Analysis of a space-time phase-field fracture complementarity model and its optimal control formulation

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Abstract

The purpose of this work is the formulation of optimality conditions for phase-field optimal control problems. The forward problem is first stated as an abstract nonlinear optimization problem, and then the necessary optimality conditions are derived. The sufficient optimality conditions are also examined. The choice of suitable function spaces to ensure the regularity of the nonlinear optimization problem is a true challenge here. Afterwards the optimal control problem with a tracking type cost functional is formulated. The constraints are given by the previously derived first order optimality conditions of the forward problem. Herein regularity is proven under certain conditions and first order optimality conditions are formulated.

Keywords: phase-field fracture propagation; optimal control; necessary optimality conditions; complementarity system

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1 Introduction

Variational phase-field methods for the modeling of fracture propagation are an important research area in applied mathematics and engineering. First works establishing phase-field methods for fracture propagation from a mathematical and mechanical point of view are [3, 2, 6, 34, 25]. There are numerous additional references cited in the overview articles and monographs [4, 5, 1, 51, 50, 11, 10] as well. The large majority of studies is concerned with forward modeling of phase-field fracture with applications in numerous fields. Since the year 2017, optimization with phase-field fracture as forward problem is being investigated within optimal control [19, 39, 40, 41, 21, 18, 22] as well as topology optimization [9] and stochastic phase-field fracture settings [15].

Phase-field fracture forward problems can be classified as coupled variational inequality systems (CVIS) [50] in which vector-valued displacements couple with a smoothed indicator phase-field function. In situations where fracture healing is not allowed, as in our work and most often the case in the literature, the phase-field function is subject to an inequality constraint in time. Various approaches have been employed to represent the inequality constraint, such as imposing Dirichlet values in the fracture zone [3, 2], strain history function [33], simple penalization [38, 14], augmented Lagrangian formulations [48], a closely related inexact augmented Lagrangian method [49], primal-dual active set methods [20], interior-point methods [47], recursive multilevel trust region methods in which the corrections satisfy the irreversibility condition [24], truncated nonsmooth Newton multigrid methods in which the variational structure handles the irreversibility constraint pointwise [16], and complementarity formulations [30]. In this work, the latter is of interest for which we notice that [30] formally introduced and implemented a complementarity condition, but without rigorous mathematical analysis and still in time-incremental form, thus not within a space-time setting. In this respect, we notice that the first space-time phase-field fracture formulation (with penalization of the irreversibility constraint) as forward problem and within optimal control was proposed in [21].

The main objective of this work is the rigorous investigation of optimality conditions in terms of KKT (Karush-Kuhn-Tucker) systems for phase-field fracture forward and optimal control problems in a continuous space-time setting. In optimal control, a cost functional is minimized subject to some forward problem that acts as a (physical) constraint. Within this upper level control problem, the fracture is driven by the control, which can act as a boundary condition or a right hand side force [19, 39, 40, 41, 21, 18, 22]. In our case the forward problem constitutes a second (lower level) Nonlinear Optimization Problem (NLP), i.e., a phase-field fracture NLP. The objective of that lower level NLP consists in minimizing the energy of the crack as it was formulated in the pioneering work [12].

The theoretical derivations on optimization in Banach spaces that we employ are based on [32, 31, 53]. Applying these methods to a continuous space-time phase-field fracture model and rigorously deriving the KKT conditions is novel. Further we introduce these KKT conditions as a lower level problem within the upper level optimal control problem and prove its regularity under certain conditions.

Concerning the mathematical analysis, well-posedness with existence and convergence of quasi-static brittle fracture settings was investigated in [13], and in nonlinear elasticity in [7]. In the year 2020, fracture nucleation was revisited as this is heavily used in numerous applications, but less clear from a theoretical viewpoint [26]. Related works governing the analysis of phase-field fracture and damage models are [23, 28, 37, 42, 46]. Phase-field fracture for finite stresses was analysed in [46]. In particular, the convergence of time-discrete solutions to solutions of the time-continuous problem was investigated. The relationships between gradient damage, rate-independent damage and phase-field fracture are discussed in [8, 43] and [28]. For rate-independent damage models, [23] introduced a vanishing viscosity approach. Additionally, [37] emphasized complete (quasi-static) damage in particular, avoiding the use of displacement fields in favour of stress and energy terms. A monograph and a book chapter on rate independent systems and damage models are available in [36, 35], respectively.

In summary, the main novelties in this work are: The rigorous derivation of phase-field fracture as a complementarity system, including the careful selection of suitable function spaces that are required for the regularity of the resulting problems. Design of a space-time formulation of forward phase-field fracture posed as complementarity system involving KKT conditions in Banach spaces rather than a penalized space time-formulation [21, 22]. Here, corresponding cones and regularity results are rigorously investigated, followed by second order necessary conditions and sufficient conditions.

Then, the upper level optimal control NLP with tracking type cost functional and with the phase-field fracture KKT system as a constraint is studied and KKT conditions, regularity properties, and further optimality conditions are rigorously established.

The outline of this paper is as follows: In Section 2, the function spaces and the basic notation are introduced. In addition, the required abstract NLP theory is presented. The phase-field fracture forward model is then introduced, along with its formulation as an abstract NLP, in Section 3. Regular points of that lower level NLP and its KKT system are given specific emphasis. In Section 4, second order optimality conditions for the phase-field NLP are presented. Then in Section 5, the upper level optimal control problem is formulated, where the constraints are given by the previously derived phase-field fracture KKT system. Further, regular points of the optimal control NLP are characterized, and its KKT conditions are derived. Our work is summarized in Section 6.

2 Theory for optimization in Banach spaces

In this section, we introduce our notation, recapitulate known results in the area of functional analysis from the literature, and define function spaces required for space-time phase-field fracture.

2.1 Notation

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitz domain with boundary partitioned as $\partial\Omega = \Gamma_N \cup \Gamma_D \cup \Gamma_F$, where both Γ_D and Γ_N have nonzero one dimensional Hausdorff measure and $\Omega \cup \Gamma_N$ is regular in the sense of Gröger [17]. Next, define Hilbert spaces $Q := L^2(\Gamma_N)$ for the control force q, $V_\varphi := H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ for the phase-field φ, $V_u := H^1_D(\Omega;\mathbb{R}^2)$ for the two dimensional displacement field u, where $H^1_D(\Omega;\mathbb{R}^2) := \{v \in H^1(\Omega;\mathbb{R}^2) \colon v|_{\Gamma_D} = 0\}$, and the product space $V := V_u \times V_\varphi$. Finally consider a compact time interval $I := [0,T]$ and define the spaces

$$Y := Y_u \times Y_\varphi := L^2(I,V_u) \times H^1(I,V_\varphi) \quad \text{and} \quad W := L^2(I,Q). \tag{1}$$

We denote natural scalar products and norms with their space as index, such as $(\,\cdot\,,\,\cdot\,)_{V_u} \equiv (\,\cdot\,,\,\cdot\,)_{H^1_D(\Omega)}$ or $\|\cdot\|_{Y_\varphi} \equiv \|\cdot\|_{H^1(I,H^2(\Omega))}$, and L^2 scalar products and norms with their domain, such as $(\,\cdot\,,\,\cdot\,)_\Omega := (\,\cdot\,,\,\cdot\,)_{L^2(\Omega)}$ or $(\,\cdot\,,\,\cdot\,)_{I\times\Omega} := (\,\cdot\,,\,\cdot\,)_{L^2(I,L^2(\Omega))}$. Consequently the norm on V is given by

$$\|\boldsymbol{u}\|_V^2 = (\boldsymbol{u},\boldsymbol{u})_V = (u,u)_{V_u} + (\varphi,\varphi)_{V_\varphi} = \sum_{|\alpha|\le 1} (D^\alpha u, D^\alpha u)_\Omega + \sum_{|\alpha|\le 2} (D^\alpha \varphi, D^\alpha \varphi)_\Omega.$$

The norm on Y is given by

$$\|\boldsymbol{u}\|_Y^2 = \int_I \big(\|u(t)\|_{V_u}^2 + \|\varphi(t)\|_{V_\varphi}^2 + \|\dot\varphi(t)\|_{V_\varphi}^2\big)\,\mathrm{d}t.$$

Occasionally we will need the norm of a component $\varphi \in H^1(I,V_\varphi)$ or $u \in L^2(I,V_u)$ and not of the combined function $\boldsymbol{u} = (u,\varphi)$:

$$\|u\|_{Y_u}^2 = \int_I \|u(t)\|_{V_u}^2 \mathrm{d}t, \qquad \|\varphi\|_{Y_\varphi}^2 = \int_I \big(\|\varphi(t)\|_{V_\varphi}^2 + \|\dot\varphi(t)\|_{V_\varphi}^2\big)\,\mathrm{d}t.$$

2.2 Abstract NLP theory

We consider the following constrained nonlinear optimization problem of NLP type, which was studied by Maurer and Zowe [32, 31] based on prior work by Robinson and Kurcyusz [45, 27, 53]: given Banach spaces Y, Z, a closed convex set $C \subseteq Y$, a closed convex cone $K \subset Z$, a cost functional $f : Y \to \mathbb{R}$, and a constraint map $g : Y \to Z$, the problem reads

$$\min_{y \in C} f(y) \quad \text{s.t.} \quad g(y) \in K. \tag{2}$$

As always in nonconvex optimization, we regard every local minimizer as a solution, and we are interested in first and second order conditions that characterize these local minimizers.

The feasible set of (2) is $M := C \cap g^{-1}(K)$. For any feasible point $\bar{y} \in M$, the *tangent cone* $T(M, \bar{y})$ and the *linearized cone* $L(M, \bar{y})$ are defined as

$$\begin{aligned} T(M, \bar{y}) &:= \{h \in C_{\bar{y}} : h = \lim (y_n - \bar{y})/t_n,\ y_n \in M,\ t_n > 0,\ t_n \to 0\}, \\ L(M, \bar{y}) &:= \{h \in C_{\bar{y}} : g'(\bar{y})h \in K_{g(\bar{y})}\} = C_{\bar{y}} \cap g'(\bar{y})^{-1}(K_{g(\bar{y})}). \end{aligned}$$

Here we assume that the Fréchet derivatives $f'(\bar{y}) \in L(Y, \mathbb{R}) = Y^*$ and $g'(\bar{y}) \in L(Y, Z)$ at $\bar{y}$ exist, and by $C_{\bar{y}} := \operatorname{cone}(C - \bar{y})$ and $K_{g(\bar{y})} := \operatorname{cone}(K - g(\bar{y}))$ we denote the conical hulls of $C - \bar{y}$ and $K - g(\bar{y})$, respectively, with $\operatorname{cone}(S) := \{\alpha s : s \in S,\ \alpha \geq 0\}$. By Y^* we denote the topological dual space of Y, and for any nonempty subset $S \subseteq Y$ we consider the *dual cone* $S^* := \{l \in Y^* : ls \geq 0 \text{ for all } s \in S\}$.

Definition 2.1. *A feasible point $\bar{y} \in M$ is called* regular for (2) (in the sense of Zowe and Kurcyusz) *if $g'(\bar{y})C_{\bar{y}} - K_{g(\bar{y})} = Z$.*

An important consequence of regularity is the inclusion $L(M, \bar{y}) \subseteq T(M, \bar{y})$. KKT type optimality conditions for local minimizers of (2) are now given in the following theorem [32, 31] in terms of the Lagrangian $\mathcal{L} : Y \times Z^* \to \mathbb{R}$ with $\mathcal{L}(y, l) := f(y) - lg(y)$.

Theorem 2.2. *If $\bar{y} \in M$ is a minimizer, then $f'(\bar{y})h \geq 0$ for all $h \in T(M, \bar{y})$, i.e., $f'(\bar{y}) \in T(M, \bar{y})^*$. If, additionally, $\bar{y}$ is regular, then $f'(\bar{y})h \geq 0$ for all $h \in L(M, \bar{y})$, i.e., $f'(\bar{y}) \in L(M, \bar{y})^*$. Equivalently, there is a Lagrange multiplier $l \in K^*$ such that*

$$\partial_y \mathcal{L}(\bar{y}, l) \equiv f'(\bar{y}) - lg'(\bar{y}) \in C_{\bar{y}}^* \quad \text{and} \quad lg(\bar{y}) = 0. \tag{3}$$

In order to solve (2) we have to find a *KKT point*, i.e., a regular solution $\bar{y}$ of the KKT conditions eq. (3). Assuming that second order Fréchet derivatives $f''(\bar{y}) \in L(Y, L(Y, \mathbb{R})) \cong L(Y, Y; \mathbb{R})$ and $g''(\bar{y}) \in L(Y, L(Y, Z)) \cong L(Y, Y; Z)$ exist and that $C = Y$ (or $\bar{y} \in \operatorname{int} C$), hence $C_{\bar{y}} = Y$ and $C_{\bar{y}}^* = \{0\}$, [32, 31] also provide second order necessary optimality conditions at a given KKT point $(\bar{y}, l)$. These conditions are stated in terms of the cones $K^l := K \cap \ker l$ and $T(M^l, \bar{y})$ with $M^l := g^{-1}(K^l)$ as well as

$$L(M^l, \bar{y}) := \{h \in Y : g'(\bar{y})h \in K^l_{g(\bar{y})}\} \quad \text{with} \quad K^l_{g(\bar{y})} := K_{g(\bar{y})} \cap \ker l.$$

The cone $L(M^l, \bar{y})$ is called the *critical cone* at $(\bar{y}, l)$.

Theorem 2.3. *If $\bar{y} \in M$ is a minimizer with an associated Lagrange multiplier l, then*

$$\partial_{yy}\mathcal{L}(\bar{y}, l)(h, h) \geq 0 \quad \textit{for all} \quad h \in T(M^l, \bar{y}).$$

If, additionally, $\bar{y}$ is regular w.r.t. K^l, *that is, $g'(\bar{y})Y - K^l_{g(\bar{y})} = Z$, then*

$$\partial_{yy}\mathcal{L}(\bar{y}, l)(h, h) \geq 0 \quad \textit{for all} \quad h \in L(M^l, \bar{y}).$$

In order to formulate sufficient optimality conditions, the linearized cone $L(M, \bar{y})$ has to be a good approximation of the admissible set M in a neighbourhood of $\bar{y}$.

Definition 2.4. *We say that the linearized cone $L(M, \bar{y})$* approximates *M at $\bar{y}$ if there exists a map $h \colon M \to L(M, \bar{y})$ such that*

$$\|h(y) - (y - \bar{y})\| \in o(\|y - \bar{y}\|) \quad \textit{as} \quad M \ni y \to \bar{y}.$$

Using the notation $\bar{B}^Y_r(\bar{y}) := \{y \in Y \colon \|y - \bar{y}\| \leq r\}$, sufficient optimality conditions of first and second order are now given in the following theorem [32, 31].

Theorem 2.5. *Assume that $L(M, \bar{y})$ approximates M at $\bar{y}$. If there exists $\gamma > 0$ such that*

$$f'(\bar{y})h \geq \gamma\|h\| \quad \textit{for all} \quad h \in L(M, \bar{y}),$$

then there exist $\alpha > 0$ and $\delta > 0$ with

$$f(y) \geq f(\bar{y}) + \alpha\|y - \bar{y}\| \quad \textit{for all} \quad y \in M \cap \bar{B}^Y_\delta(\bar{y}).$$

If $(\bar{y}, l)$ is a KKT point and there exist $\gamma > 0$ and $\beta > 0$ such that

$$\partial_{yy}\mathcal{L}(\bar{y}, l)(h, h) \geq \gamma\|h\|^2 \quad \textit{for all} \quad h \in L(M, \bar{y}) \cap \{h \in C_{\bar{y}} \colon lg'(\bar{y})h \leq \beta\|h\|\},$$

then there exist $\alpha > 0$ and $\delta > 0$ with

$$f(y) \geq f(\bar{y}) + \alpha\|y - \bar{y}\|^2 \quad \textit{for all} \quad y \in M \cap \bar{B}^Y_\delta(\bar{y}).$$

3 Phase-field fracture as nonlinear energy minimization problem

In this section, we formulate phase-field fracture as an energy minimization problem with the crack irreversibility as inequality constraint and the initial condition as equality constraint. We formulate the corresponding cones and establish regularity results and the KKT conditions.

3.1 Problem statement

Our phase-field fracture formulation differs from most works found in the literature in that the crack irreversibility condition is treated in a continuous-time fashion [21, 22] rather than by an (incremental) discrete-time formulation [3, 2, 6, 1, 34, 25]. We refer to the introduction for the discussion of various possibilities of imposing the irreversibility constraint. The continuous-time constraint enables us to formulate phase-field fracture in a space-time setting, which we continue to utilize in this work. The forward problem NLP_E reads as follows:

Problem 3.1. *Given the phase-field regularization $\varepsilon > 0$, the bulk regularization $\kappa \in (0,1)$, the Lamé parameters $\mu > 0$, $\lambda > -\frac{2}{3}\mu$, the critical energy release rate G_c, an initial phase-field $\varphi_0 \in V_\varphi$ and a space-time control $q \in W$, find a function $\boldsymbol{u} \in Y = Y_u \times Y_\varphi$ consisting of a displacement field*

$$u = (u_1, u_2) \in Y_u = L^2(I, V_u)$$

and a phase-field $\varphi \in Y_\varphi = H^1(I, V_\varphi)$ that minimize the crack energy $f\colon Y \to \mathbb{R}$ subject to the initial condition and the crack irreversibility constraint:

$$\begin{aligned} \min_{\boldsymbol{u}\in Y} \quad & f(\boldsymbol{u}) := \frac{1}{2}(g_\kappa(\varphi)\mathbb{C}e(u), e(u))_{I\times\Omega} + \\ & \qquad \frac{G_c}{2\varepsilon}\|1-\varphi\|^2_{I\times\Omega} + \frac{G_c\varepsilon}{2}\|\nabla\varphi\|^2_{I\times\Omega} - (q,u)_{I\times\Gamma_N} \\ \text{s.t.} \quad & \varphi(0) = \varphi_0 \quad in \quad V_\varphi, \\ & -\dot{\varphi}(t) \geq 0 \quad in \quad V_\varphi \ a.e.\ in\ I. \end{aligned} \tag{4}$$

In the integrand of the first term we use the Frobenius scalar product $\mathbb{C}e(u) : e(u)$ of matrices $\mathbb{C}e(u)$ and $e(u)$ in $\mathbb{R}^{2\times 2}$, where $e(u) := \frac{1}{2}(\nabla u + \nabla u^T)$ denotes the symmetric strain gradient and $\mathbb{C}e(u) := 2\mu e(u) + \lambda \operatorname{tr}(e(u))I_2$ the stress tensor with the identity matrix $I_2 \in \mathbb{R}^{2\times 2}$. This product is multiplied with the nonlinear degradation function $g_\kappa(\varphi) = (1-\kappa)\varphi^2 + \kappa$.

3.2 Constraints and cones

In order to formulate the KKT system that corresponds to (4), we have to define the operator g (which is affine linear in this case), the spaces Z, Z^* and the cones K, K^*. There is no set constraint, i.e., $C = Y$. First we collect the equality and inequality constraints $g_\mathcal{E}$ and $g_\mathcal{I}$, respectively, to define $g\colon Y \to Z$ as

$$g(\boldsymbol{u}) = \begin{pmatrix} g_\mathcal{E}(\boldsymbol{u}) \\ g_\mathcal{I}(\boldsymbol{u}) \end{pmatrix} := \begin{pmatrix} \varphi(0) - \varphi_0 \\ -\dot{\varphi} \end{pmatrix} \quad \text{for all} \quad \boldsymbol{u} \in Y.$$

It is clear that the upper term belongs to V_φ for each $\varphi_0 \in V_\varphi$ since $\varphi(t) \in V_\varphi$ for all $t \in I$, particularly $\varphi \in H^1(I, V_\varphi) \hookrightarrow C(I, V_\varphi)$. Moreover, the point evaluation $\varphi \mapsto \varphi(0)$ is surjective onto V_φ. By definition, the second component always belongs to $L^2(I, V_\varphi)$. Consequently we define the image space Z as

$$Z := Z_1 \times Z_2 \quad \text{with} \quad Z_1 := V_\varphi, \quad Z_2 := L^2(I, V_\varphi).$$

The dual space is

$$Z^* = Z_1^* \times Z_2^* = V_\varphi^* \times L^2(I, V_\varphi^*).$$

Next we define the constraints cone $K \subset Z$ as

$$K := K_1 \times K_2 \quad \text{with} \quad K_1 := \{0\} \subset Z_1, \quad K_2 := \{z_2 \in Z_2 \colon z_2 \geq 0\}.$$

More precisely, K_2 has to be understood as

$$K_2 = \{z_2 \in Z_2 \colon z_2(t) \geq 0 \text{ in } V_\varphi \text{ for a.e. } t \in I\}.$$

It is clear that K_2 and hence K are closed convex cones. Finally we need the dual cone $K^* \subset Z^*$. Since $K = \{0\} \times K_2$, K^* has the product structure

$$
\begin{aligned}
K^* &= Z_1^* \times K_2^* = Z_1^* \times \{l_2 \in Z_2^* \colon l_2 z_2 \geq 0 \text{ for all } z_2 \in K_2\} \\
&= Z_1^* \times \left\{ l_2 \in L^2(I, V_\varphi^*) \colon \int_I \langle l_2(t), z_2(t) \rangle_{V_\varphi^*, V_\varphi} \, \mathrm{d}t \geq 0 \text{ for all } z_2 \in K_2 \right\},
\end{aligned}
$$

where $\langle u, v \rangle_{V_\varphi^*, V_\varphi}$ denotes the dual pairing between V_φ^* and V_φ, i.e., between $H^2(\Omega)^*$ and $H^2(\Omega)$. Given a solution candidate $\bar{\boldsymbol{u}} \in M$ with feasible set

$$
M = \{\boldsymbol{u} = (u, \varphi) \in Y \colon g(\boldsymbol{u}) \in K\} = V_u \times \{\varphi \in V_\varphi \colon \varphi(0) = \varphi_0, \, -\dot{\varphi} \geq 0\},
$$

we have $\bar{\varphi}(t) = \bar{\varphi}_0 + \int_0^t \dot{\bar{\varphi}}(s) \, \mathrm{d}s \leq \bar{\varphi}_0$ for all $t \in I$ and the relevant cones are

$$
C_{\bar{\boldsymbol{u}}} = Y, \qquad C_{\bar{\boldsymbol{u}}}^* = \{0\}, \qquad K_{g(\bar{\boldsymbol{u}})} = \{0\} \times (K_2 + \operatorname{span}\{\dot{\bar{\varphi}}\}). \tag{5}
$$

Next we have to compute the derivatives $f'(\bar{\boldsymbol{u}}) \in Y^*$ and $g'(\bar{\boldsymbol{u}}) \in L(Y, Z)$. For $f'(\bar{\boldsymbol{u}})$ see the following proposition. Since g is affine linear, for any given direction $\boldsymbol{\Phi} := (\Phi_u, \Phi_\varphi) \in Y$ we obtain

$$
g'(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}) = \begin{pmatrix} \Phi_\varphi(0) \\ -\dot{\Phi}_\varphi \end{pmatrix}.
$$

Finally, given any multiplier $\boldsymbol{l} = (l_1, l_2) \in K^*$, we have $\boldsymbol{l} g'(\bar{\boldsymbol{u}}) \in Y^*$ with

$$
\boldsymbol{l} g'(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}) = \langle l_1, \Phi_\varphi(0) \rangle_{V_\varphi^*, V_\varphi} - \int_I \langle l_2(t), \dot{\Phi}_\varphi(t) \rangle_{V_\varphi^*, V_\varphi} \, \mathrm{d}t.
$$

In preparation of some estimates to be employed in the proof of proposition 3.1, we relate certain expressions to the norm in Y:

Lemma 3.2. *Let $\mu > 0$, $\lambda > -\frac{2}{3}\mu$. Then there is $C > 0$ such that the following estimates hold for all $\boldsymbol{u} = (u, \varphi) \in Y$, $\boldsymbol{u}_1, \boldsymbol{u}_2 \in Y$:*

$$
\begin{aligned}
(\psi \mathbb{C} e(u_1), e(u_2))_{I \times \Omega} &\leq C \|\psi\|_{L^\infty(I \times \Omega)} \|\boldsymbol{u}_1\|_Y \|\boldsymbol{u}_2\|_Y \quad \textit{for all} \quad \psi \in L^\infty(I \times \Omega), \\
\|\varphi\|_{L^\infty(I \times \Omega)} &\leq C \|\boldsymbol{u}\|_Y, \\
\max\{\|\nabla \varphi\|_{I \times \Omega}, \|\varphi\|_{I \times \Omega}\} &\leq \|\boldsymbol{u}\|_Y.
\end{aligned}
$$

Proof. The last inequality is straightforward, as

$$
\begin{aligned}
\|\nabla \varphi\|_{I \times \Omega} &\leq \|\varphi\|_{L^2(I, H^2(\Omega))} \leq \|\boldsymbol{u}\|_Y, \\
\|\varphi\|_{I \times \Omega} &\leq \|\varphi\|_{L^2(I, H^2(\Omega))} \leq \|\boldsymbol{u}\|_Y,
\end{aligned}
$$

whereas the second estimate holds due to the embedding $Y_\varphi = H^1(I, H^2(\Omega)) \hookrightarrow L^\infty(I, L^\infty(\Omega))$. The first one mainly relies on Hölder's inequality: With some $C > 0$ (depending on μ and λ),

$$
\begin{aligned}
(\psi \mathbb{C} e(u_1), e(u_2))_{I \times \Omega} &= \int_{I \times \Omega} \psi(t, x) \mathbb{C} e(u_1(t, x)) : e(u_2(t, x)) \, \mathrm{d}x \, \mathrm{d}t \\
&\leq C \|\psi\|_{L^\infty(I \times \Omega)} \|\nabla u_1\|_{I \times \Omega} \|\nabla u_2\|_{I \times \Omega} \\
&\leq C \|\psi\|_{L^\infty(I \times \Omega)} \|\boldsymbol{u}_1\|_Y \|\boldsymbol{u}_2\|_Y.
\end{aligned}
$$

□

Proposition 3.1. *The energy functional f defined in (4) is twice Fréchet differentiable in Y. For any direction $\boldsymbol{\Phi} \in Y$ the first and second derivatives at any element $\boldsymbol{u} \in Y$ are given by*

$$\begin{aligned} f'(\boldsymbol{u})(\boldsymbol{\Phi}) &= (g_\kappa(\varphi)\mathbb{C}e(u), e(\Phi_u))_{I\times\Omega} - (q, \Phi_u)_{I\times\Gamma_N} + G_c\varepsilon(\nabla\varphi, \nabla\Phi_\varphi)_{I\times\Omega} \\ &\quad - \frac{G_c}{\varepsilon}(1-\varphi, \Phi_\varphi)_{I\times\Omega} + (1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(u), e(u))_{I\times\Omega}, \\ f''(\boldsymbol{u})(\boldsymbol{\Phi}, \boldsymbol{\Phi}) &= (g_\kappa(\varphi)\mathbb{C}e(\Phi_u), e(\Phi_u))_{I\times\Omega} + 4(1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(u), e(\Phi_u))_{I\times\Omega} \\ &\quad + G_c\varepsilon\|\nabla\Phi_\varphi\|^2_{I\times\Omega} + \frac{G_c}{\varepsilon}\|\Phi_\varphi\|^2_{I\times\Omega} + (1-\kappa)(\Phi_\varphi^2\mathbb{C}e(u), e(u))_{I\times\Omega}. \end{aligned} \tag{6}$$

Proof. The expressions in (6) are easily confirmed to be Gâteaux derivatives. Moreover, for any $\boldsymbol{u}, \boldsymbol{\Phi}, \boldsymbol{\Psi} \in Y$, by lemma 3.2 in combination with the identity $g_\kappa(\varphi+\Psi_\varphi) = g_\kappa(\varphi) + (1-\kappa)(2\varphi\Psi_\varphi + \Psi_\varphi^2)$ we have

$$\begin{aligned} &|f'(\boldsymbol{u}+\boldsymbol{\Psi})\boldsymbol{\Phi} - f'(\boldsymbol{u})\boldsymbol{\Phi}| \\ &\quad = \Big|(g_\kappa(\varphi+\Psi_\varphi)\mathbb{C}e(\Psi_u), e(\Phi_u))_{I\times\Omega} \\ &\qquad + (1-\kappa)((2\varphi\Psi_\varphi + \Psi_\varphi^2)\mathbb{C}e(u), e(\Phi_u))_{I\times\Omega} + G_c\varepsilon(\nabla\Psi_\varphi, \nabla\Phi_\varphi)_{I\times\Omega} \\ &\qquad + \frac{G_c}{\varepsilon}(\Psi_\varphi, \Phi_\varphi)_{I\times\Omega} + (1-\kappa)(\Psi_\varphi\Phi_\varphi\mathbb{C}e(u+\Psi_u), e(u+\Psi_u))_{I\times\Omega} \\ &\qquad + 2(1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(u), e(\Psi_u))_{I\times\Omega} + (1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(\Psi_u), e(\Psi_u))_{I\times\Omega}\Big| \\ &\quad \leq C\|g_\kappa(\varphi+\Psi_\varphi)\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{\Phi}\|_Y \\ &\qquad + (1-\kappa)C\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}\|_Y\|\boldsymbol{\Phi}\|_Y + G_c\varepsilon\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{\Phi}\|_Y \\ &\qquad + \frac{G_c}{\varepsilon}\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{\Phi}\|_Y + (1-\kappa)C\|\Psi_\varphi\Phi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}+\boldsymbol{\Psi}\|_Y^2 \\ &\qquad + 2(1-\kappa)C\|\varphi\Phi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}\|_Y\|\boldsymbol{\Psi}\|_Y + (1-\kappa)C\|\varphi\Phi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\Psi}\|_Y^2, \end{aligned}$$

where $C > 0$ is the constant from lemma 3.2, another application of which yields

$$\begin{aligned} \|f'(\boldsymbol{u}+\boldsymbol{\Psi}) - f'(\boldsymbol{u})\|_{Y^*} &\leq C\|g_\kappa(\varphi+\Psi_\varphi)\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\Psi}\|_Y \\ &\quad + (1-\kappa)C\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}\|_Y + G_c\varepsilon\|\boldsymbol{\Psi}\|_Y \\ &\quad + \frac{G_c}{\varepsilon}\|\boldsymbol{\Psi}\|_Y + (1-\kappa)C^3\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{u}+\boldsymbol{\Psi}\|_Y^2 \\ &\quad + 2(1-\kappa)C^3\|\boldsymbol{u}\|_Y^2\|\boldsymbol{\Psi}\|_Y + (1-\kappa)C^3\|\boldsymbol{u}\|_Y\|\boldsymbol{\Psi}\|_Y^2. \end{aligned}$$

Hence, apparently, $f'(\boldsymbol{u}+\boldsymbol{\Psi}) \to f'(\boldsymbol{u})$ in Y^* as $\boldsymbol{\Psi} \to 0$. Continuity of the Gâteaux derivative implies Fréchet differentiability (cf. [52, Prop. 4.8(c)]).

For the second derivative, we similarly obtain for any $\boldsymbol{u}, \boldsymbol{\Phi}, \boldsymbol{\Psi} \in Y$

$$\begin{aligned}
&|f''(\boldsymbol{u}+\boldsymbol{\Psi})(\boldsymbol{\Phi},\boldsymbol{\Phi}) - f''(\boldsymbol{u})(\boldsymbol{\Phi},\boldsymbol{\Phi})| \\
&\quad = \Big|(1-\kappa)((2\varphi\Psi_\varphi + \Psi_\varphi^2)\mathbb{C}e(\Phi_u), e(\Phi_u))_{I\times\Omega} + 4(1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(\Psi_u), e(\Phi_u))_{I\times\Omega} \\
&\qquad + 4(1-\kappa)(\Psi_\varphi\Phi_\varphi\mathbb{C}e(u+\Psi_u), e(\Phi_u))_{I\times\Omega} + 2(1-\kappa)(\Phi_\varphi^2\mathbb{C}e(u), e(\Psi_u))_{I\times\Omega} \\
&\qquad + (1-\kappa)(\Phi_\varphi^2\mathbb{C}e(\Psi_u), e(\Psi_u))_{I\times\Omega}\Big| \\
&\quad \le (1-\kappa)C\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\Phi}\|_Y^2 + 4(1-\kappa)C^3\|\boldsymbol{u}\|_Y\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{\Phi}\|_Y^2 \\
&\qquad + 4(1-\kappa)C^3\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{u}+\boldsymbol{\Psi}\|_Y\|\boldsymbol{\Phi}\|_Y^2 + 2(1-\kappa)C^3\|\boldsymbol{\Phi}\|_Y^2\|\boldsymbol{u}\|_Y\|\boldsymbol{\Psi}\|_Y \\
&\qquad + (1-\kappa)C^3\|\boldsymbol{\Phi}\|_Y^2\|\boldsymbol{\Psi}\|_Y^2,
\end{aligned}$$

so that

$$\begin{aligned}
\|f''(\boldsymbol{u}+\boldsymbol{\Psi}) - f''(\boldsymbol{u})\|_{L(Y,Y;\mathbb{R})} \le\ & (1-\kappa)C\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)} \\
& + 6(1-\kappa)C^3\|\boldsymbol{u}\|_Y\|\boldsymbol{\Psi}\|_Y \\
& + 4(1-\kappa)C^3\|\boldsymbol{\Psi}\|_Y\|\boldsymbol{u}+\boldsymbol{\Psi}\|_Y + (1-\kappa)C^3\|\boldsymbol{\Psi}\|_Y^2.
\end{aligned}$$

Once more continuity of the Gâteaux derivative ensures Fréchet differentiability. ☐

3.3 Regularity and KKT system

Recall that a feasible point $\bar{\boldsymbol{u}} \in M$ is regular for (4) if

$$Z = g'(\bar{\boldsymbol{u}})Y - K_{g(\bar{\boldsymbol{u}})},$$

where in our case

$$\begin{aligned}
Z &= Z_1 \times Z_2 = V_\varphi \times L^2(I, V_\varphi), \\
g'(\bar{\boldsymbol{u}})Y &= \left\{ \begin{pmatrix} \Phi_\varphi(0) \\ -\dot{\Phi}_\varphi \end{pmatrix} : (\Phi_u, \Phi_\varphi) \in Y \right\}, \\
K_{g(\bar{\boldsymbol{u}})} &= \left\{ \begin{pmatrix} 0 \\ k_2 \end{pmatrix} + \alpha \begin{pmatrix} 0 \\ \dot{\varphi} \end{pmatrix} : k_2 \in K_2 \text{ and } \alpha \in \mathbb{R} \right\}.
\end{aligned}$$

In fact, *every* feasible point is regular since $Z = g'(\bar{\boldsymbol{u}})Y$ by the following result.

Lemma 3.3. *The derivative $g'(\bar{\boldsymbol{u}})\colon Y \to Z$ is surjective for every $\bar{u} \in M$.*

Proof. Given $\bar{\boldsymbol{u}} \in M$ and $z = (z_1, z_2) \in Z$, simply choose any $\Phi_u \in Y_u$ and set $\Phi_\varphi(t) := z_1 - \int_0^t z_2(s)\,\mathrm{d}s$ to obtain $\boldsymbol{\Phi} \in Y$ with $g'(\bar{\boldsymbol{u}})\boldsymbol{\Phi} = z$. ☐

We work with $\varphi \in H^1(I, H^2(\Omega))$ to make use of the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ in proving proposition 3.1. A seemingly natural alternative would be to require less spatial regularity, for example by merely assuming $\varphi(t) \in H^1(\Omega)$ for every $t \in I$. In this case, however, it would be unclear whether f was well-defined as a functional $f\colon Y \to \mathbb{R}$, because finiteness of the term $(g_\kappa(\varphi)\mathbb{C}e(u), e(u))_\Omega$ could not be guaranteed for each $\boldsymbol{u} \in Y$. Of course, it would be possible to replace g_κ by a bounded (cut off) variant, but even then, related terms (and thus the same problem) would re-emerge when dealing with derivatives. Another common space for φ is $L^2(I, H^1(\Omega))$ with $\dot{\varphi} \in L^2(I, H^1(\Omega)^*)$. The following counterexample shows that this choice of function spaces cannot ensure that any feasible point is regular for (4).

Lemma 3.4. *Let $I = [0,1]$ and $\Omega = (0,1)^2$, let $\bar{\varphi}$ be a nonnegative function in $L^2(I, H^1(\Omega))$ such that $\dot{\bar{\varphi}} \in L^2(I, H^1(\Omega)^*)$ with $\dot{\bar{\varphi}} \leq 0$. Then there exists a function $z \in V_\varphi \times L^2(I, H^1(\Omega)^*)$ for which the equations $z_1 = \Phi_\varphi(0)$, $z_2 = -\dot{\Phi}_\varphi + k_2 + \alpha\dot{\bar{\varphi}}$ cannot be fulfilled with any $\boldsymbol{\Phi} \in L^2(I, H^1(\Omega))$ that satisfies $\dot{\Phi}_\varphi \in L^2(I, H^1(\Omega)^*)$, any $k_2 \in L^2(I, H^1(\Omega)^*)$ that satisfies $k_2 \geq 0$, and any $\alpha \in \mathbb{R}$.*

Proof. Let $z_1 = \bar{\varphi}(0) \in L^2(\Omega)$, and $z_2(t,x,y) = -x^{-\frac{1}{4}}$ for every $t \in I$ and $(x,y) \in \Omega$. Then, for each $t \in I$, $z_2(t) \in L^2(\Omega) \subset H^1(\Omega)^*$ since

$$\int_0^1 \int_0^1 |z_2(t,x,y)|^2 \,\mathrm{d}x \,\mathrm{d}y = \int_0^1 \int_0^1 |-x^{-\frac{1}{4}}|^2 \,\mathrm{d}x \,\mathrm{d}y = \int_0^1 x^{-\frac{1}{2}} \,\mathrm{d}x = 2 < \infty.$$

Moreover, this shows $z_2 \in L^2(I, H^1(\Omega)^*)$. Now we seek functions $\Phi_\varphi \in L^2(I, H^1(\Omega))$ satisfying $\dot{\Phi}_\varphi \in L^2(I, H^1(\Omega)^*)$ and $k_2 \in L^2(I, H^1(\Omega)^*)$ with $k_2 \geq 0$ and constant $\alpha \in \mathbb{R}$ such that

$$\Phi_\varphi(0) = z_1 \quad \text{and} \quad \dot{\Phi}_\varphi = -z_2 + k_2 + \alpha\dot{\bar{\varphi}}.$$

If such a function Φ_φ exists, then for almost every $t \in I$ we have $\Phi_\varphi(t) \in H^1(\Omega)$ and

$$\Phi_\varphi(t) = \int_0^t [k_2(s) - z_2(s) + \alpha\dot{\bar{\varphi}}(s)] \,\mathrm{d}s \tag{7}$$

in $H^1(\Omega)$. If $\alpha \leq 0$, then due to $k_2 \geq 0$ and $\dot{\bar{\varphi}} \leq 0$ this ensures

$$\Phi_\varphi(t) \geq -\int_0^t z_2(s) \,\mathrm{d}s = -tz_2(0).$$

If, on the other hand $\alpha > 0$, eq. (7) shows that $\Phi_\varphi(t) \geq -tz_2(0) + \alpha\bar{\varphi}(t) \geq -tz_2(0)$. In both cases this implies the existence of a function $g \in H^1(\Omega)$ with $g(x,y) \geq -z_2(0,x,y) = x^{-\frac{1}{4}}$, namely $g(x,y) = \frac{1}{t}\Phi_\varphi(t,x,y)$ for some $t > 0$ for which (7) is valid. Now let $\tilde{g}(x) = \int_0^1 g(x,y) \,\mathrm{d}y$. Then $\tilde{g} \in H^1((0,1)) \subset C([0,1])$ and $\tilde{g}(x) \geq x^{-\frac{1}{4}}$ for all $x \in (0,1)$, which contradicts $\tilde{g} \in C([0,1])$ since continuous functions are bounded. Therefore such functions Φ_φ and k_2 cannot exist. □

Now we are ready to formulate the KKT system that corresponds to (4).

Proposition 3.2. *Let the data and parameters be as in problem 3.1. Since every local minimizer $\bar{\boldsymbol{u}} = (\bar{u}, \bar{\varphi}) \in M$ of NLP$_E$ is regular by lemma 3.3, there exists a multiplier $\boldsymbol{l} = (l_1, l_2) \in Z^*$ such that the KKT conditions of theorem 2.2 hold:*

$$-\dot{\bar{\varphi}}(t) \geq 0 \textit{ in } V_\varphi \textit{ for a.e. } t \in I, \tag{KKT 1}$$

$$\bar{\varphi}(0) = \varphi_0 \textit{ in } V_\varphi, \tag{KKT 2}$$

$$l_2(t) \geq 0 \textit{ in } V_\varphi^* \textit{ for a.e. } t \in I, \tag{KKT 3}$$

$$
\begin{aligned}
(g_\kappa(\bar\varphi)\mathbb{C}e(\bar u), e(P_u(\,\cdot\,)))_{I\times\Omega} - (q, P_u(\,\cdot\,))_{I\times\Gamma_N} + G_c\varepsilon(\nabla\bar\varphi, \nabla P_\varphi(\,\cdot\,))_{I\times\Omega}& \\
- \frac{G_c}{\varepsilon}(1-\bar\varphi, P_\varphi(\,\cdot\,))_{I\times\Omega} + (1-\kappa)(\bar\varphi P_\varphi(\,\cdot\,)\mathbb{C}e(\bar u), e(\bar u))_{I\times\Omega}& \\
- \langle l_1, P_\varphi(\,\cdot\,)(0)\rangle_{V_\varphi^*,V_\varphi} + \int_I \langle l_2(t), \partial_t P_\varphi(\,\cdot\,)(t)\rangle_{V_\varphi^*,V_\varphi}\,\mathrm{d}t = 0,& \qquad \text{(KKT 4)}
\end{aligned}
$$

$$
\langle l_1, \bar\varphi(0)-\varphi_0\rangle_{V_\varphi^*,V_\varphi} - \int_I \langle l_2(t), \dot{\bar\varphi}(t)\rangle_{V_\varphi^*,V_\varphi}\,\mathrm{d}t = 0, \qquad \text{(KKT 5)}
$$

where we introduce canonical projections $P_u(\boldsymbol{\Phi}) = \Phi_u$ *and* $P_\varphi(\boldsymbol{\Phi}) = \Phi_\varphi$.

Proof. Conditions (KKT 1) and (KKT 2) are just feasibility $\bar{\boldsymbol{u}} \in M$. Condition (KKT 3) is equivalent to $\boldsymbol{l} \in K^*$. The stationarity condition $f'(\bar{\boldsymbol{u}}) - \boldsymbol{l}g'(\bar{\boldsymbol{u}}) \in C^*_{\bar{\boldsymbol{u}}}$ in the form (KKT 4) is immediate from the representation of f' in proposition 3.1 since $C^*_{\bar{\boldsymbol{u}}} = \{0\}$. Finally, (KKT 5) is the complementarity condition $\boldsymbol{l}g(\bar{\boldsymbol{u}}) = 0$. □

4 Further optimality conditions

Here we formulate the specific second order necessary conditions as well as first and second order sufficient conditions of the forward problem NLP_E.

4.1 Necessary optimality conditions of second order

The Lagrangian corresponding to (4) reads

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{u}, \boldsymbol{l}) &= f(\boldsymbol{u}) - \boldsymbol{l}g(\boldsymbol{u}) \\
&= \frac{1}{2}(g_\kappa(\varphi)\mathbb{C}e(u), e(u))_{I\times\Omega} + \frac{G_c}{2\varepsilon}\|1-\varphi\|^2_{I\times\Omega} + \frac{G_c\varepsilon}{2}\|\nabla\varphi\|^2_{I\times\Omega} - (q, u)_{I\times\Gamma_N} \\
&\quad - \langle l_1, \varphi(0)-\varphi_0\rangle_{V_\varphi^*,V_\varphi} + \int_I \langle l_2(t), \dot\varphi(t)\rangle_{V_\varphi^*,V_\varphi}\,\mathrm{d}t.
\end{aligned}
$$

By affine linearity of g and proposition 3.1, the derivative $\partial_{\boldsymbol{uu}}\mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}, \boldsymbol{\Phi})$ for a pair $(\bar{\boldsymbol{u}}, \boldsymbol{l}) \in Y \times Z^*$ and a direction $\boldsymbol{\Phi} = (\Phi_u, \Phi_\varphi) \in Y$ becomes

$$
\begin{aligned}
\partial_{\boldsymbol{uu}}\mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}, \boldsymbol{\Phi}) &= f''(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}, \boldsymbol{\Phi}) \\
&= (g_\kappa(\bar\varphi)\mathbb{C}e(\Phi_u), e(\Phi_u))_{I\times\Omega} + 4(1-\kappa)(\bar\varphi\Phi_\varphi\mathbb{C}e(\bar u), e(\Phi_u))_{I\times\Omega} \\
&\quad + G_c\varepsilon\|\nabla\Phi_\varphi\|^2_{I\times\Omega} + \frac{G_c}{\varepsilon}\|\Phi_\varphi\|^2_{I\times\Omega} + (1-\kappa)(\Phi_\varphi^2\mathbb{C}e(\bar u), e(\bar u))_{I\times\Omega}.
\end{aligned}
$$

In order to ensure the required regularity of some minimizer $\bar{\boldsymbol{u}} \in M$ with a multiplier $\boldsymbol{l} \in K^*$ for the second order necessary optimality conditions, we have to show that

$$
g'(\bar{\boldsymbol{u}})Y - K^{\boldsymbol{l}}_{g(\bar{\boldsymbol{u}})} = Z.
$$

This is indeed the case for *every* feasible point since $g'(\bar{\boldsymbol{u}})\colon Y \to Z$ is surjective, as shown in lemma 3.3. Finally we can apply theorem 2.3 to problem 3.1:

Proposition 4.1. *Every local minimizer* $\bar{\boldsymbol{u}}$ *of* NLP_E *is regular with respect to* $K^{\boldsymbol{l}}$*, and for every* $\boldsymbol{\Phi} \in L(M^{\boldsymbol{l}}, \bar{\boldsymbol{u}}) = \{h \in Y \colon g'(\bar{\boldsymbol{u}})h \in K^{\boldsymbol{l}}_{g(\bar{\boldsymbol{u}})}\}$ *it holds*

$$
\begin{aligned}
&(g_\kappa(\bar\varphi)\mathbb{C}e(\Phi_u), e(\Phi_u))_{I\times\Omega} + 4(1-\kappa)(\bar\varphi\Phi_\varphi\mathbb{C}e(\bar u), e(\Phi_u))_{I\times\Omega} \\
&+ G_c\varepsilon\|\nabla\Phi_\varphi\|^2_{I\times\Omega} + \frac{G_c}{\varepsilon}\|\Phi_\varphi\|^2_{I\times\Omega} + (1-\kappa)(\Phi_\varphi^2\mathbb{C}e(\bar u), e(\bar u))_{I\times\Omega} \geq 0.
\end{aligned}
$$

4.2 Sufficient optimality conditions

First of all we note that the approximation property of definition 2.4 is trivially satisfied at every feasible point $\bar{\boldsymbol{u}} \in M$ since $M \subseteq L(M, \bar{\boldsymbol{u}})$. The sufficient optimality conditions theorem 2.5 of first and second order for eq. (4) take the following form.

Proposition 4.2. *Let $(\bar{\boldsymbol{u}}, \boldsymbol{l}) \in Y \times Z^*$ be a KKT point for problem 3.1. The first order sufficient condition holds if there exists $\gamma > 0$ such that*

$$f'(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}) \geq \gamma \|\boldsymbol{\Phi}\|_Y \quad \text{for all} \quad \boldsymbol{\Phi} \in L(M, \bar{\boldsymbol{u}}),$$

where

$$L(M, \bar{\boldsymbol{u}}) := \{\boldsymbol{\Phi} \in Y : \Phi_\varphi(0) = 0,\, -\dot{\Phi}_\varphi \in K_2 + \operatorname{span}\{\dot{\bar{\varphi}}\}\}.$$

The second order sufficient condition holds if there exist $\gamma > 0$ and $\beta > 0$ such that

$$\partial_{\boldsymbol{uu}} \mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}, \boldsymbol{\Phi}) \geq \gamma \|\boldsymbol{\Phi}\|_Y^2 \quad \text{for all} \quad \boldsymbol{\Phi} \in L_\beta(M, \bar{\boldsymbol{u}}),$$

where

$$L_\beta(M, \bar{\boldsymbol{u}}) := \Big\{\boldsymbol{\Phi} \in Y : \Phi_\varphi(0) = 0,\, -\dot{\Phi}_\varphi \in K_2 + \operatorname{span}\{\dot{\bar{\varphi}}\}, \\ -\int_I \langle l_2(t), \dot{\Phi}_\varphi(t) \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t \leq \beta \|\boldsymbol{\Phi}\|_Y \Big\}$$

In lemma 4.1 and lemma 4.3 we show that the sufficient optimality conditions of first and second order do *not* hold at any KKT point.

Lemma 4.1. *Let $(\bar{\boldsymbol{u}}, \boldsymbol{l}) \in Y \times Z^*$ be a KKT point for problem 3.1 with $\bar{\varphi} \not\equiv \varphi_0$. For each $\gamma > 0$ there exists $\boldsymbol{\Phi} \in L(M, \bar{\boldsymbol{u}})$ such that $f'(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}) = 0 < \gamma \|\boldsymbol{\Phi}\|_Y$.*

Proof. Set $\Phi_u = 0$ and $\Phi_\varphi = -\varphi_0 + \bar{\varphi}$. Then $\boldsymbol{\Phi} \in L(M, \bar{\boldsymbol{u}})$ since $\Phi_\varphi(0) = 0$ by (KKT 2) and $-\dot{\Phi}_\varphi = -\dot{\bar{\varphi}} \in K_2 + \operatorname{span}\{\dot{\bar{\varphi}}\}$. Further, due to (6), (KKT 4) and (KKT 5), we get

$$\begin{aligned} f'(\bar{\boldsymbol{u}})(\boldsymbol{\Phi}) = \boldsymbol{l} g'(\bar{\boldsymbol{u}}) &= \langle l_1, \Phi_\varphi(0) \rangle_{V_\varphi^*, V_\varphi} - \int_I \langle l_2(t), \dot{\Phi}_\varphi(t) \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t \\ &= \langle l_1, \bar{\varphi}(0) - \varphi_0 \rangle_{V_\varphi^*, V_\varphi} - \int_I \langle l_2(t), \dot{\bar{\varphi}}(t) \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t = 0. \end{aligned}$$

□

The following lemma serves as technical preliminary for the treatment of the sufficient second order condition. It will be applied to $g = -\dot{\bar{\varphi}}$ and its use could be entirely avoided under the additional assumption that $\dot{\bar{\varphi}}$ be continuous.

Lemma 4.2. *Let $g \in L^2(I, \mathcal{H}(\Omega)) \setminus \{0\}$ satisfy $g \geq 0$, where $\mathcal{H}(\Omega)$ is a separable Banach space of functions with continuous embedding $\mathcal{H}(\Omega) \hookrightarrow C^0(\overline{\Omega})$. Then there are a subset $J \subset I$ of positive (Lebesgue) measure $\mu(J)$ and a function $\Psi \in C_0^\infty(\Omega) \setminus \{0\}$ such that $0 \leq \Psi(x) \leq g(t, x)$ for almost every $(t, x) \in J \times \Omega$.*

Proof. As $g \not\equiv 0$, there is $\varepsilon > 0$ such that the set $S_\varepsilon := \{(t,x) \in I \times \Omega \mid g(t,x) > 2\varepsilon\}$ fulfills $\mu(S_\varepsilon) > 0$. We use Lusin's theorem (for a variant in Bochner spaces we refer to [29]) to find a set $K \subset I$ with $\mu(I \setminus K) < \mu(S_\varepsilon)/(2\mu(\Omega))$ such that $g|_K \colon K \to \mathcal{H}(\Omega)$ is continuous. Noting that the set $S := (K \times \Omega) \cap S_\varepsilon$ has positive measure, we pick $(t_0, x_0) \in S$ such that for all $\delta > 0$ we have $\mu(K \cap (t_0 - \delta, t_0 + \delta)) > 0$. Relying on the continuity of $g(t_0, \cdot)$, we pick $\delta_1 > 0$ such that for every $x \in B := B_{\delta_1}(x_0)$ we have $g(t_0, x) > 2\varepsilon$, and from continuity of $g|_K$ and the embedding $\mathcal{H}(\Omega) \hookrightarrow C^0(\overline{\Omega})$ we obtain some $\delta_2 > 0$ such that for every $\tau \in J := K \cap (t_0 - \delta_2, t_0 + \delta_2)$ we have $\|g(\tau, \cdot) - g(t_0, \cdot)\|_{C^0(\overline{\Omega})} < \varepsilon$. For every $\tau \in J$ and $x \in B$ we thus have

$$g(\tau, x) = (g(\tau, x) - g(t_0, x)) + g(t_0, x) > -\varepsilon + 2\varepsilon = \varepsilon.$$

We finally choose any nonnegative $\Psi \in C_0^\infty(\Omega) \setminus \{0\}$ which vanishes on $\Omega \setminus B$ and satisfies $\Psi(x) \in [0, \varepsilon]$ for every $x \in B$. $\square$

Lemma 4.3. *Let $(\bar{\boldsymbol{u}}, \boldsymbol{l}) \in Y \times Z^*$ be a KKT point for problem 3.1. Then for all $\gamma > 0$ and $\beta > 0$ there exists $\boldsymbol{\Phi} \in L_\beta(M, \bar{\boldsymbol{u}})$ such that $\partial_{\boldsymbol{uu}} \mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}, \boldsymbol{\Phi}) < \gamma \|\boldsymbol{\Phi}\|_Y^2$.*

Proof. Applying lemma 4.2 to $-\dot{\bar{\varphi}}$ with $\mathcal{H}(\Omega) = V_\varphi = H^2(\Omega) \hookrightarrow C^0(\overline{\Omega})$ leads to a set $J \subset I$ and $\Psi \in V_\varphi$ such that $0 \le \Psi(x) \le -\dot{\bar{\varphi}}(t,x)$ for a.e. $(t,x) \in J \times \Omega$. For $\eta \in (0, \mu(J))$ choose $J_\eta \subset J$ with $\mu(J_\eta) = \eta$ and set $f_\eta(t) = \frac{1}{\eta} \int_0^t \chi_{J_\eta}(s) \,\mathrm{d}s$, where χ_{J_η} denotes the characteristic function of J_η. We define $\boldsymbol{\Phi}_\eta = (\Phi_u, \Phi_\varphi)$ by setting $\Phi_u \equiv 0$ and $\Phi_\varphi(t,x) = -f_\eta(t)\Psi(x)$. Then $\Phi_\varphi(0,x) = 0\Psi(x) = 0$, $-\dot{\Phi}_{\varphi,\eta}(t,x) = \frac{1}{\eta}\chi_{J_\eta}(t)\Psi(x) \ge 0$, and (KKT 3) and (KKT 5) in conjunction with (KKT 2) yields

$$\begin{aligned} -\int_I \langle l_2(t), \dot{\Phi}_\varphi(t) \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t &= \int_I \langle l_2(t), \tfrac{1}{\eta}\chi_{J_\eta}(t)\Psi \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t = \frac{1}{\eta} \int_{J_\eta} \langle l_2(t), \Psi \rangle_{V_\varphi^*, V_\varphi} \,\mathrm{d}t \\ &\le \frac{1}{\eta} \int_{J_\eta} \langle l_2(t), -\dot{\bar{\varphi}}(t) \rangle_{V_\varphi^*, V_\varphi} = 0 \le \beta \|\Phi_\eta\|_Y. \end{aligned}$$

Therefore $\boldsymbol{\Phi}_\eta \in L_\beta(M, \bar{\boldsymbol{u}})$ for every $\beta > 0$. From

$$\begin{aligned} \|\boldsymbol{\Phi}_\eta\|_Y^2 &= \int_I (\|\Phi_\varphi(t)\|_{V_\varphi}^2 + \|\dot{\Phi}_\varphi(t)\|_{V_\varphi}^2) \,\mathrm{d}t \ge \int_I \|\dot{\Phi}_\varphi(t)\|_{V_\varphi}^2 \,\mathrm{d}t \\ &= \int_I \dot{f}_\eta(t)^2 \|\Psi\|_{V_\varphi}^2 \,\mathrm{d}t = \frac{\|\Psi\|_{V_\varphi}^2}{\eta^2} \int_I \chi_{J_\eta}(t)^2 \,\mathrm{d}t = \frac{1}{\eta} \|\Psi\|_{V_\varphi}^2 \end{aligned}$$

we can conclude $\|\boldsymbol{\Phi}_\eta\|_Y^2 \to \infty$ as $\eta \to 0$. With $c_1 > 0$ being the constant introduced in lemma 3.2, we obtain

$$\begin{aligned} \partial_{\boldsymbol{uu}} \mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}_\eta, \boldsymbol{\Phi}_\eta) &= G_c \varepsilon \|\nabla \Phi_\varphi\|_{I \times \Omega}^2 + \frac{G_c}{\varepsilon} \|\Phi_\varphi\|_{I \times \Omega}^2 + (1 - \kappa)(\Phi_\varphi^2 \mathbb{C} e(\bar{u}), e(\bar{u}))_{I \times \Omega} \\ &\le G_c \varepsilon \|\nabla \Phi_\varphi\|_{I \times \Omega}^2 + \frac{G_c}{\varepsilon} \|\Phi_\varphi\|_{I \times \Omega}^2 + c_1 \|\Phi_\varphi\|_{L^\infty(I \times \Omega)}^2 \|\bar{u}\|_{I \times \Omega}^2. \end{aligned}$$

As $\Phi_\varphi(t) = -f_\eta(t)\Psi$ and $|f_\eta(t)| \le 1$ for all $t \in I$, this estimate together with the embedding $V_\varphi = H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ shows that there exists a constant $C > 0$ such that $\partial_{\boldsymbol{uu}} \mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}_\eta, \boldsymbol{\Phi}_\eta) \le C \|\Psi\|_{V_\varphi}^2$ for all $\eta \in (0, \mu(J))$. Consequently for every $\gamma > 0$ we can find η small enough such that $\partial_{\boldsymbol{uu}} \mathcal{L}(\bar{\boldsymbol{u}}, \boldsymbol{l})(\boldsymbol{\Phi}_\eta, \boldsymbol{\Phi}_\eta) < \gamma \|\boldsymbol{\Phi}_\eta\|_Y^2$. $\square$

5 Upper level NLP with phase-field constraint

In this section we consider an optimal control NLP whose constraints are given by (KKT 1)–(KKT 4). The chosen tracking type cost functional models the goal of approximating a desired fracture pattern by finding a suitable control. However, the results extend to all Fréchet differentiable cost functionals. We start by defining the required function spaces and cones. Then, in section 5.3, we characterize the regular points for the upper level NLP and conclude with the full KKT system.

Note that we drop the complementarity condition (KKT 5) in order to obtain a Banach space NLP rather than a Banach space MPCC (mathematical program with complementarity constraints) on the upper level. This optimal control NLP is already novel and hard to solve. The corresponding MPCC would not admit any regular point and would be significantly more complicated both in theory and computation. Of course, after solving the NLP it is easily checked whether the omitted complementarity condition holds anyway, i.e., whether we have a physically valid solution.

5.1 Problem statement

The upper level NLP is defined on the Hilbert space $\mathcal{Y} := W \times Y \times Z^*$ which is equipped with the natural norm

$$\begin{aligned}\|(q, \boldsymbol{u}, \boldsymbol{l})\|_{\mathcal{Y}}^2 &= \|q\|_W^2 + \|\boldsymbol{u}\|_Y^2 + \|\boldsymbol{l}\|_{Z^*}^2 \\ &= \|q\|_{L^2(I,Q)}^2 + \|u\|_{Y_u}^2 + \|\varphi\|_{Y_\varphi}^2 + \|l_1\|_{V_\varphi^*}^2 + \|l_2\|_{L^2(I,V_\varphi^*)}^2.\end{aligned}$$

To simplify the notation, we introduce a semilinear map $a\colon \mathcal{Y} \to Y^*$ representing the stationarity condition (KKT 4),

$$\begin{aligned}a(q, \boldsymbol{u}, \boldsymbol{l}) := {}&(g_\kappa(\varphi)\mathbb{C}e(u), e(P_u(\,\cdot\,)))_{I\times\Omega} - (q, P_u(\,\cdot\,))_{I\times\Gamma_N} + G_c\varepsilon(\nabla\varphi, \nabla P_\varphi(\,\cdot\,))_{I\times\Omega} \\ &- \frac{G_c}{\varepsilon}(1-\varphi, P_\varphi(\,\cdot\,))_{I\times\Omega} + (1-\kappa)(\varphi\mathbb{C}e(u)P_\varphi(\,\cdot\,), e(u))_{I\times\Omega} \\ &- \langle l_1, P_\varphi(\,\cdot\,)(0)\rangle_{V_\varphi^*,V_\varphi} + \int_I \langle l_2(t), \partial_t P_\varphi(\,\cdot\,)(t)\rangle_{V_\varphi^*,V_\varphi}\,\mathrm{d}t.\end{aligned}$$

The map a is nonlinear in $\boldsymbol{u}$ and linear in q and $\boldsymbol{l}$. The cost functional is of tracking type, including a Tikhonov regularization term which is beneficial for numerical stabilization [21, 40, 41]. For some desired spatial phase-field $\varphi_d \in V_\varphi$, a nominal control $q_r \in Q$ and a Tikhonov parameter $\alpha > 0$ the cost functional $\mathcal{J}\colon W \times Y \to \mathbb{R}$ is defined as

$$\mathcal{J}(q, \boldsymbol{u}) := \frac{1}{2}\int_I \left(\|\varphi(t) - \varphi_d\|_\Omega^2 + \alpha\|q(t) - q_r\|_{\Gamma_N}^2\right)\mathrm{d}t. \tag{8}$$

Problem 5.1. *Let the parameters ε, κ, μ, λ and φ_0 be as in problem 3.1. For given $\varphi_d \in V_\varphi$, $q_r \in Q$ and $\alpha > 0$, find a control $q \in W$ and functions $\boldsymbol{u} \in Y$, $\boldsymbol{l} \in Z^*$ that minimize the cost functional $\mathcal{J}$*

subject to eqs. (KKT 1) *to* (KKT 4)*:*

$$\begin{aligned} \min_{(q,\boldsymbol{u},\boldsymbol{l})\in\mathcal{Y}} \quad & \mathcal{J}(q,\boldsymbol{u}) \\ \text{s.t.} \quad & \varphi(0) = \varphi_0 \ \textit{in } V_\varphi, \\ & -\dot{\varphi}(t) \geq 0 \ \textit{in } V_\varphi \ \textit{a.e. in } I, \\ & a(q,\boldsymbol{u},\boldsymbol{l}) = 0 \ \textit{in } Y^*, \\ & l_2(t) \geq 0 \ \textit{in } V_\varphi^* \ \textit{a.e. in } I. \end{aligned} \tag{9}$$

We define the constraints operator $\mathcal{G}\colon \mathcal{Y} \to \mathcal{Z}$ as

$$\mathcal{G} := \begin{pmatrix} \mathcal{G}_\mathcal{E} \\ \mathcal{G}_\mathcal{I} \end{pmatrix}, \quad \mathcal{G}_\mathcal{E}(q,\boldsymbol{u},\boldsymbol{l}) := \begin{pmatrix} \varphi(0) - \varphi_0 \\ a(q,\boldsymbol{u},\boldsymbol{l}) \end{pmatrix} \in V_\varphi \times Y^*,$$

$$\mathcal{G}_\mathcal{I}(q,\boldsymbol{u},\boldsymbol{l}) := \begin{pmatrix} -\dot{\varphi} \\ l_2 \end{pmatrix} \in L^2(I,V_\varphi) \times L^2(I,V_\varphi^*) \quad \text{for all} \quad (q,\boldsymbol{u},\boldsymbol{l}) \in \mathcal{Y}.$$

Consequently the image space of $\mathcal{G}$ reads as $\mathcal{Z} := \mathcal{Z}_1 \times \mathcal{Z}_2 \times \mathcal{Z}_3 \times \mathcal{Z}_4$ where

$$\mathcal{Z}_1 := V_\varphi, \qquad \mathcal{Z}_2 := Y^*, \qquad \mathcal{Z}_3 := L^2(I,V_\varphi), \qquad \mathcal{Z}_4 := L^2(I,V_\varphi^*).$$

The dual space is then

$$\mathcal{Z}^* = V_\varphi^* \times Y^{**} \times L^2(I,V_\varphi^*) \times L^2(I,V_\varphi^{**}),$$

and the constraints cone becomes $\mathcal{K} := \mathcal{K}_1 \times \mathcal{K}_2 \times \mathcal{K}_3 \times \mathcal{K}_4$ where

$$\begin{aligned} \mathcal{K}_1 &:= \{0\} \subset V_\varphi, & \mathcal{K}_3 &:= \{v \in \mathcal{Z}_3 \colon v \geq 0\} \subset L^2(I,V_\varphi), \\ \mathcal{K}_2 &:= \{0\} \subset Y^*, & \mathcal{K}_4 &:= \{v \in \mathcal{Z}_4 \colon v \geq 0\} \subset L^2(I,V_\varphi^*). \end{aligned}$$

Finally the dual cone $\mathcal{K}^*$ of $\mathcal{K} \subset \mathcal{Z}$ is defined as

$$\begin{aligned} \mathcal{K}^* &:= \{\boldsymbol{k} = (k_1,k_2,k_3,k_4) \in \mathcal{Z}^* \colon \boldsymbol{k}\boldsymbol{z} \geq 0 \text{ for all } \boldsymbol{z} = (0,0,z_3,z_4) \in \mathcal{K}\} \\ &= V_\varphi^* \times Y^{**} \times \Big\{ (k_3,k_4) \in L^2(I,V_\varphi^*) \times L^2(I,V_\varphi^{**}) \colon \\ &\qquad \int_I \big(\langle k_3, z_3\rangle_{V_\varphi^*,V_\varphi} + \langle k_4, z_4\rangle_{V_\varphi^{**},V_\varphi^*}\big)\,\mathrm{d}t \geq 0 \text{ for all } (z_3,z_4) \in \mathcal{K}_3 \times \mathcal{K}_4 \Big\}. \end{aligned}$$

5.2 Derivatives

Next we compute the derivatives of $\mathcal{J}\colon \mathcal{Y} \to \mathbb{R}$ and $\mathcal{G}\colon \mathcal{Y} \to \mathcal{Z}$ for all $(q,\boldsymbol{u},\boldsymbol{l}) \in \mathcal{Y}$ and any given direction $h = (\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \in \mathcal{Y}$, where $\boldsymbol{\delta u} = (\delta u, \delta\varphi)$ and $\boldsymbol{\delta l} = (\delta l_1, \delta l_2)$. The quadratic functional $\mathcal{J}$ is infinitely often Fréchet differentiable as a functional $\mathcal{J}\colon (\mathcal{Y}, \|\cdot\|_{L^2}) \to \mathbb{R}$ and hence also as a functional $\mathcal{J}\colon (\mathcal{Y}, \|\cdot\|_\mathcal{Y}) \to \mathbb{R}$:

$$\begin{aligned} \mathcal{J}(q,\boldsymbol{u},\boldsymbol{l}) &= \frac{1}{2}\left(\|\varphi - \varphi_d\|_{I\times\Omega}^2 + \alpha\|q - q_r\|_{I\times\Gamma_N}^2\right), \\ \mathcal{J}'(q,\boldsymbol{u},\boldsymbol{l})h &= (\varphi - \varphi_d, \delta\varphi)_{I\times\Omega} + \alpha(q - q_r, \delta q)_{I\times\Gamma_N}, \\ \mathcal{J}''(q,\boldsymbol{u},\boldsymbol{l})(h_1,h_2) &= (\delta\varphi_1, \delta\varphi_2)_{I\times\Omega} + \alpha(\delta q_1, \delta q_2)_{I\times\Gamma_N}, \end{aligned}$$

and $\mathcal{J}^{(k)} = 0$ for $k > 2$. For the constraint map $\mathcal{G}$ we obtain the derivative

$$\mathcal{G}'(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) = \begin{pmatrix} \delta\varphi(0) \\ a'(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \\ -\delta\dot{\varphi} \\ \delta l_2 \end{pmatrix},$$

and we show in the following proposition that this actually is a Fréchet derivative, focusing on the only nontrivial component.

Proposition 5.1. *The semilinear form $a\colon \mathcal{Y} \to Y^*$ is Fréchet differentiable at every point $(q, \boldsymbol{u}, \boldsymbol{l}) \in \mathcal{Y}$. For each direction $(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \in \mathcal{Y}$, the derivative reads*

$$\begin{aligned} a'(q, \boldsymbol{u}, \boldsymbol{l})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) = {} & (g_\kappa(\varphi)\mathbb{C}e(\delta u), e(P_u(\,\cdot\,)))_{I\times\Omega} \\ & + 2(1-\kappa)(\delta\varphi\varphi\mathbb{C}e(u), e(P_u(\,\cdot\,)))_{I\times\Omega} \\ & - (\delta q, P_u(\,\cdot\,))_{I\times\Gamma_N} + G_c\varepsilon(\nabla\delta\varphi, \nabla P_\varphi(\cdot))_{I\times\Omega} \\ & + \frac{G_c}{\varepsilon}(\delta\varphi, P_\varphi(\,\cdot\,))_{I\times\Omega} + 2(1-\kappa)(\varphi P_\varphi(\,\cdot\,)\mathbb{C}e(\delta u), e(u))_{I\times\Omega} \\ & + (1-\kappa)(\delta\varphi P_\varphi(\,\cdot\,)\mathbb{C}e(u), e(u))_{I\times\Omega} \\ & - \langle \delta l_1, P_\varphi(\,\cdot\,)(0)\rangle_{V_\varphi^*, V_\varphi} + \int_I \langle \delta l_2, \partial_t P_\varphi(\,\cdot\,)\rangle_{V_\varphi^*, V_\varphi}\,\mathrm{d}t. \end{aligned}$$

Proof. We proceed as in the proof of proposition 3.1. Straightforward computations confirm that the expression for a' is indeed the Gâteaux derivative of a. For arbitrary $(q, \boldsymbol{u}, \boldsymbol{l})$, $(\Psi_q, \Psi_{\boldsymbol{u}}, \Psi_{\boldsymbol{l}})$, $(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \in \mathcal{Y}$ and $\boldsymbol{\Phi} \in Y$ we apply lemma 3.2 and the identity $g_\kappa(\varphi + \Psi_\varphi) = g_\kappa(\varphi) + (1-\kappa)(2\varphi\Psi_\varphi + \Psi_\varphi^2)$ to obtain

$$\begin{aligned} & |a'(q + \Psi_q, \boldsymbol{u} + \Psi_{\boldsymbol{u}}, \boldsymbol{l} + \Psi_{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l})(\boldsymbol{\Phi}) - a'(q, \boldsymbol{u}, \boldsymbol{l})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l})(\boldsymbol{\Phi})| \\ & \quad = \big|(1-\kappa)((2\varphi\Psi_\varphi + \Psi_\varphi^2)\mathbb{C}e(\delta u), e(\Phi_u))_{I\times\Omega} + 2(1-\kappa)(\varphi\delta\varphi\mathbb{C}e(\Psi_u), e(\Phi_u))_{I\times\Omega} \\ & \qquad + 2(1-\kappa)(\Psi_\varphi\delta\varphi\mathbb{C}e(u), e(\Phi_u))_{I\times\Omega} + 2(1-\kappa)(\Psi_\varphi\delta\varphi\mathbb{C}e(\Psi_u), e(\Phi_u))_{I\times\Omega} \\ & \qquad + 2(1-\kappa)(\varphi\Phi_\varphi\mathbb{C}e(\delta u), e(\Psi_u))_{I\times\Omega} + 2(1-\kappa)(\Psi_\varphi\Phi_\varphi\mathbb{C}e(\delta u), e(u))_{I\times\Omega} \\ & \qquad + 2(1-\kappa)(\Psi_\varphi\Phi_\varphi\mathbb{C}e(\delta u), e(\Psi_u))_{I\times\Omega} + 2(1-\kappa)(\delta\varphi\Phi_\varphi\mathbb{C}e(u), e(\Psi_u))_{I\times\Omega} \\ & \qquad + (1-\kappa)(\delta\varphi\Phi_\varphi\mathbb{C}e(\Psi_u), e(\Psi_u))_{I\times\Omega}\big| \\ & \quad \le (1-\kappa)C\big(\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y + 2\|\varphi\delta\varphi\|_{L^\infty(I\times\Omega)}\|\Psi_{\boldsymbol{u}}\|_Y \\ & \qquad\qquad + 2\|\Psi_\varphi\delta\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}\|_Y + 2\|\Psi_\varphi\delta\varphi\|_{L^\infty(I\times\Omega)}\|\Psi_{\boldsymbol{u}}\|_Y\big)\|\boldsymbol{\Phi}\|_Y \\ & \qquad + (1-\kappa)C^2\big(2\|\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y + 2\|\Psi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\boldsymbol{u}\|_Y \\ & \qquad\qquad + 2\|\Psi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y + 2\|\delta\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y \\ & \qquad\qquad + \|\delta\varphi\|_{L^\infty(I\times\Omega)}\|\Psi_{\boldsymbol{u}}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y\big)\|\boldsymbol{\Phi}\|_Y, \end{aligned}$$

where C is from lemma 3.2. Consequently it holds that

$$\begin{aligned}
&\|a'(q+\Psi_q, \boldsymbol{u}+\Psi_{\boldsymbol{u}}, \boldsymbol{l}+\Psi_{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) - a'(q, \boldsymbol{u}, \boldsymbol{l})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l})\|_{Y^*} \\
&\quad \le (1-\kappa)C\big(\|2\varphi\Psi_\varphi + \Psi_\varphi^2\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y + 2C^2\|\boldsymbol{u}\|_Y\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y \\
&\qquad\qquad + 2C^2\|\Psi_{\boldsymbol{u}}\|_Y\|\boldsymbol{\delta u}\|_Y\|\boldsymbol{u}\|_Y + 2C^2\|\Psi_{\boldsymbol{u}}\|_Y\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y\big) \\
&\qquad + (1-\kappa)C^2\big(2\|\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y + 2\|\Psi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\boldsymbol{u}\|_Y \\
&\qquad\qquad + 2\|\Psi_\varphi\|_{L^\infty(I\times\Omega)}\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y + 2C\|\boldsymbol{\delta u}\|_Y\|\boldsymbol{u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y \\
&\qquad\qquad + C\|\boldsymbol{\delta u}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y\|\Psi_{\boldsymbol{u}}\|_Y\big),
\end{aligned}$$

and therefore $a'(q+\Psi_q, \boldsymbol{u}+\Psi_{\boldsymbol{u}}, \boldsymbol{l}+\Psi_{\boldsymbol{l}}) \to a'(q, \boldsymbol{u}, \boldsymbol{l})$ in $L(\mathcal{Y}, Y^*)$ as $(\Psi_q, \Psi_{\boldsymbol{u}}, \Psi_{\boldsymbol{l}}) \to 0$. This implies continuity of the Gâteaux derivative, which ensures Fréchet differentiability. ☐

Given any multiplier $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3, \pi_4) \in \mathcal{K}^*$, we thus have

$$\begin{aligned}
\boldsymbol{\pi}\mathcal{G}'(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) &= \langle \pi_1, \delta\varphi(0)\rangle_{V_\varphi^*, V_\varphi} + \langle \pi_2, a'(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l})\rangle_{Y^{**}, Y^*} \\
&\quad - \int_I \langle \pi_3, \delta\dot\varphi\rangle_{V_\varphi^*, V_\varphi}\,\mathrm{d}t - \int_I \langle \pi_4, \delta l_2\rangle_{V_\varphi^{**}, V_\varphi^*}\,\mathrm{d}t.
\end{aligned}$$

5.3 Regularity for the upper level NLP

A feasible point $(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) \in \mathcal{M}$ with $\mathcal{M} = \{(q, \boldsymbol{u}, \boldsymbol{l}) \in \mathcal{Y} \colon \mathcal{G}(q, \boldsymbol{u}, \boldsymbol{l}) \in \mathcal{K}\}$ will be regular for problem 5.1 if

$$\mathcal{Z} = \mathcal{G}'(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})\mathcal{Y} - \mathcal{K}_{\mathcal{G}(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})},$$

where $\mathcal{K}_{\mathcal{G}(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})} = \mathcal{K} + \{\alpha(0, 0, -\dot{\bar\varphi}, -\bar l_2) \colon \alpha \in \mathbb{R}\}$. Thus, given $(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) \in \mathcal{M}$ and any $\boldsymbol{z} = (z_1, z_2, z_3, z_4) \in \mathcal{Z}$, we seek $(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \in \mathcal{Y}$, $(k_3, k_4) \in \mathcal{K}_3 \times \mathcal{K}_4$, and $\alpha \in \mathbb{R}$ such that

$$\begin{aligned}
z_1 &= \delta\varphi(0) \text{ in } V_\varphi, \\
z_2 &= a'(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \text{ in } Y^*, \\
z_3 &= -\delta\dot\varphi - k_3 - \alpha\dot{\bar\varphi} \text{ in } L^2(I, V_\varphi), \\
z_4 &= -\delta l_2 - k_4 - \alpha\bar l_2 \text{ in } L^2(I, V_\varphi^*).
\end{aligned} \tag{10}$$

The following proposition provides a sufficient condition for the characterization of regular points.

Proposition 5.2. *Let $\bar{\boldsymbol{u}} = (\bar u, \bar\varphi) \in Y$ be given such that*

$$\mathbb{C}[g_\kappa(\bar\varphi)e(w_u) + 2(1-\kappa)\bar\varphi e(\bar u)w_\varphi] \not\perp \mathcal{E} \quad \textit{for all} \quad \boldsymbol{w} := (w_u, w_\varphi) \neq 0, \tag{11}$$

where $\mathcal{E} := \{e(v) \colon v \in Y_u\} \subset [L^2(I, L^2(\Omega))]^{2\times 2}$. Then the equation system (10) admits a solution $(\delta q, \delta u, \delta\varphi, \delta l_1, \delta l_2, k_3, k_4, \alpha) \in \mathcal{Y} \times \mathcal{K}_3 \times \mathcal{K}_4 \times \mathbb{R}$.

Proof. Let $\boldsymbol{z} = (z_1, z_2, z_3, z_4) \in \mathcal{Z}$ be arbitrary. Set $\delta\varphi(t) = z_1 - \int_0^t z_3(s)\,\mathrm{d}s$, $k_3 = 0$, $k_4 = 0$, $\delta l_2 = -z_4$, $\alpha = 0$, and $\delta q = 0$. Then the first, third and fourth equations of (10) hold and $\sup_{t\in I}\|\delta\varphi(t)\|_{V_\varphi} < \infty$. It remains to show that we can find solution components $(\delta u, \delta l_1) \in Y_u \times V_\varphi^*$ for the second equation,

$$a'(\bar q, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l})(\boldsymbol{w}) = \langle z_2, \boldsymbol{w}\rangle_{V_\varphi^*, V_\varphi} \quad \text{for all} \quad \boldsymbol{w} := (w_u, w_\varphi) \in Y.$$

This is equivalent to solving $b((\delta u, \delta l_1), \boldsymbol{w}) = r(\boldsymbol{w})$ for all $\boldsymbol{w} \in Y$, where $b\colon \tilde{\mathcal{Y}} \times Y \to \mathbb{R}$ with $\tilde{\mathcal{Y}} := Y_u \times V_\varphi^*$ denotes the bilinear form defined as

$$
\begin{aligned}
b((\delta u, \delta l_1), \boldsymbol{w}) := (g_\kappa(\bar\varphi)\mathbb{C}e(\delta u), e(w_u))_{I\times\Omega} + 2(1-\kappa)(\bar\varphi w_\varphi \mathbb{C}e(\delta u), e(\bar u))_{I\times\Omega} \\
- \langle \delta l_1, w_\varphi(0)\rangle_{V_\varphi^*, V_\varphi} \quad \text{for all} \quad (\delta u, \delta l) \in \mathcal{Y},\ \boldsymbol{w} \in Y,
\end{aligned}
$$

and $r(\boldsymbol{w})$ denotes the corresponding right hand side

$$
\begin{aligned}
r(\boldsymbol{w}) := \langle z_2, \boldsymbol{w}\rangle_{V_\varphi^*, V_\varphi} - \Big(& 2(1-\kappa)(\delta\varphi\bar\varphi\mathbb{C}e(\bar u), e(w_u))_{I\times\Omega} + G_c\varepsilon(\nabla\delta\varphi, \nabla w_\varphi)_{I\times\Omega} \\
&+ (1-\kappa)(\delta\varphi w_\varphi \mathbb{C}e(\bar u), e(\bar u))_{I\times\Omega} \\
&+ \frac{G_c}{\varepsilon}(\delta\varphi, w_\varphi)_{I\times\Omega} + \int_I \langle \delta l_2, \partial_t w_\varphi\rangle_{V_\varphi^*, V_\varphi}\,\mathrm{d}t\Big), \quad \boldsymbol{w} \in Y.
\end{aligned}
$$

Clearly, $r \in Y^*$. In order to apply the Babuška-Lax-Milgram theorem [44, Theorem 5.1.2], we have to show that b is continuous and weakly coercive:

$$
\exists C > 0\colon \sup_{\|\boldsymbol{w}\|_Y = 1} |b((\delta u, \delta l_1), \boldsymbol{w})| \geq C\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}} \quad \text{for all} \quad (\delta u, \delta l_1) \in \tilde{\mathcal{Y}}, \tag{12}
$$

$$
\sup_{\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}} = 1} |b((\delta u, \delta l_1), \boldsymbol{w})| > 0 \quad \text{for all} \quad 0 \neq \boldsymbol{w} \in Y, \tag{13}
$$

where $\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}} := \|\delta u\|_{Y_u} + \|\delta l_1\|_{V_\varphi^*}$. Setting $U := L^\infty(I \times \Omega)$ for brevity, we obtain continuity from the fact that there is $c > 0$ such that

$$
\begin{aligned}
|b((\delta u, \delta l_1), \boldsymbol{w})| &\leq |(g_\kappa(\bar\varphi)\mathbb{C}e(\delta u), e(w_u))_{I\times\Omega}| + |2(1-\kappa)(\bar\varphi w_\varphi \mathbb{C}e(\delta u), e(\bar u))_{I\times\Omega}| \\
&\quad + |\langle \delta l_1, w_\varphi(0)\rangle_{V_\varphi^*, V_\varphi}| \\
&\leq c\big(\|\bar\varphi\|_U^2 \|\nabla\delta u\|_{I\times\Omega}\|\nabla w_u\|_{I\times\Omega} + \|\bar\varphi\|_U\|\nabla\delta u\|_{I\times\Omega}\|\nabla\bar u\|_{I\times\Omega}\|w_\varphi\|_U \\
&\quad + \|\delta l_1\|_{V_\varphi^*}\|w_\varphi(0)\|_{V_\varphi}\big)
\end{aligned}
$$

for all $(\delta u, \delta l_1, \boldsymbol{w}) \in \tilde{\mathcal{Y}} \times Y$. With $c_1 := \|\bar\varphi\|_U$, $c_2 := \|\nabla\bar u\|_{I\times\Omega}$ and $\tilde c = c(c_1^2 + c_1c_2 + 1)$ it holds that

$$
\begin{aligned}
|b((\delta u, \delta l_1), \boldsymbol{w})| &\leq c\big(c_1^2\|\nabla\delta u\|_{I\times\Omega}\|\nabla w_u\|_{I\times\Omega} + c_1c_2\|\nabla\delta u\|_{I\times\Omega}\|w_\varphi\|_U \\
&\quad + \|\delta l_1\|_{V_\varphi^*}\|w_\varphi(0)\|_{V_\varphi}\big) \\
&\leq c\big(c_1^2\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}}\|\boldsymbol{w}\|_Y + c_1c_2\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}}\|\boldsymbol{w}\|_Y \\
&\quad + \|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}}\|\boldsymbol{w}\|_Y\big) \\
&\leq \tilde c\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}}\|\boldsymbol{w}\|_Y.
\end{aligned}
$$

Now the first coercivity condition eq. (12) can be seen to hold by setting $(w_u, w_\varphi) = (\delta u/\|\delta u\|_{Y_u}, 0)$ in the supremum,

$$
\begin{aligned}
\sup_{\|(w_u, w_\varphi)\|_Y = 1} &\big|(g_\kappa(\bar\varphi)\mathbb{C}e(\delta u), e(w_u))_{I\times\Omega} + (1-\kappa)(\bar\varphi w_\varphi\mathbb{C}e(\delta u), e(\bar u))_{I\times\Omega} \\
&+ \langle \delta l_1, w_\varphi(0)\rangle_{V_\varphi^*, V_\varphi}\big| \\
&\geq \left|\frac{1}{\|\delta u\|_{Y_u}}(g_\kappa(\bar\varphi)\mathbb{C}e(\delta u), e(\delta u))_{I\times\Omega}\right| \geq \frac{C}{\|\delta u\|_{Y_u}}\|\delta u\|_{Y_u}^2 = C\|\delta u\|_{Y_u},
\end{aligned}
$$

where C in the last inequality is taken from Korn's inequality. To prove the second coercivity condition eq. (13), we distinguish the cases $w_\varphi(0) = 0$ and $w_\varphi(0) \neq 0$. If $w_\varphi(0) \neq 0$, then there exists $\delta l_1 \in Z_1^*$ with $\|\delta l_1\|_{Z_1^*} = 1$ such that

$$\langle \delta l_1, w_\varphi(0)\rangle_{V_\varphi^*, V_\varphi} \neq 0.$$

By setting $\delta u = 0$ we have $\|(\delta u, \delta l_1)\|_{\tilde{\mathcal{Y}}} = 1$, and it holds that

$$|b((\delta u, \delta l_1), \boldsymbol{w})| = |\langle \delta l_1, w_\varphi(0)\rangle_{V_\varphi^*, V_\varphi}| > 0.$$

If $w_\varphi(0) = 0$, we set $\delta l_1 = 0$ and conclude from eq. (11) that there exists $\delta u \in Y_u$ with $\|\delta u\|_{Y_u} = 1$ such that

$$(e(\delta u), \mathbb{C}[g_\kappa(\bar{\varphi})e(w_u) + 2(1-\kappa)\bar{\varphi}e(\bar{u})w_\varphi])_{I\times\Omega} \neq 0$$

and thus

$$|b((\delta u, \delta l_1), \boldsymbol{w})| = |(g_\kappa(\bar{\varphi})\mathbb{C}e(\delta u), e(w_u))_{I\times\Omega} + 2(1-\kappa)(\bar{\varphi}w_\varphi\mathbb{C}e(\delta u), e(\bar{u}))_{I\times\Omega}| > 0.$$

Consequently eq. (12) and eq. (13) hold and, due to the Babuška-Lax-Milgram theorem, there exists a solution $(\delta q, \boldsymbol{\delta u}, \boldsymbol{\delta l}) \in \mathcal{Y}$ of the second equation of eq. (10), and hence a solution of the entire system eq. (10). □

By proposition 5.2 we can ensure that every feasible point $(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) \in \mathcal{M}$ which fulfills condition eq. (11) is regular for problem 5.1.

Remark 5.2. *It is apparent that every pair $(\bar{u}, \bar{\varphi})$ with $e(\bar{u}) = 0$ or $\bar{\varphi} = 0$ violates the condition eq. (11): simply choose $\boldsymbol{w} = (0, w_\varphi)$ with $w_\varphi \neq 0$. From a mechanics viewpoint, we first notice that a similar condition for the phase-field part exists, in which $2\mathbb{C}(1-\kappa)\bar{\varphi}e(\bar{u})w_\varphi$ is interpreted as some force that drives the fracture field ([33, Section 3]; see also [50, Section 4.5.3]). This interpretation is related to the complementarity condition that relates the bulk energy to crack growth. The situation is similar in eq. (11) except that $\mathbb{C}(1-\kappa)\bar{\varphi}e(\bar{u})w_\varphi$ acts as a right hand side driving force for the displacement equation. This can be compared with classical elasticity, where the conservation of momentum is driven by right hand side volume and traction forces. Clearly, when the right hand sides are zero, and having $u \in V_u$, i.e., $u = 0$ on Γ_D, we obtain trivial solutions, which are not of interest from the mechanics viewpoint. Thus, condition eq. (11) simply excludes mechanically irrelevant solutions.*

5.4 Optimality conditions

In order to formulate optimality conditions, we finally translate theorem 2.2 to the setting of problem (9).

Proposition 5.3. *Let $(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) \in \mathcal{M}$ be a regular minimizer of (9). Then there is a multiplier $\boldsymbol{\pi} =$*

$(\pi_1, \pi_2, \pi_3, \pi_4) \in \mathcal{Z}^*$ *such that the KKT system*

$$\bar{\varphi}(0) = \varphi_0 \text{ in } V_\varphi, \tag{KKTN 1}$$

$$-\dot{\bar{\varphi}}(t) \geq 0 \text{ in } V_\varphi \text{ a.e. in } I, \tag{KKTN 2}$$

$$a(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) = 0 \text{ in } Y^*, \tag{KKTN 3}$$

$$-\bar{l}_2(t) \geq 0 \text{ in } V_\varphi^* \text{ a.e. in } I, \tag{KKTN 4}$$

$$\pi_3(t) \geq 0 \text{ in } V_\varphi^* \text{ a.e. in } I, \tag{KKTN 5}$$

$$\pi_4(t) \geq 0 \text{ in } V_\varphi^{**} \text{ a.e. in } I, \tag{KKTN 6}$$

$$\begin{aligned} &\int_I \left[(P_\varphi(\,\cdot\,), \bar{\varphi} - \varphi_d)_\Omega + (P_q(\,\cdot\,), \bar{q} - q_r)_\Omega\right] \mathrm{d}t \\ &- \langle \pi_1, P_\varphi(\,\cdot\,)(0)\rangle_{V_\varphi^*, V_\varphi} - \langle \pi_2, a'(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})(P_q(\,\cdot\,), P_{\boldsymbol{u}}(\,\cdot\,), P_{\boldsymbol{l}}(\,\cdot\,))\rangle_{Y^{**}, Y^*} \\ &\qquad + \int_I \left(\langle \pi_3, \partial_t P_\varphi(\,\cdot\,)\rangle_{V_\varphi^*, V_\varphi} + \langle \pi_4, P_{l_2}(\,\cdot\,)\rangle_{V_\varphi^{**}, V_\varphi^*}\right) \mathrm{d}t = 0, \end{aligned} \tag{KKTN 7}$$

$$\begin{aligned} &\langle \pi_1, \bar{\varphi}(0) - \varphi_0\rangle_{V_\varphi^*, V_\varphi} + \langle \pi_2, a(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}})\rangle_{Y^{**}, Y^*} \\ &\qquad - \int_I \left(\langle \pi_3, \dot{\bar{\varphi}}\rangle_{V_\varphi^*, V_\varphi} - \langle \pi_4, \bar{l}_2\rangle_{V_\varphi^{**}, V_\varphi^*}\right) \mathrm{d}t = 0 \end{aligned} \tag{KKTN 8}$$

is satisfied, where we have used the projections defined by $P_q(\boldsymbol{\Phi}) = \Phi_q$, $P_{\boldsymbol{u}}(\boldsymbol{\Phi}) = \Phi_{\boldsymbol{u}}$, $P_{\boldsymbol{l}}(\boldsymbol{\Phi}) = \Phi_{\boldsymbol{l}}$, $P_{l_2}(\boldsymbol{\Phi}) = \Phi_{l_2}$.

Proof. Conditions (KKTN 1)–(KKTN 4) are just feasibility $(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) \in \mathcal{M}$ for the primal variables. Conditions (KKTN 5) and (KKTN 6) are feasibility for the multiplier, that is, $\boldsymbol{\pi} \in \mathcal{K}^*$. The stationarity condition $\mathcal{J}'(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) - \boldsymbol{\pi}\mathcal{G}'(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) = 0 \in \mathcal{Y}^*$ from theorem 2.2 is presented in (KKTN 7). At last (KKTN 8) is the complementarity condition $\boldsymbol{\pi}\mathcal{G}(\bar{q}, \bar{\boldsymbol{u}}, \bar{\boldsymbol{l}}) = 0$, again asserted by theorem 2.2. ☐

Remark 5.3. *For the sake of clarity, throughout the article, we have kept* V_φ^* *and* V_φ *separate, although, being a Hilbert space and its dual, they are isomorphic and could be identified with each other.*

6 Conclusions

In this paper, we rigorously established a space-time phase-field fracture complementarity model in combination with an optimal control problem. By formulating phase-field fracture as an abstract NLP in Banach spaces, a complementarity system was obtained. This derivation includes all cones necessary to characterize the multiplier. Within this formulation the crack irreversibility was treated as an inequality constraint for the time derivative of the phase-field. Hence a careful selection of a suitable functional framework was necessary to obtain regularity results for the lower-level phase-field NLP. In this process, all required differentiability results, i.e., Fréchet differentiability of the energy and the constraints, were rigorously shown. In section 4, we discussed necessary optimality conditions of second order together with first and second order sufficient conditions. The KKT system resulting from the lower level problem then served as the constraint for the optimal control problem, which is again formulated as an abstract NLP in Banach spaces. Under certain conditions, regularity results for the higher level NLP were shown. These conditions were then briefly interpreted from a mechanical viewpoint. Finally, we presented the full KKT system for the optimal control problem.

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