time, we use the convex continuous functional

$$g(\mathbf{u}) = g(u_1, u_2) := g_T(u_1) + g_T(u_2) = g_T(I_1\mathbf{u}) + g_T(I_2\mathbf{u}), \tag{4.16}$$

where I_i denotes the linear and continuous projection mapping $I_i : \mathbf{u} = (u_1, u_2) \mapsto u_i$, $i = 1, 2$, from $L^1(0, T; L^2(\Omega))^2$ to $L^1(0, T; L^2(\Omega))$.

Since the convex functional g_T is continuous on the whole space $L^1(0, T; L^2(\Omega))$, we obtain from the sum and chain rules for subdifferentials (see, e.g., [18, Sect. 4.2.2, Thm. 1 and Thm.2]) that

$$\partial g(\mathbf{u}) = I_1^* \, \partial g_T(I_1\mathbf{u}) + I_2^* \, \partial g_T(I_2\mathbf{u}) = (I, 0)^\top \partial g_T(u_1) + (0, I)^\top \partial g_T(u_2),$$

with the identical mapping $I \in \mathcal{L}(L^1(0, T; L^2(\Omega)))$. Therefore, we have

$$\partial g(\mathbf{u}) = \{(\lambda_1, \lambda_2) \in L^\infty(0, T; L^2(\Omega))^2 : \lambda_i \in \partial g_T(u_i),\ i = 1, 2\}.$$

The variational inequality (3.14) is equivalent to two independent variational inequalities for $\overline{u}_1$ and $\overline{u}_2$ that have to hold jointly, namely,

$$\int_Q \big(-\overline{\psi}_1 h(\overline{\varphi}) + \kappa\overline{\lambda}_1 + \nu\, \overline{u}_1\big)\, (u - \overline{u}_1)\, dx\, dt \ \geq\ 0 \quad \forall\, u \in C_1, \tag{4.17}$$

$$\int_Q \big(\overline{\psi}_3 + \kappa\overline{\lambda}_2 + \nu\, \overline{u}_2\big)\, (u - \overline{u}_2)\, dx\, dt \ \geq\ 0 \quad \forall\, u \in C_2, \tag{4.18}$$

where the sets C_i, $i = 1, 2$, are defined by

$$C_i = \{u \in L^\infty(Q) : \underline{u}_i(x, t) \leq u(x, t) \leq \widehat{u}_i(x, t) \text{ for a.a. } (x, t) \in Q\},$$

and where $\overline{\lambda}_i$, $i = 1, 2$, obey for almost every $t \in (0, T)$ the conditions

$$\overline{\lambda}_i(\cdot, t) \begin{cases} \in B(0, 1) & \text{if } \|\overline{u}_i(\cdot, t)\|_{L^2(\Omega)} = 0 \\ = \dfrac{\overline{u}_i(\cdot, t)}{\|\overline{u}_i(\cdot, t)\|_{L^2(\Omega)}} & \text{if } \|\overline{u}_i(\cdot, t)\|_{L^2(\Omega)} \neq 0 \end{cases}. \tag{4.19}$$

Applying Lemma 4.1 to each of the variational inequalities (4.17) and (4.18) separately, we arrive at the following result:

Theorem 4.2. (Directional sparsity in time) *Suppose that the general assumptions* **(F1)–(F4)** *and* **(A1)–(A6)** *are fulfilled, and assume in addition that* $\underline{u}_i, \widehat{u}_i$ *are constants satisfying* $\underline{u}_i < 0 < \widehat{u}_i$, *for* $i = 1, 2$. *Let* $\overline{\mathbf{u}} = (\overline{u}_1, \overline{u}_2)$ *be an optimal control of the problem* $(\mathcal{CP})$ *with sparsity functional* g *defined in* (4.16)*, and with associated state* $(\overline{\mu}, \overline{\varphi}, \overline{\sigma}) = \mathcal{S}(\overline{\mathbf{u}})$ *solving* (1.2)–(1.6) *and adjoint state* $\overline{\boldsymbol{\psi}} = (\overline{\psi}_1, \overline{\psi}_2, \overline{\psi}_3)$ *solving* (3.7)–(3.11)*. Then, there are functions* $\overline{\lambda}_i$, $i = 1, 2$, *that satisfy* (4.19) *and* (4.17)–(4.18)*. In addition, for almost every* $t \in (0, T)$*, we have that*

$$\|\overline{u}_1(\cdot, t)\|_{L^2(\Omega)} = 0 \quad \iff \quad \|\overline{\psi}_1(\cdot, t) h(\overline{\varphi}(\cdot, t))\|_{L^2(\Omega)} \leq \kappa, \tag{4.20}$$

$$\|\overline{u}_2(\cdot, t)\|_{L^2(\Omega)} = 0 \quad \iff \quad \|\overline{\psi}_3(\cdot, t)\|_{L^2(\Omega)} \leq \kappa. \tag{4.21}$$

Moreover, if $\overline{\psi}$ *and* $\overline{\lambda}_1, \overline{\lambda}_2$ *are given, then the optimal controls* $\overline{u}_1$, $\overline{u}_2$ *are obtained from the projection formulas*

$$\begin{aligned}
\overline{u}_1(x,t) &= \mathbb{P}_{[\underline{u}_1(x,t),\widehat{u}_1(x,t)]}\left(-\nu^{-1}\left(-\overline{\psi}_1(x,t)h(\overline{\varphi}(x,t)) + \kappa\overline{\lambda}_1(x,t)\right)\right), \\
\overline{u}_2(x,t) &= \mathbb{P}_{[\underline{u}_2(x,t),\widehat{u}_2(x,t)]}\left(-\nu^{-1}\left(\overline{\psi}_3(x,t) + \kappa\overline{\lambda}_2(x,t)\right)\right), \quad \textit{for a.e. } (x,t) \in Q.
\end{aligned}$$

Remark 4.3. In the medical context, where the controls u_1, u_2 have the meaning of medications or of nutrients supplied to the patients, it does not seem to be meaningful to allow for negative controls, unfortunately.

It is to be expected that the support of optimal controls will shrink with increasing sparsity parameter κ. Although this can hardly be quantified or proved, it is useful to confirm that optimal controls vanish for all sufficiently large values of κ. We are going to derive a corresponding result now.

For this purpose, let us indicate for a while the dependence of optimal controls, optimal states, and the associated adjoint states, on κ by an index κ. An inspection of the conditions (4.20) and/or (4.21) reveals that $\overline{u}_{1,\kappa} = 0$ holds true for all $\kappa > \kappa_1$, if

$$\kappa_1 := \sup_{\kappa>0} \sup_{t\in(0,T)} \|\overline{\psi}_{1,\kappa}(\cdot,t)h(\overline{\varphi}_\kappa(\cdot,t))\|_{L^2(\Omega)} < \infty, \tag{4.22}$$

and $\overline{u}_{2,\kappa} = 0$ holds true for all $\kappa > \kappa_2$, if

$$\kappa_2 = \sup_{\kappa>0} \sup_{t\in(0,T)} \|\overline{\psi}_{3,\kappa}(\cdot,t)\|_{L^2(\Omega)} < \infty. \tag{4.23}$$

These boundedness conditions hold simultaneously for $\kappa > \kappa_0 = \max\{\kappa_1, \kappa_2\}$. The existence of such a constant κ_0 will be confirmed next. In order to avoid an overloaded notation, we omit the index κ in the following.

First, we derive bounds for the adjoint state variables $\overline{\psi}_1, \overline{\psi}_3$ (the function $h(\overline{\varphi})$ is globally bounded by **(A2)**). To this end, recall the global estimates (2.6)–(2.8) from Theorem 2.1, which have to be satisfied by all possible states (μ, φ, σ) corresponding to controls $\mathbf{u} \in \mathcal{U}_{\rm ad}$. It follows that also the "right-hand sides" $\beta_1(\overline{\varphi} - \varphi_Q)$ and $\beta_2(\overline{\varphi}(T) - \varphi_\Omega)$ are uniformly bounded, independently of κ. It remains to show that this implies the boundedness of all possible adjoint states.

To this end, recall that by virtue of (3.12), (3.13) we know that $\overline{\psi}_1 \in C^0([0,T];V)$ and $\overline{\psi}_3 \in C^0([0,T];H)$. Now indeed, a closer look at the proof of [10, Thm. 2.8] reveals that the bounds derived there are in fact uniform with respect to the choice of $\mathbf{u} \in \mathcal{U}_{\rm ad}$. Therefore, there is some $\kappa_0 > 0$ such that $\overline{\mathbf{u}}_\kappa = \mathbf{0}$ for every $\kappa \geq \kappa_0$. For the reader's convenience, we now give some insight how such bounds can be derived.

In the following, we argue formally, noting that in a rigorous proof the following arguments would have to be carried out on a Faedo–Galerkin system approximating the weak form of the adjoint system (3.7)–(3.11) satisfied by the adjoint variables $(\psi_1, \psi_2, \psi_3) = (\overline{\psi}_1, \overline{\psi}_2, \overline{\psi}_3)$. The arguments are similar to those in the proof of Lemma 2.4.

Indeed, we (formally) multiply (3.7) by $-\beta\partial_t\overline{\psi}_1$, (3.8) by $\overline{\psi}_2$, and (3.9) by $\delta\overline{\psi}_3$, where $\delta > 0$ is yet to be specified. Then we add the three resulting equations, whence a cancellation of two terms occurs, and integrate the result over $Q^t := \Omega \times (t,T)$, where $t \in [0,T)$. Using formal integration by parts and the endpoint conditions, we then obtain the identity

$$\begin{aligned}
&\alpha\beta \int_{Q^t} |\partial_t \overline{\psi}_1|^2 + \frac{\beta}{2}\|\nabla\overline{\psi}_1(t)\|_2^2 + \frac{\beta}{2}\|\overline{\psi}_2(t)\|_2^2 + \frac{\delta}{2}\|\overline{\psi}_3(t)\|_2^2 \\
&\quad + \int_{Q^t} \big(|\nabla\overline{\psi}_2|^2 + \delta|\nabla\overline{\psi}_3|^2\big) + \int_{Q^t} F_1''(\overline{\varphi})|\overline{\psi}_2|^2 \\
&= \frac{\beta_2^2}{2\beta}\int_\Omega |\overline{\varphi}(T)-\varphi_\Omega|^2 + \chi\int_{Q^t} \nabla\overline{\psi}_2\cdot\nabla\overline{\psi}_3 + \beta_1\int_{Q^t}(\overline{\varphi}-\varphi_Q)\overline{\psi}_2 - \int_{Q^t} F_2''(\overline{\varphi})|\overline{\psi}_2|^2 \\
&\quad + \int_{Q^t}(P\overline{\sigma}-A-\overline{u}_1)h'(\overline{\varphi})\overline{\psi}_1\overline{\psi}_3 - \int_{Q^t} E\overline{\sigma}h'(\overline{\varphi})\overline{\psi}_2\overline{\psi}_3 - \delta\int_{Q^t}(Eh(\overline{\varphi})+B)|\overline{\psi}_3|^2 \\
&\quad + \delta\int_{Q^t}(Ph(\overline{\varphi})\overline{\psi}_1 + \chi\overline{\psi}_2)\overline{\psi}_3. \qquad (4.24)
\end{aligned}$$

Since $F_1'' \geq 0$, all of the terms on the left-hand side are nonnegative. Moreover, Young's inequality implies that

$$\chi\int_{Q^t}\nabla\overline{\psi}_2\cdot\nabla\overline{\psi}_3 \le \frac{1}{2}\int_{Q^t}|\nabla\overline{\psi}_2|^2 + \frac{\chi^2}{2}\int_{Q^t}|\nabla\overline{\psi}_3|^2.$$

Hence, invoking the known bounds for the state variables, and applying Young's inequality appropriately to the terms on the right-hand side, we obtain from (4.24) the estimate

$$\begin{aligned}
&\alpha\beta \int_{Q^t} |\partial_t \overline{\psi}_1|^2 + \frac{\beta}{2}\|\nabla\overline{\psi}_1(t)\|_2^2 + \frac{\beta}{2}\|\overline{\psi}_2(t)\|_2^2 + \frac{\delta}{2}\|\overline{\psi}_3(t)\|_2^2 \\
&\quad + \frac{1}{2}\int_{Q^t}|\nabla\overline{\psi}_2|^2 + \big(\delta - \tfrac{1}{2}\chi^2\big)\int_{Q^t}|\nabla\overline{\psi}_3|^2 \\
&\le C_1 + C_2(1+\delta)\int_{Q^t}\big(|\overline{\psi}_1|^2 + |\overline{\psi}_2|^2 + |\overline{\psi}_3|^2\big), \qquad (4.25)
\end{aligned}$$

with constants C_1, C_2 that depend neither on $\mathcal{U}_{\rm ad}$ nor on κ.

Next observe that $\overline{\psi}_1(T)=0$ and thus $\frac{1}{2}\|\overline{\psi}_1(t)\|_2^2 = -\int_t^T(\partial_t\overline{\psi}_1(s),\overline{\psi}_1(s))\,ds$. Hence, owing to Young's inequality,

$$\frac{1}{2}\|\overline{\psi}_1(t)\|_2^2 \le \frac{\alpha\beta}{2}\int_{Q^t}|\partial_t\overline{\psi}_1|^2 + \frac{1}{2\alpha\beta}\int_{Q^t}|\overline{\psi}_1|^2. \qquad (4.26)$$

Now we add (4.25) and (4.26) and choose $\delta = \chi^2$. Using Gronwall's lemma backward in time, it then easily follows that, in particular,

$$\|\overline{\psi}_1\|_{L^\infty(0,T;V)} + \|\overline{\psi}_3\|_{L^\infty(0,T;H)} \le C_3,$$

where $C_3 > 0$ is independent of both $\mathcal{U}_{\rm ad}$ and κ. Then,

$$\|\overline{\psi}_1 h(\overline{\varphi})\|_{L^\infty(0,T;H)} + \|\overline{\psi}_3\|_{L^\infty(0,T;H)} \le \big(1+\|h\|_{L^\infty(\mathbb{R})}\big)\,C_3 =: \kappa_0.$$

The asserted existence of the constant κ_0 is thus shown.

4.3 Spatial directional sparsity and full sparsity

Let us briefly sketch the other types of sparsity that are obtained from the choices $g = g_\Omega$ and $g = g_Q$, respectively.

With the functional g_Ω, we obtain regions in Ω where the optimal controls are zero for a.e. $t \in (0,T)$. The theory is analogous to that of directional sparsity in time: indeed, it is obtained by simply interchanging the roles of t and x. For instance, instead of the equivalences (4.20), (4.21), one obtains for a.e. $x \in \Omega$ that

$$\begin{aligned} \|\overline{u}_1(x,\cdot)\|_{L^2(0,T)} = 0 \quad &\Longleftrightarrow \quad \|\overline{\psi}_1(x,\cdot)h(\overline{\varphi}(x,\cdot))\|_{L^2(0,T)} \le \kappa, \\ \|\overline{u}_2(x,\cdot)\|_{L^2(0,T)} = 0 \quad &\Longleftrightarrow \quad \|\overline{\psi}_3(x,\cdot)\|_{L^2(0,T)} \le \kappa. \end{aligned}$$

For the choice $g = g_Q$, the equivalence relations

$$\begin{aligned} \overline{u}_1(x,t) = 0 \quad &\Longleftrightarrow \quad |\overline{\psi}_1(x,t)h(\overline{\varphi}(x,t))| \le \kappa, \\ \overline{u}_2(x,t) = 0 \quad &\Longleftrightarrow \quad |\overline{\psi}_3(x,t)| \le \kappa, \end{aligned}$$

can be deduced for almost every $(x,t) \in Q$. We refer to the discussion of the variational inequality (4.8) in [3]. Therefore, the optimal controls vanish in certain spatio-temporal subsets of Q.

Moreover, in this case a usually unexpected property of the function $\overline{\boldsymbol{\lambda}} \in g(\overline{\mathbf{u}})$ is obtained: $\overline{\boldsymbol{\lambda}}$ is unique, that is, for an optimal control, the subdifferential is a singleton; we again refer to [3]. This fact can easily be explained. Consider, e.g., the function $\overline{\lambda}_2 \in \partial g_Q(\overline{u}_2)$:

Thanks to (4.7), it holds that

$$\overline{\lambda}_2(x,t) = \begin{cases} 1 & \text{if} \quad \overline{u}_2(x,t) > 0 \\ -1 & \text{if} \quad \overline{u}_2(x,t) < 0 \end{cases}$$

Therefore, the only points, at which $\overline{\lambda}_2(x,t)$ might not be uniquely determined, are those where $\overline{u}_2(x,t)$ vanishes. At these points, however, $\overline{u}_2(x,t) = 0$ is away from the thresholds, and hence the reduced gradient must be zero, i.e.,

$$0 = \overline{\psi}_3(x,t) + \kappa\overline{\lambda}_2(x,t) + \nu \cdot 0.$$

This implies that $\overline{\lambda}_2(x,t) = -\kappa^{-1}\overline{\psi}_3(x,t)$ at these points. With a little more effort, finally the projection formula

$$\overline{\lambda}_2(x,t) = \mathbb{P}_{[-1,1]}\left(-\frac{1}{\kappa}\overline{\psi}_3(x,t)\right)$$

results. By similar reasoning, the identity

$$\overline{\lambda}_1(x,t) = \mathbb{P}_{[-1,1]}\left(\frac{1}{\kappa}\overline{\psi}_1(x,t)h(\overline{\varphi}(x,t))\right)$$

can be derived.

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