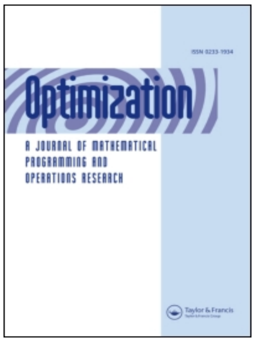

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Identification of some nonsmooth evolution systems with illustration on adhesive contacts at small strains

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A class of evolution quasi-static systems which leads, after a suitable time discretization, to recursive non-linear programs, is considered and optimal control or identification problems governed by such systems are investigated. The resulting problem is an evolutionary Mathematical Programs with Equilibrium Constraints. A subgradient information of the (in general nonsmooth) composite objective function is evaluated and the problem is solved by the implicit programming approach. The abstract theory is illustrated on an identification problem governed by delamination of a unilateral adhesive contact of elastic bodies discretized by finite-element method in space and a semiimplicit formula in time. Being motivated by practical tasks, an identification problem of the fracture toughness and of the elasticity moduli of the adhesive is computationally implemented and tested numerically on a two-dimensional example. Other applications including frictional contacts or bulk damage, plasticity or phase transformations are outlined.

Keywords: rate-independent systems; optimal control; identification; fractional-step time discretization; quadratic programming; gradient evaluation; variational analysis; implicit programming approach; limiting subdifferential; coderivative; nonsmooth contact mechanics; delamination

AMS Subject Classifications: 35Q90; 49N10; 65K15; 65M32; 74M15; 74P10; 90C20

1. Introduction

Many evolution systems have the structure of the *generalized gradient flow*

$$\dot{q} \in \partial_\xi \mathscr{R}^*(q; -\partial_q \mathscr{E}(t, q))$$

with functionals $\mathscr{E}(t, q)$ and $\mathscr{R}^*(q; \xi)$. Here, q is an abstract state of the system and $\dot{q}$ denotes its time derivative. Quite typically, $\mathscr{R}^*(q; \cdot)$ is convex and, making the conjugate of $\mathscr{R}^*(q; \xi)$ with respect to the 'driving force' variable ξ, i.e. $\mathscr{R}(q; v) = \sup_\xi[\langle v, \xi\rangle - \mathscr{R}^*(q; \xi)]$, the generalized gradient flow can equivalently be written in the Biot-equation form

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$$\partial_{\dot{q}}\mathscr{R}(q;\dot{q}) + \partial_q\mathscr{E}(t,q) \ni 0. \tag{1}$$

In many cases, the problem is nonsmooth due to a nonsmoothness of $\mathscr{R}(q;\cdot)$ or $\mathscr{E}(t,q)$, which is why we wrote inclusion in (1) rather than equality. Ansatz (1) is very general and covers great variety of problems in particular in nonsmooth continuum mechanics. The state variable q may involve displacements and various internal parameters (but also various concentrations of some constituents subjected to diffusive processes). In this paper, we focus on a subclass of such problems where the state has the structure

$$q = (u, z) \tag{2}$$

for each time instance t in a Banach space $U \times Z$. In this way, a quasi-static *plasticity*, or *damage* or various *phase transformations* at small strains can be modelled, and also various problems in *contact mechanics* like friction or adhesion, together with various combinations of these phenomena.

After a suitable time discretization, (1) gives rise to recursive optimization problems. Often (or, in applications in continuum mechanics we have in mind, rather typically) q ranges over an infinite-dimensional Banach space and, after a possible 'spatial' discretization, these minimization problems have a structure of strictly convex *Quadratic Programming* problems. It is then relatively easy to use such a discretized evolution problem as a governing system for some optimization problem, e.g. optimal control or identification of parameters. This leads to *Mathematical Programs with Evolution Equilibrium Constraints* (MPEEC) which have been studied, e.g. in [1–3].

The functionals in (1) depend also on an abstract parameter π and have a special form

$$\begin{aligned}\mathscr{R}(\pi,q;\dot{q}) &= \mathscr{R}_1(\pi,u,z;\dot{u}) + \mathscr{R}_2(\pi,u,z;\dot{z}),\\ \mathscr{E}(t,\pi,q) &= \mathscr{E}(t,\pi,u,z).\end{aligned}$$

We then consider an optimal-control or an identification problem on a fixed time interval $[0,T]$:

$$\begin{aligned}&\text{Minimize } \int_0^T j(u,z)\,\mathrm{d}t + H(\pi)\\ &\text{subject to } \partial_{\dot{u}}\mathscr{R}_1(\pi,u,z;\dot{u}) + \partial_u\mathscr{E}(t,\pi,u,z) \ni 0 \quad \text{for a.a. } t\in[0,T], \quad u(0)=u_0,\\ &\qquad\qquad\ \partial_{\dot{z}}\mathscr{R}_2(\pi,u,z;\dot{z}) + \partial_z\mathscr{E}(t,\pi,u,z) \ni 0 \quad \text{for a.a. } t\in[0,T], \quad z(0)=z_0,\\ &\qquad\qquad\ u\in L^\infty(0,T;U), \quad z\in L^\infty(0,T;Z), \quad \pi\in\Pi\end{aligned} \tag{3}$$

with some $j : U \times Z \to \mathbb{R}$ and $H : \Pi \to \mathbb{R}$ specified later; here Π is a closed convex set of a Banach space where π lives. In some models, the flow rule for u in (3) is purely static, i.e. $\mathscr{R}_1 = 0$. In this case, if there is no dissipation in this part, then only z_0, but not u_0 is decisive when considering $\partial_u\mathscr{E}(t,\pi,u_0,z_0) \ni 0$. We use the standard notation for Bochner space $L^\infty(0,T;\cdot)$ of Banach-space-valued Bochner measurable functions on $[0,T]$.

The main aim of the paper is a deep analysis of a discretized version of MPEEC (3) leading both to sharp necessary optimality conditions as well as to an efficient numerical procedure based on the so-called *Implicit Programming* approach (ImP), cf. [4,5]. In particular, on the basis of the subdifferential calculus of Mordukhovich [6,7] we will show that the *solution map* $S : \pi \mapsto (u,z)$ defined via the discretized equilibrium relations in (3), is single-valued and locally Lipschitz and satisfies henceforth the basic ImP hypothesis. In the respective proof, one has to deal with a difficult multifunction arising in connection with our *evolving* constraint sets. The application of standard tools of generalized differential calculus provides us in this case only with an upper estimate of the coderivative of the normal cone mapping to the *overall* constraint set, which could be a substantial drawback both in the optimality conditions as well as in the used numerical approach. To overcome this hurdle, we have employed a new result from [8], which enables us to compute the limiting coderivative of the mentioned normal cone mapping *exactly*.

The plan of the paper is the following. In Section 2, we briefly introduce a suitable discretization of the identification problem (3) that yields a unique response (u, z) of the constraint system of (3) for a given π and allows for efficient optimization technique. After introducing some notation and notions from variational analysis in Section 3, we formulate in Section 4 first-order necessary optimality condition for the discrete version of MPEEC (3) and derive a subgradient formula for the composite objective function of the discretized problem. In Section 5, we formulate a specific application-motivated identification problem from contact continuum mechanics that fits (and illustrates) the system (3). Eventually, in Section 6, we illustrate the usage of the subgradient evaluation procedure via an adhesive contact problem in a non-trivial two-dimensional example involving a spatial discretization by *Finite-Element-Method* (FEM).

2. Discretization of the identification problem (3)

The natural procedure is to discretize the problem (3) in time. This might be a rather delicate problem, especially when the inclusions in the controlled system (3) exhibit responses of different time scales, and in particular with tendencies for jumping, which quite typically happens in rate-independent systems governed by non-convex potentials $\mathscr{E}(t, \pi, \cdot, \cdot)$.

We consider (for simplicity) an equidistant partition of the time interval $[0, T]$ with a time step $\tau > 0$ such that $T/\tau =: K \in \mathbb{N}$ and then a fractional-step-type semi-implicit time discretization of (3). Moreover, if U, Z or Π is infinite-dimensional, the time-discrete problem still remains infinite-dimensional, and to implement it on computers, we need to apply also an abstract space discretization controlled by a parameter, let us denote it by $h > 0$. Such an approximation can be considered by replacing U, Z and Π in (4) by their finite-dimensional subsets U_h, Z_h, and Π_h. Counting also a possible numerical approximation of $\mathscr{E}$, denoted by $\mathscr{E}_h$, altogether, (3) turns into the problem:

$$\begin{aligned}
&\text{Minimize } \tau \textstyle\sum_{k=1}^{K} j(u_{\tau h}^k, z_{\tau h}^k) + H(\pi)\\
&\text{subject to } \partial_{\dot{u}}\mathscr{R}_1\Big(\pi, u_{\tau h}^{k-1}, z_{\tau h}^{k-1}; \frac{u_{\tau h}^k - u_{\tau h}^{k-1}}{\tau}\Big) + \partial_u \mathscr{E}_h(k\tau, \pi, u_{\tau h}^k, z_{\tau h}^{k-1}) \ni 0, \quad u_{\tau h}^0 = u_{0h},\\
&\qquad \partial_{\dot{z}}\mathscr{R}_2\Big(\pi, u_{\tau h}^{k-1}, z_{\tau h}^{k-1}; \frac{z_{\tau h}^k - z_{\tau h}^{k-1}}{\tau}\Big) + \partial_z \mathscr{E}_h(k\tau, \pi, u_{\tau h}^k, z_{\tau h}^k) \ni 0, \qquad z_{\tau h}^0 = z_{0h},\\
&\qquad u_{\tau h}^k \in U_h \ \text{ and } \ z_{\tau h}^k \in Z_h \ \text{ for } k = 1, \ldots, K, \quad \pi \in \Pi_h,
\end{aligned} \tag{4}$$

where $(u_{0h}, z_{0h}) \in U_h \times Z_h$ is an approximation of the initial condition (u_0, z_0). Let us note that the controlled system (4) decouples so that, for a given π, one has to solve alternating optimization problems

$$\text{Minimize } \tau\mathscr{R}_1\Big(\pi, u_{\tau h}^{k-1}, z_{\tau h}^{k-1}; \frac{u - u_{\tau h}^{k-1}}{\tau}\Big) + \mathscr{E}_h(k\tau, \pi, u, z_{\tau h}^{k-1}) \text{ subject to } u \in U_h \tag{5a}$$

and, taking (one of) its solution for $u^k_{\tau h}$, further

$$\text{Minimize } \tau\mathscr{R}_2\Big(\pi, u^{k-1}_{\tau h}, z^{k-1}_{\tau h}; \frac{z - z^{k-1}_{\tau h}}{\tau}\Big) + \mathscr{E}_h(k\tau, \pi, u^k_{\tau h}, z) \text{ subject to } z \in Z_h \tag{5b}$$

which yields $z^k_{\tau h}$ as (one of) its solution. Assuming $\mathscr{E}(t, \pi, \cdot, \cdot)$ as well as its approximation $\mathscr{E}_h(t, \pi, \cdot, \cdot)$ separately strictly convex (and, of course, coercive with compact level sets) and $\mathscr{R}_i(\pi, u, z; \cdot)$ convex, $i = 1, 2$, both problems in (5) have unique solutions $u^k_{\tau h}$ and $z^k_{\tau h}$, respectively, and thus the whole recursive problem in the constraint system of (4) has a unique response for a given π as well. This allows us to reformulate (4) as a minimization problem for a functional depending on π only, cf. (9) below. This will be exactly the situation we will consider in the rest of this article. The fully discretized system (4) can thus be understood as an MPEC for which a developed theory exists.

In what follows, we will confine ourselves to problems with a bit more detailed (but nevertheless still fairly general) structure, namely

$$\mathscr{E}(t, \pi, u, z) = \begin{cases} \mathcal{E}(t, \pi, u, z) & \text{if } u \in \Lambda^t_0,\ z \in K^t_0, \\ \infty & \text{otherwise,} \end{cases} \tag{6a}$$

$$\mathscr{R}_1(\pi, u, z, \dot{u}) = \mathcal{R}_1(\pi, u, z, \dot{u}), \tag{6b}$$

$$\mathscr{R}_2(\pi, u, z, \dot{z}) = \begin{cases} \mathcal{R}_2(\pi, u, z, \dot{z}) & \text{if } \dot{z} \in K_1, \\ \infty & \text{otherwise,} \end{cases} \tag{6c}$$

where $\mathcal{E}$, $\mathcal{R}_1$, and $\mathcal{R}_2$ are finite and smooth, Λ^t_0, K^t_0, and K_1 are convex closed set, the last one being a cone. We will use $\mathcal{E}_h$ as a possible approximation of $\mathcal{E}$.

Although, in Section 6, we will illustrate usage of this model on a rather special inverse adhesive-contact problem, most of the considerations can expectedly be applied (after possible modification) to many other problems from continuum mechanics and physics, as (various combination of) damage, phase-transformations, plasticity, etc.

Remark 1 (Stability and convergence for $\tau \to 0$ and $h \to 0$) The focus of this article is on the identification of the discrete finite-dimensional problem. Nevertheless, the convergence towards the original continuous problem when $\tau \to 0$ and $h \to 0$ is of interest.

Without going into (usually rather technical) details, let us only mention that under certain qualification of $\mathscr{R}_1$, $\mathscr{R}_2$ and $\mathscr{E}_h$, a boundedness (= numerical stability) and convergence of a solution $(u_{\tau h}, z_{\tau h})$ to the discrete state problem obtained by interpolation from values $(u^k_{\tau h}, z^k_{\tau h})^K_{k=1}$ towards a weak solution (u, z) to controlled state system for a fixed π can usually be shown at least in terms of subsequences in various situation. A rather simple situation is if $\mathscr{R}_2$, or possibly also $\mathscr{R}_1$, is uniformly convex; this corresponds to some viscosity. In a special fully rate-independent case when $\mathscr{R}_1 = 0$ and $\mathscr{R}_2(\pi, u, z; \cdot)$ is 1-homogeneous and independent of (u, z), such convergence was proved in [9]; in this case the weak solutions are called local solutions. The uniqueness is, however, not guaranteed in general. If $\mathscr{E}(t, \pi, \cdot, \cdot)$ is jointly uniformly convex, then this uniqueness and even continuous dependence on π hold, cf. [10,11] for a survey of such situations. This is, e.g. the case of linearized rate-independent plasticity with hardening. Sometimes, viscosity can help for this uniqueness. This is the case of frictional normal-compliance contact of viscoelastic bodies which, after a certain algebraic manipulation gets the structure with $\mathscr{E}(t, \pi, \cdot, \cdot)$ separately uniformly quadratic with linear constraints in two-dimensions, cf. [12], or with conical constraints in three-dimensions. The uniqueness of the response of the continuous problems was shown in [13].

As usual, the convergence of solutions to (4) towards solutions to (3) is much more delicate and it is a well-known fact that it cannot be expected unless the controlled state system in (3) has a unique response or at least any solution to (1) can be attained by the discretized solutions, which is however usually not granted unless the solution to (1) is unique. In any case, one needs to show the continuous convergence of the solution map $S_{\tau h} : \pi \mapsto (u_{\tau h}, z_{\tau h})$, i.e. that $\tau \to 0$ and $h \to 0$ and $\widetilde{\pi} \to \pi$ implies $S_{\tau h}(\widetilde{\pi}) \to S(\pi)$. This is usually a relatively simple modification of the convergence for π fixed.

3. Notation and selected notions of variational analysis

Having in mind the discrete problem with $\tau > 0$ and $h > 0$, we will use notation

$$p^k_{\tau h}(\pi, \widetilde{u}, u, \widetilde{z}) := \nabla_u \mathcal{R}_1\Big(\pi, \widetilde{u}, \widetilde{z}, \frac{u-\widetilde{u}}{\tau}\Big) + \nabla_u \mathcal{E}_h\big(k\tau, \pi, u, \widetilde{z}\big), \tag{7a}$$

$$q^k_{\tau h}(\pi, \widetilde{u}, u, \widetilde{z}, z) := \nabla_z \mathcal{R}_2\Big(\pi, \widetilde{u}, \widetilde{z}, \frac{z-\widetilde{z}}{\tau}\Big) + \nabla_z \mathcal{E}_h\big(k\tau, \pi, u, z\big), \tag{7b}$$

$$\mathfrak{K}^k(\tilde{z}) := \big(K_1 + \tilde{z}\big) \cap K_0^{k\tau}, \tag{7c}$$

$$J(\pi, \hat{u}, \hat{z}) := \tau \sum_{k=1}^{K} j(u^k, z^k) + H(\pi) \quad \text{with } \hat{u} = (u^1, \ldots, u^K) \text{ and } \hat{z} = (z^1, \ldots, z^K). \tag{7d}$$

Since problems (5) are convex, necessary optimality conditions are also sufficient and thus, taking into account structure (6), problem (4) can equivalently be written in the form:

$$\begin{aligned}
&\text{Minimize } J(\pi, u_{\tau h}, z_{\tau h}) \quad \text{with } u_{\tau h} := (u^1_{\tau h}, \ldots, u^K_{\tau h}) \text{ and } z_{\tau h} = (z^1_{\tau h}, \ldots, z^K_{\tau h})\\
&\text{subject to } 0 \in p^k_{\tau h}(\pi, u^{k-1}_{\tau h}, u^k_{\tau h}, z^{k-1}_{\tau h}) + \mathrm{N}_{\Lambda^k_\tau}(u^k_{\tau h}), \qquad k = 1, \ldots, K, \qquad u^0_{\tau h} = u_{0h},\\
&\qquad 0 \in q^k_{\tau h}(\pi, u^{k-1}_{\tau h}, u^k_{\tau h}, z^{k-1}_{\tau h}, z^k_{\tau h}) + \mathrm{N}_{\mathfrak{K}^k(z^{k-1}_{\tau h})}(z^k_{\tau h}),\ k = 1, \ldots, K,\ z^0_{\tau h} = z_{0h},\\
&\qquad \pi \in \Pi_h
\end{aligned} \tag{8}$$

with $K = T/\tau$. Defining the solution map $S_{\tau h} : \pi \mapsto (u, z)$ implicitly via the constraints in (8), we may use the so-called implicit programming approach to rewrite problem (8) equivalently into the form

$$\text{Minimize } J(\pi, S_{\tau h}(\pi)) \text{ subject to } \pi \in \Pi_h. \tag{9}$$

In the rest of the paper, we will make use of the following standing assumption, which imply in particular the single-valuedness of the solution map $S_{\tau h}$:

(A1): $\mathscr{E}_h(t, \pi, u, \cdot)$ and $\mathscr{E}_h(t, \pi, \cdot, z)$ are strictly convex,
(A2): $\mathscr{R}_1(\pi, u, z, \cdot)$ and $\mathscr{R}_2(\pi, u, z, \cdot)$ are convex,
(A3): $p^k_{\tau h}(\pi, \tilde{u}, \cdot, z)$ and $q^k_{\tau h}(\pi, \tilde{u}, u, \tilde{z}, \cdot)$ are continuously differentiable mappings, and
(A4): Λ^k and $\mathfrak{K}^k(\tilde{z})$ are closed convex sets.

Note that (A1)–(A3) imply that $p^k_{\tau h}(\pi, \tilde{u}, \cdot, z)$ and $q^k_{\tau h}(\pi, \tilde{u}, u, \tilde{z}, \cdot)$ have a positive definite Jacobian.

In what follows, we will fix time (and, if any, also space) discretization and thus we will omit τ and h in the following sections. The dimension of U_h, Z_h and Π_h will be, respectively, denoted by N, M and L.

Before devising a (necessarily) quite complicated procedure to evaluate a gradient information for the nonsmooth functional $\pi \mapsto J(\pi, S(\pi))$, let us still briefly present basic notions from variational analysis which are essential for this paper. More information can be found in [7] for finite-dimensional setting or in [6] and [14] for the general infinite-dimensional case.

All objects in this section are finite-dimensional. For a sequence of sets $A_k \subset \mathbb{R}^n$ we define the Painlevé-Kuratowski upper limit as

$$\operatorname*{Limsup}_{k\to\infty} A_k = \left\{x \mid \exists x_k \in A_k,\ x \text{ is an accumulation point of } \{x_k\}\right\}.$$

Using this construction, we define for any $\bar{x} \in A$ the Bouligand tangent cone, Fréchet normal cone and the limiting normal cone, respectively, as

$$\begin{aligned}
\mathrm{T}_A(\bar{x}) &= \left\{v \mid \exists v_k \to v,\ \lambda_k \searrow 0,\ \bar{x} + \lambda_k v_k \in A\right\},\\
\hat{\mathrm{N}}_A(\bar{x}) &= (\mathrm{T}_A(\bar{x}))^* = \left\{x^* \mid \langle x^*, v\rangle \le 0 \text{ for all } v \in T_A(\bar{x})\right\},\\
\mathrm{N}_A(\bar{x}) &= \operatorname*{Limsup}_{x \xrightarrow{A} \bar{x}} \hat{\mathrm{N}}_A(x),
\end{aligned}$$

where by $x \xrightarrow{A} \bar{x}$ we understand $x \to \bar{x}$ with $x \in A$. If $\mathrm{N}_A(\bar{\pi}) = \hat{\mathrm{N}}_A(\bar{\pi})$, then we say that $\bar{\pi}$ is a regular point of A, otherwise it is a non-regular point.

To a function $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ we can define its subdifferential at $\bar{x}$ as

$$\partial f(\bar{x}) = \left\{x^* \mid (x^*, -1) \in \mathrm{N}_{\mathrm{epi}\, f}(\bar{x}, f(\bar{x}))\right\}.$$

If A happens to be convex, both normal cones coincide and are equal to the normal cone in the standard sense of convex analysis

$$\mathrm{N}_A(\bar{x}) = \left\{x^* \mid \langle x^*, x - \bar{x}\rangle \le 0 \text{ for all } x \in A\right\}$$

and similarly, if f is continuously differentiable at $\bar{x}$, then $\partial f(\bar{x}) = \{\nabla f(\bar{x})\}$.

For a set-valued mapping $M : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ and for any $(\bar{x}, \bar{y}) \in \operatorname{gph} M$ we define the coderivative $\mathrm{D}^* M(\bar{x}, \bar{y}) : \mathbb{R}^m \rightrightarrows \mathbb{R}^n$ at this point as

$$\mathrm{D}^* M(\bar{x}, \bar{y})(y^*) = \left\{x^* \mid (x^*, -y^*) \in \mathrm{N}_{\operatorname{gph} M}(\bar{x}, \bar{y})\right\}$$

If M is single-valued, we write only $\mathrm{D}^* M(\bar{x})(y^*)$ instead of $\mathrm{D}^* M(\bar{x}, M(\bar{x}))(y^*)$. If M is single-valued and smooth, then its coderivative amounts to the adjoint Jacobian.

A set-valued mapping $M : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ has the Aubin property around $(\bar{x}, \bar{y}) \in \operatorname{gph} M$ if there exist a constant L and neighbourhoods U of $\bar{x}$ and V of $\bar{y}$ such that for all $x, x' \in U$ the following inclusion holds true

$$M(x) \cap V \subset M(x') + L|x - x'|B(0, 1),$$

where $B(0, 1) \subset \mathbb{R}^m$ is the unit ball. If M is single-valued, then the Aubin property reduces exactly to locally Lipschitzian property.

Example 3.1 For a short illustration of the aforementioned objects, we use a simple example whose extension will be used later in the text. Consider $C := [0, 1] \subset \mathbb{R}$. Since C is convex, both normal cones coincide and we have

$$\operatorname{gph} \mathrm{N}_C = \operatorname{gph} \hat{\mathrm{N}}_C = \big(\{0\}\times\mathbb{R}_-\big) \cup \big([0, 1]\times\{0\}\big) \cup \big(\{1\}\times\mathbb{R}_+\big).$$

Fix now $(\bar{x}, \bar{y}) = (0, 0)$ and compute

$$\begin{aligned}
&\hat{\mathrm{N}}_{\operatorname{gph} \mathrm{N}_C}(\bar{x}, \bar{y}) = \mathbb{R}_-\times\mathbb{R}_+,\\
&\mathrm{N}_{\operatorname{gph} \mathrm{N}_C}(\bar{x}, \bar{y}) = \big(\mathbb{R}_-\times\mathbb{R}_+\big) \cup \big(\{0\}\times\mathbb{R}_+\}\big) \cup \big(\mathbb{R}_-\times\{0\}\big).
\end{aligned}$$

One can see that in this case limiting normal cone is strictly greater than Fréchet one. This means that $(0, 0)$ is a non-regular point. Similarly, one can see that so is also $(1, 0)$.

4. Evaluation of a subgradient of $\pi \mapsto J(\pi, S(\pi))$ and first-order necessary optimality conditions for (8)

To solve problem (8) or equivalently (9) efficiently, we need to compute a subgradient information for the mapping $\pi \mapsto J(\pi, S(\pi))$. Unfortunately, we cannot expect that S is a differentiable function and thus, we need first to compute some kind of generalized derivative of S.

We will work with the generalized differential calculus of Mordukhovich [6,7] and compute the limiting subdifferential of the objective in (9). To be able to do so, we first have to compute the so-called coderivative $\mathrm{D}^* S$, which for continuously differentiable functions amounts to the adjoint Jacobian. First we state a lemma which links these two concepts together.

Lemma 4.1 *Consider the solution mapping $S : \pi \mapsto (\bar{u}, \bar{z})$ being implicitly defined by system* (8) *and fix some $(\bar{u}, \bar{z}) = S(\bar{\pi})$. Assume that S is Lipschitz continuous on some neighborhood of $\bar{\pi}$ and that J is continuously differentiable on some neighbourhood of $(\bar{\pi}, \bar{u}, \bar{z})$. Denoting $\tilde{J}(\pi) := J(\pi, S(\pi))$, we have*

$$\partial \tilde{J}(\bar{\pi}) = \nabla_\pi J(\bar{\pi}, \bar{u}, \bar{z}) + \mathrm{D}^* S(\bar{\pi}, \bar{u}, \bar{z})(\nabla_u J(\bar{\pi}, \bar{u}, \bar{z}), \nabla_z J(\bar{\pi}, \bar{u}, \bar{z})).$$

Proof It follows directly from [6, Theorem 3.13] and [7, Exercise 8.8]. □

To obtain the necessary optimality conditions in the form of original data, we need to compute $\mathrm{D}^* S$. This is carried out in the next lemma which will also be the basis for proving the Lipschitzian continuity of S later in Corollary 4.4.

Lemma 4.2 *Consider the setting of the solution mapping $S : \pi \mapsto (\bar{u}, \bar{z})$ being implicitly defined by system* (8) *and fix some $(\bar{u}, \bar{z}) = S(\bar{\pi})$. Assuming (A1)–(A4), the upper estimate of $\mathrm{D}^* S(\bar{\pi}, \bar{u}, \bar{z})(u^*, z^*)$ is the collection of all quantities*

$$-\sum_{k=1}^{K} (\nabla_\pi p^k)^\top \beta^k - \sum_{k=1}^{K} (\nabla_\pi q^k)^\top \delta^k \tag{10}$$

such that for $k = 1, \dots, K$ the adjoint equations

$$-u^{*k} = \alpha^k - (\nabla_u p^k)^\top \beta^k - (\nabla_u q^k)^\top \delta^k - (\nabla_{\tilde{u}} p^{k+1})^\top \beta^{k+1} - (\nabla_{\tilde{u}} q^{k+1})^\top \delta^{k+1}, \quad (11a)$$

$$-z^{*k} = \gamma^k - (\nabla_z q^k)^\top \delta^k - (\nabla_{\tilde{z}} p^{k+1})^\top \beta^{k+1} - (\nabla_{\tilde{z}} q^{k+1})^\top \delta^{k+1} \quad (11b)$$

with the terminal conditions $\beta^{K+1} = 0$ and $\delta^{K+1} = 0$ are fulfilled. For the multipliers $\alpha, \beta, \gamma, \delta$ we have the relations

$$\begin{pmatrix} \alpha^k \\ \beta^k \end{pmatrix} \in \mathrm{N}_{\mathrm{gph}\, \mathrm{N}_{\Lambda^k}}(\bar{u}^k, -p^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})), \quad (12a)$$

$$\begin{pmatrix} \gamma \\ \delta \end{pmatrix} \in \mathrm{N}_{\mathrm{gph}\, Q}(\bar{z}, -q(\bar{\pi}, \bar{u}, \bar{z})), \quad (12b)$$

where $\gamma = (\gamma^1, \dots, \gamma^K)$ and $\delta = (\delta^1, \dots, \delta^K)$ and where, for $u = (u^1, \dots, u^K)$ and $z = (z^1, \dots, z^K)$, we have defined

$$\begin{aligned} q(\pi, u, z) &:= \begin{pmatrix} q^1(\pi, u^0, u^1, z^0, z^1) \\ \dots \\ q^K(\pi, u^{K-1}, u^K, z^{K-1}, z^K) \end{pmatrix} : \mathbb{R}^L \times \mathbb{R}^{KN} \times \mathbb{R}^{KM} \to \mathbb{R}^{KM}, \\ Q(z) &:= \textstyle\prod_{k=1}^K \mathrm{N}_{\mathfrak{K}^k(z^{k-1})}(z^k) \qquad : \mathbb{R}^{KM} \rightrightarrows \mathbb{R}^{KM}. \end{aligned}$$

Proof Similarly to q and Q, we define

$$\begin{aligned} p(\pi, u, z) &:= \begin{pmatrix} p^1(\pi, u^0, u^1, z^0) \\ \dots \\ p^K(\pi, u^{K-1}, u^K, z^{K-1}) \end{pmatrix} : \mathbb{R}^L \times \mathbb{R}^{KN} \times \mathbb{R}^{KM} \to \mathbb{R}^{KN}, \\ P(u) &:= \textstyle\prod_{k=1}^K \mathrm{N}_{\Lambda^k}(u^k) : \mathbb{R}^{KN} \rightrightarrows \mathbb{R}^{KN}. \end{aligned}$$

We define the following partially linearized mapping

$$\begin{aligned} M(\mu, \nu) := \Big\{ (\pi, u, z) \,\Big|\, & \mu \in p(\bar{\pi}, \bar{u}, \bar{z}) + \nabla_u p(\bar{\pi}, \bar{u}, \bar{z})(u - \bar{u}) + \nabla_z p(\bar{\pi}, \bar{u}, \bar{z})(z - \bar{z}) \\ & + P(u) \nu \in q(\bar{\pi}, \bar{u}, \bar{z}) + \nabla_u q(\bar{\pi}, \bar{u}, \bar{z})(u - \bar{u}) + \nabla_z q(\bar{\pi}, \bar{u}, \bar{z})(z - \bar{z}) + Q(z) \Big\} \end{aligned}$$

and show that it is single–valued and locally Lipschitz around $(0, 0)$. Indeed, the relations defining M read for $k = 1, \dots, K$

$$\begin{aligned} \mu^k \in\; & p^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1}) + \nabla_u p^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})(u^k - \bar{u}^k) \\ & + \nabla_{\tilde{u}} p^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})(u^{k-1} - \bar{u}^{k-1}) \\ & + \nabla_{\tilde{z}} p^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})(z^{k-1} - \bar{z}^{k-1}) + \mathrm{N}_{\Lambda^k}(u^k), \\ \nu^k \in\; & q^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1}, \bar{z}^k) + \nabla_u q^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1} \bar{z}^k)(u^k - \bar{u}^k) \\ & + \nabla_{\tilde{u}} q^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1}, \bar{z}^k)(u^{k-1} - \bar{u}^{k-1}) + \nabla_z q^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})(z^k - \bar{z}^k) \\ & + \nabla_{\tilde{z}} q^k(\bar{\pi}, \bar{u}^{k-1}, \bar{u}^k, \bar{z}^{k-1})(z^{k-1} - \bar{z}^{k-1}) + \mathrm{N}_{\mathfrak{K}^k(z^{k-1})}(z^k) \end{aligned}$$

with $u^0 = \bar{u}^0$ and $z^0 = \bar{z}^0$. Since the first inclusion is solved for u^k and the second one for z^k, we obtain that M is single-valued due to (A1)–(A4). By virtue of [16, Corollary 3D.5] we further obtain that M is Lipschitz continuous around $\bar{\pi}$, so that the system defining S is strongly regular (in the sense of Robinson [17]) at $(0, 0, \bar{\pi}, \bar{u}, \bar{z})$.

This enables us to use [3, Proposition 3.2] and [7, Theorem 6.14] to obtain, with I being the identity matrix, that

$$\mathrm{N}_{\mathrm{gph}\,S}(\bar{\pi},\bar{u},\bar{z}) \subset \begin{pmatrix} 0 & I & 0 \\ -\nabla_\pi p(\bar{\pi},\bar{u},\bar{z}) & -\nabla_u p(\bar{\pi},\bar{u},\bar{z}) & -\nabla_z p(\bar{\pi},\bar{u},\bar{z}) \\ 0 & 0 & I \\ -\nabla_\pi q(\bar{\pi},\bar{u},\bar{z}) & -\nabla_u q(\bar{\pi},\bar{u},\bar{z}) & -\nabla_z q(\bar{\pi},\bar{u},\bar{z}) \end{pmatrix}^\top \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix}.$$

with some $\alpha, \beta \in \mathbb{R}^{KN}$ and $\gamma, \delta \in \mathbb{R}^{KM}$ satisfying

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathrm{N}_{\mathrm{gph}\,P}(\bar{u}, -p(\bar{\pi},\bar{u},\bar{z})) \quad \text{and} \quad \begin{pmatrix} \gamma \\ \delta \end{pmatrix} \in \mathrm{N}_{\mathrm{gph}\,Q}(\bar{z}, -q(\bar{\pi},\bar{u},\bar{z})).$$

Applying the product rule for normal cones [7, Proposition 6.41] we obtain the statement of the lemma. □

If Λ^k is a (convex) polyhedral set, then $\mathrm{N}_{\mathrm{gph}\,\Lambda^k}(\cdot)$ can be computed due to [18, Theorem 2] or [19, Proposition 3.2]. For the computation of $\mathrm{N}_{\mathrm{gph}\,Q}(\cdot)$, we will consider two cases of $\mathfrak{K}^k$, specifically

$$\mathfrak{K}^k(z^{k-1}) = \mathbb{R}^M \quad \text{or} \tag{13a}$$

$$\mathfrak{K}^k(z^{k-1}) = \{z \in \mathbb{R}^M \mid 0 \le z \le z^{k-1}\}, \tag{13b}$$

where in (13b), the inequality is understood componentwise.

The former case (13a) corresponds to $K_0^t = K_1 = \mathbb{R}^M$, while the latter case (13b) corresponds to $K_0^t = \mathbb{R}^M_+$ and $K_1 = \mathbb{R}^M_-$. The former case is simple because from (12b) we immediately obtain that $\gamma^k = 0$ and $\delta^k \in \mathbb{R}^M$.

For the analysis of the more complicated case (13b) we recall the definition of Q and define its counterpart $\tilde{Q}$ for a single time instant

$$Q(z) = \{v \in \mathbb{R}^{KM} \mid v^k \in \mathrm{N}_{[0,z^{k-1}]}(z^k),\ k = 1,\dots,K\},$$
$$\tilde{Q}(\tilde{z}) := \{(z,v) \in \mathbb{R}^M \times \mathbb{R}^M \mid v \in \mathrm{N}_{[0,\tilde{z}]}(z)\}.$$

This case is more involved than the previous one, because in Q one has to do with normal cones to moving sets whereby (components of) z arise simultaneously both as the arguments as well as parameters specifying the movement of the constraint sets. Such a situation occurs typically in quasi-variational inequalities and has been studied, e.g. in [20]. Unfortunately, the results of [20] cannot be directly applied here because the set

$$\mathfrak{K}^k(0) = \{0\}$$

does not satisfy even the Mangasarian–Fromovitz constraint qualification when described in the form (13b).

As we have mentioned in the introduction, it would be possible to use standard calculus rules to obtain a formula for $\mathrm{N}_{\mathrm{gph}\,Q}$ based on multiple computations of $\mathrm{N}_{\mathrm{gph}\,\tilde{Q}}$. The graph of $\tilde{Q}$ can easily be visualized in Figure 1 and thus, $\mathrm{N}_{\mathrm{gph}\,\tilde{Q}}$ can be computed by analysing 8 parts of gph $\tilde{Q}$ separately, see definition of $\tilde{Q}_i$ below. However, when computing $\mathrm{N}_{\mathrm{gph}\,Q}$ on the basis of $\mathrm{N}_{\mathrm{gph}\,\tilde{Q}}$ and the chain rule from [21, Theorem 4.1] one obtains only an upper estimate and not equality.

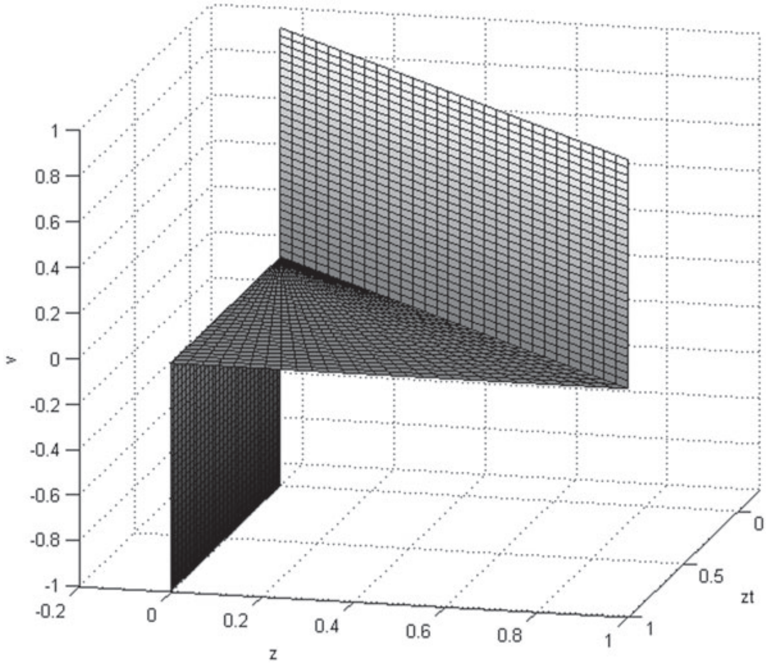

Figure 1. Visualization of gph $\tilde{Q}$.

That is why we make use of [8] where formulas for Fréchet and limiting normal cones to a finite union of polyhedral sets have been derived and then applied to a special structure arising in time dependent problems. For simplicity, we will show the result only for the simplest case of $M = 1$. However, the generalization to a more–dimensional space is straightforward and can be conducted in componentwise way.

In the following text, we will assume that $i^0 = 1$. Define now the following sets

$$\begin{aligned}
\tilde{Q}_1 &= \left\{(\tilde{z}, z, v) \in \mathbb{R}^3 \,|\, \tilde{z} \in (0, \infty), z = \tilde{z}, v \in (0, \infty)\right\},\\
\tilde{Q}_2 &= \left\{(\tilde{z}, z, v) \in \mathbb{R}^3 \,|\, \tilde{z} \in (0, \infty), z = \tilde{z}, v = 0\right\},\\
\tilde{Q}_3 &= \left\{(\tilde{z}, z, v) \in \mathbb{R}^3 \,|\, \tilde{z} \in (0, \infty), z \in (0, \tilde{z}), v = 0\right\},\\
\tilde{Q}_4 &= (0, \infty) \times \{0\} \times \{0\},\\
\tilde{Q}_5 &= (0, \infty) \times \{0\} \times (-\infty, 0),\\
\tilde{Q}_6 &= \{0\} \times \{0\} \times (-\infty, 0),\\
\tilde{Q}_7 &= \{0\} \times \{0\} \times \{0\},\\
\tilde{Q}_8 &= \{0\} \times \{0\} \times (0, \infty).
\end{aligned}$$

It is not difficult to show that $\cup_{i=1}^{8} \tilde{Q}_i = \operatorname{gph} \tilde{Q}$. Moreover, $\{\tilde{Q}_i \,|\, i = 1, \ldots, 8\}$ forms the so-called normally admissible stratification of gph $\tilde{Q}$ as defined in [8]. Now, define the following index sets

$$\Theta = \left\{ (i^1, \ldots, i^K) \middle| \begin{array}{l} i^k \in \{1, \ldots, 8\} \\ i^{k-1} \in \{1, 2, 3\} \implies i^k \in \{1, 2, 3, 4, 5\} \\ i^{k-1} \in \{4, 5, 6, 7, 8\} \implies i^k \in \{6, 7, 8\} \end{array} \right\},$$

$$I(s) = \left\{ (i^1, \ldots, i^K) \in \Theta \middle| \begin{array}{ll} s^k = 1 \implies i^k = 1, & s^k = 5 \implies i^k = 5 \\ s^k = 2 \implies i^k \in \{1, 2, 3\}, & s^k = 6 \implies i^k \in \{5, 6\} \\ s^k = 3 \implies i^k = 3, & s^k = 7 \implies i^k \in \{1, \ldots, 8\} \\ s^k = 4 \implies i^k \in \{3, 4, 5\}, & s^k = 8 \implies i^k \in \{1, 8\} \end{array} \right\},$$

where we assume that $s = (s^1, \ldots, s^K) \in \{1, \ldots, 8\}^K$ and all relations are required to hold for all $k = 1, \ldots, K$. Further define

$$Q_i := \left\{ (z, v) \in \mathbb{R}^{2K} \,\middle|\, (z^{k-1}, z^k, v^k) \in \tilde{Q}_{i^k},\ k = 1, \ldots, K \right\}.$$

As shown in [8], we obtain that $\cup_{i\in\Theta} Q_i = \operatorname{gph} Q$ and that $\{Q_i |\, i \in \Theta\}$ forms a normally admissible statification of gph Q. Now, we may state the result concerning the computation of $\mathrm{N}_{\operatorname{gph} Q}(\bar{z}, \bar{v})$, which replaces the computation of normal cone to a non-convex set by the computation of multiple normal cones to convex sets.

Proposition 4.3 [8, Section 4] *Fix any $(\bar{z}, \bar{v}) \in \operatorname{gph} Q$ and denote by $\bar{s}$ the index of the unique component $Q_{\bar{s}}$ such that $(\bar{z}, \bar{v}) \in Q_{\bar{s}}$. Then*

$$\mathrm{N}_{\operatorname{gph} Q}(\bar{z}, \bar{v}) = \bigcup_{s\in I(\bar{s})} \bigcap_{i\in I(s)} \mathrm{N}_{\operatorname{cl} Q_i}(Q_s),$$

where $\mathrm{N}_{\operatorname{cl} Q_i}(Q_s)$ denotes the common value $\mathrm{N}_{\operatorname{cl} Q_i}(z, v)$ for any $(z, v) \in Q_s$. For any $s \in \Theta$ and $i \in I(s)$, this value can be computed as

$$\mathrm{N}_{\operatorname{cl} Q_i}(Q_s) = \left\{ \begin{pmatrix} \mu^1 + \tilde{\mu}^1 \\ \vdots \\ \mu^K + \tilde{\mu}^K \\ \nu^1 \\ \ldots \\ \nu^K \end{pmatrix} \in \mathbb{R}^{2K} \middle| \begin{array}{l} \begin{pmatrix} \tilde{\mu}^{k-1} \\ \mu^k \\ \nu^k \end{pmatrix} \in \mathrm{N}_{\operatorname{cl} \tilde{Q}_{i^k}}(\tilde{Q}_{s^k}),\ k = 1, \ldots, K \\ \tilde{\mu}^K = 0 \end{array} \right\}.$$

Note that the computation of $\mathrm{N}_{\operatorname{cl} Q_i}(z, v)$ is simple as long as $z > 0$ in which case standard results can be used. The situation changes, however, if there exists i such that $z_{i-1} = 0$. Then $\mathrm{N}_{\operatorname{cl} \tilde{Q}_i}(z_{i-1}, z, v)$ is generated by normal cones to all 'neighboring' components. This is the reason why we have to consider all $\tilde{Q}_1, \ldots, \tilde{Q}_8$.

Now we have enough information to prove the Lipschitz continuity of S for both cases in (13). Due to assumptions (A1)–(A3) and [18, Proof of Theorem 2] we obtain that if a pair (α^k, β^k) satisfies (12a), then we have $\alpha^{k\top}\beta^k \leq 0$. However, for (γ, δ) satisfying (12b), it may happen that $\gamma^{k\top}\delta^k > 0$ (see formula (17) below). Nevertheless, we are able to overcome this problem by making use of the specific structure of gph Q.

Corollary 4.4 *In the setting of Lemma 4.2 assume that $\mathfrak{K}^k$ is defined via (13a) or (13b). Fix some $(\bar{u}, \bar{z}) = S(\bar{\pi})$. Then S is Lipschitz continuous around $\bar{\pi}$.*

Proof Without loss of generality we may assume that $M = 1$. Since S is single-valued, it is locally Lipschitz around $\bar{\pi}$ if and only if it has the so-called Aubin property around $(\bar{\pi}, \bar{u}, \bar{z})$. Moreover, this property is according to [7, Theorem 9.40] equivalent to

$$\mathrm{D}^* S(\bar{\pi}, \bar{u}, \bar{z})(0, 0) = \{0\}. \tag{14}$$

To show this, we plug $u^* = z^* = 0$ into system (11)–(12) and attempt to deduce that $\beta = \delta = 0$, which would imply that (10) is equal to zero as well, and thus condition (14) is fulfilled.

To this end, we first realize that the first case (13a) implies $\gamma^k = 0$ and $\delta^k \in \mathbb{R}^M$. In the rest of the proof, we will consider only the second case (13b) with a note that case (13a) can be shown by a slight modification of the last paragraph. Fix any $(\gamma, \delta) \in \mathrm{N}_{\mathrm{gph}\, Q}(\bar{z}, -q(\bar{\pi}, \bar{u}, \bar{z}))$. From Proposition 4.3 we know that there is some $s \in I(\bar{s})$ such that for all $i \in I(s)$ there exist some μ_i^k, $\tilde{\mu}_i^k$ and ν_i^k such that $\gamma^k = \mu_i^k + \tilde{\mu}_i^k$, $\delta^k = \nu_i^k$, $\tilde{\mu}_i^K = 0$ and relation

$$\begin{pmatrix} \tilde{\mu}_i^{k-1} \\ \mu_i^k \\ \nu_i^k \end{pmatrix} \in \mathrm{N}_{\mathrm{cl}\, \tilde{Q}_{i^k}}(\tilde{Q}_{s^k}) \tag{15}$$

holds for all $k = 1, \dots, K$.

We will define now the index set

$$I = \left\{ (i^1, \dots, i^K) \,\middle|\, \begin{array}{l} s^k = 1 \implies i^k = 1,\ s^k = 2 \implies i^k \in \{1, 3\} \\ s^k = 3 \implies i^k = 3,\ s^k = 4 \implies i^k \in \{3, 5\} \\ s^k = 5 \implies i^k = 5 \\ s^k = 6,\ i^{k-1} \in \{1, 3\} \implies i^k = 5 \\ s^k = 6,\ i^{k-1} \in \{5, 6, 8\} \implies i^k = 6 \\ s^k = 7,\ i^{k-1} \in \{1, 3\} \implies i^k \in \{1, 5\} \\ s^k = 7,\ i^{k-1} \in \{5, 6, 8\} \implies i^k \in \{6, 8\} \\ s^k = 8,\ i^{k-1} \in \{1, 3\} \implies i^k = 1 \\ s^k = 8,\ i^{k-1} \in \{5, 6, 8\} \implies i^k = 8 \end{array} \right\}$$

and say that property (P^k) holds if

$$s^k \in \{1, 2\} \implies \mu_i^k = 0 \text{ for all } i \in I, \text{ and} \tag{16a}$$

$$\exists j < k : s^j = 4,\ s^{j+1} = \dots = s^k = 8 \implies \mu_i^k \geq 0 \text{ for some } i \in I \text{ with } i^j = 3 \text{ and } i^{j+1} = \dots = i^k = 1. \tag{16b}$$

Naturally, this property is satisfied if $s^k \notin \{1, 2, 8\}$ and it can be shown that $I \subset I(s)$. We will now show that for all $k = 1, \dots, K - 1$ we have the following implication

$$\gamma^{k+1\top} \delta^{k+1} \leq 0 \text{ and } (P^{k+1}) \text{ holds} \implies \gamma^{k\top} \delta^k \leq 0 \text{ and } (P^k) \text{ holds}. \tag{17}$$

Thus, we assume $\gamma^{k+1\top} \delta^{k+1} \leq 0$ and that property (P^{k+1}) holds. We will now make use of the fact that $\delta^k = \nu_i^k$, and thus ν_i^k does not depend on i. By evaluating (15), we obtain that there exists $i \in I \subset I(s)$ such that

$$\begin{aligned} s^{k+1} &= 1 \implies \tilde{\mu}_i^k = -\mu_i^{k+1}, & s^k &= 1 \implies & \nu_i^k &= 0,\\ s^{k+1} &= 2 \implies \tilde{\mu}_i^k = -\mu_i^{k+1}, & s^k &= 2 \implies \mu_i^k \geq 0, & \nu_i^k &\leq 0,\\ s^{k+1} &= 3 \implies \tilde{\mu}_i^k = 0, & s^k &= 3 \implies \mu_i^k = 0, & &\\ s^{k+1} &= 4 \implies \tilde{\mu}_i^k = 0, & s^k &= 4 \implies \mu_i^k \leq 0, & \nu_i^k &\geq 0,\\ s^{k+1} &= 5 \implies \tilde{\mu}_i^k = 0, & s^k &= 5 \implies & \nu_i^k &= 0,\\ & & s^k &= 6 \implies & \nu_i^k &= 0,\\ & & s^k &= 7 \implies & \nu_i^k &= 0,\\ & & s^k &= 8 \implies & \nu_i^k &= 0. \end{aligned}$$

The implication $s^k = 7 \implies \nu_i^k = 0$ follows from $I \subset I(s)$, the non-dependence of ν_i^k on i and from the possibility to choose either $i^k \in \{1, 5\}$ or $i^k \in \{6, 8\}$. We observe now that in any case we have $\mu_i^{k\top}\delta^k = \mu_i^{k\top}\nu_i^k \leq 0$. This means that we have managed to prove $\gamma^{k\top}\delta^k \leq 0$ provided $\tilde{\mu}_i^k = 0$ or $\nu_i^k = 0$.

Thus, to prove the first part of (17) it remains to investigate cases $s^{k+1} \in \{1, 2, 6, 7, 8\}$ and $s^k \in \{2, 3, 4\}$. We will restrict now to these problematic cases. If $s^{k+1} \in \{1, 2\}$, then (P^{k+1}) implies $\tilde{\mu}_i^k = -\mu_i^{k+1} = 0$ and we may apply the previous result. If $s^{k+1} \in \{6, 7\}$ and $s^k = 4$, then choosing $i^{k+1} = 5$ and $i^k = 3$ results in $\tilde{\mu}_i^k \leq 0$ and $\mu_i^k \leq 0$, which together with $\nu_i^k \geq 0$ implies $\gamma^{k\top}\delta^k \leq 0$. Due to definition of Θ, it remains to investigate the last case: $s^{k+1} = 8$ and $s^k = 4$. In this case, we choose $i^{k+1} = 1$ and $i^k = 3$, which leads to $\mu_i^{k+1} + \tilde{\mu}_i^k \leq 0$ and $\mu_i^k \leq 0$. But since $\mu_i^{k+1} \geq 0$ due to (P^{k+1}), we have $\tilde{\mu}_i^k \leq 0$, and thus we again obtain $\gamma^{k\top}\delta^k \leq 0$. So far, we have managed to prove that if the left-hand side of (17) holds true, then we have $\gamma^{k\top}\delta^k \leq 0$.

To show the validity of formula (17), we need to verify that (P^k) holds as well. To do so, we multiply the adjoint Equation (11b) by δ^k, which due to assumption (A1)–(A2) and the already proven $\gamma^{k\top}\delta^k \leq 0$ results in $\gamma^k = \mu_i^k + \tilde{\mu}_i^k = 0$ and $\delta^k = \nu_i^k = 0$ for all $i \in I$. We will now investigate the cases described on the left-hand side of (16).

For (16a) we have $s^k \in \{1, 2\}$. This by definition of Θ yields $s^{k+1} \in \{1, 2, 3, 4, 5\}$. If $s^{k+1} \in \{3, 4, 5\}$, then $\tilde{\mu}_i^k = 0$ and thus $\mu_i^k = 0$ follows. If on the other hand we have $s^k \in \{1, 2\}$, then from assumed (P^{k+1}) we get $\tilde{\mu}_i^k = -\mu_i^{k+1} = 0$, and thus $\mu_i^k = 0$ follows for this case as well. To prove (16b) consider some $j < k$ and $s^j = 4$, $s^{j+1} = \cdots = s^k = 8$, $i^j = 3$ and $i^{j+1} = \cdots = i^k = 1$. If $s^{k+1} = 8$, then $i^{k+1} = 1$ and we may apply (P^{k+1}) to obtain $\mu_i^{k+1} \geq 0$, which together with $\tilde{\mu}_i^k + \mu_i^{k+1} \leq 0$ and $\mu_i^k + \tilde{\mu}_i^k = 0$ implies $\mu_i^k \geq 0$. If $s^{k+1} \in \{6, 7\}$, then choosing $i^{k+1} = 5$ results in $\tilde{\mu}_i^k \leq 0$, which again implies $\mu_i^k \geq 0$. Since these are all possibilities due to the definition of Θ, we have showed formula (17).

Having this formula at hand, the rest of the proof is performed by a finite induction. Since $\tilde{\mu}_i^K = 0$, by similar arguments as in the previous text we obtain that $\gamma^{K\top}\delta^K = \mu_i^{K\top}\nu_i^K \leq 0$, which further yields $\gamma^K = \mu_i^K = \delta^K = 0$, and thus property (P^K) is satisfied. Hence, we have obtained the validity of the first step for finite induction. Plugging this into the first adjoint Equation (11a) and multiplying it by β^K, we obtain that $\alpha^K = \beta^K = 0$. Since the left-hand side of (17) is satisfied, we immediately obtain that $\gamma^{K-1\top}\delta^{K-1} \leq 0$ and that (P^{K-1}) holds. Performing this procedure K times, we obtain that (14) indeed holds, which finishes the proof. □

Finally, we summarize the derivation of the necessary optimality conditions in Theorem 4.5 below. Thereby, the normal cone $\mathrm{N}_{\mathrm{gph}\, Q}(\cdot)$ is computed in Proposition 4.3 and for the computation of $\mathrm{N}_{\mathrm{gph}\, \Lambda^k}(\cdot)$ we refer the reader to [18, Theorem 2] or [19, Proposition

3.2]. Moreover, when solving system (12) and (19), one may use [22, Lemma 4.7] to its advantage.

THEOREM 4.5 *(First-order optimality conditions)* *Consider the setting of the solution mapping $S : \pi \mapsto (\bar{u}, \bar{z})$ implicitly defined by system (8) and fix some $(\bar{u}, \bar{z}) = S(\bar{\pi})$. Assume (A1)–(A4) and that J is continuously differentiable at $(\bar{\pi}, \bar{u}, \bar{z})$. If $(\bar{\pi}, \bar{y}, \bar{z})$ is a local minimum of problem (8), then there exists multipliers $(\alpha, \beta, \gamma, \delta)$ satisfying (12) such that the optimality condition*

$$0 \in \nabla_\pi J(\bar{\pi}, \bar{u}, \bar{z}) - \sum_{k=1}^{K} (\nabla_\pi p^k)^\top \beta^k - \sum_{k=1}^{K} (\nabla_\pi q^k)^\top \delta^k + \mathrm{N}_\Pi(\bar{\pi}), \tag{18}$$

the adjoint equations with $k = 1, \ldots, K$

$$-\nabla_{u^k} J(\bar{\pi}, \bar{u}, \bar{z}) = \alpha^k - (\nabla_u p^k)^\top \beta^k - (\nabla_u q^k)^\top \delta^k - (\nabla_{\tilde{u}} p^{k+1})^\top \beta^{k+1} - (\nabla_{\tilde{u}} q^{k+1})^\top \delta^{k+1}, \tag{19a}$$

$$-\nabla_{z^k} J(\bar{\pi}, \bar{u}, \bar{z}) = \gamma^k - (\nabla_z q^k)^\top \delta^k - (\nabla_{\tilde{z}} p^{k+1})^\top \beta^{k+1} - (\nabla_{\tilde{z}} q^{k+1})^\top \delta^{k+1} \tag{19b}$$

and terminal conditions $\beta^{K+1} = 0$ and $\delta^{K+1} = 0$ are satisfied.

Remark 2 (More general dissipation I) In a number of applications $\mathscr{R}_2$ is finite, but nonsmooth at 0 and $K_1 = Z$. In this case, in the generalized equation system defining S, one has generally a sum of multifunctions which is typically very difficult to handle, cf. [7, Theorem 10.41]. Sometimes, however, an analytic formula for the behaviour of S at the single time instances can be obtained and then D^*S can be computed by applying the (first-order) generalized differential calculus, see [6,7].

Another possible approach to this situation is to transform it into the form considered here, i.e. $\mathscr{R}_2$ smooth and a suitable K_1. Let us illustrate this on a one-dimensional case $Z = \mathbb{R}$ with $\mathscr{R}_2(\dot{z}) = a \max(0, \dot{z}) + b \max(0, -\dot{z})$ with some $a, b \geq 0$ and, e.g. $\mathscr{E}(z) = \frac{1}{2} z^2$. Considering artificial variable (z_1, z_2) such that $z_1 + z_2 = z$, we may write

$$\mathscr{E}(z_1, z_2) = \frac{1}{2}(z_1 + z_2)^2 \quad \text{and} \quad \mathscr{R}_2(\dot{z}_1, \dot{z}_2) = \begin{cases} a\dot{z}_1 - b\dot{z}_2 & \text{if } \dot{z}_1 \geq 0 \text{ and } \dot{z}_2 \leq 0, \\ \infty & \text{otherwise.} \end{cases} \tag{20}$$

Such a transformation allows to widen the application range towards e.g. damage or delamination problems with healing in arbitrary space dimension. Another application can be frictional contact [23] or adhesive contact with an interfacial plasticity [24] allowing to distinguish less dissipative mode I (opening) from more dissipative mode II (shear) in two-dimensional cases. Another, rather academical, application is the bulk plasticity with kinematic hardening in one dimension. Naturally, all these applications are considered with a suitable space discretization.

Remark 3 (More general dissipation II) In some applications, the cone K_1 could be the second-order (Lorentz, or colloquially also called ‘ice-cream’) cone, defined in $\mathbb{R}^l$ by

$$\{x \in \mathbb{R}^l \mid x_l \geq |(x_1, \ldots, x_{l-1})|\}.$$

where $|\cdot|$ stands for the Euclidean norm. In this case, it is possible to make use of coderivatives of the normal cone mapping associated with second-order cones, which have been computed in [25]. Then, however, the special technique of [8], tailored to polyhedral multifunctions, cannot be used anymore and we have to confine ourselves to standard calculus rules, which leads to less selective necessary optimality conditions.

Typical applications of this type with $K_1 = Z$ are a frictional contact in three-dimensional case or plasticity with kinematic hardening in two- or three-dimensional case, again having in mind a suitable space discretization in each case. An example which uses a combination of $K_1 \neq Z$ with a nonsmooth potential $\mathscr{R}_2$, both being of the 'ice-cream-type', is plasticity with isotropic hardening, cf. [10,26,27] which has the dissipation potential acting on the rate of $z = (p, \eta)$ of the form:

$$\delta_S^*(\dot{p}) + \delta_{K_1}(\dot{p}, \dot{\eta}) \quad \text{with} \;\; 0 \in S \subset \mathbb{R}^{d\times d}_{\text{dev}} \;\; \text{and} \;\; K_1 := \big\{(\dot{p}, \dot{\eta}) \in \mathbb{R}^{d\times d}_{\text{dev}} \times \mathbb{R};\; \dot{\eta} \geq q_{\text{H}} \delta_S^*(\dot{p})\big\} \tag{21}$$

where $q_{\text{H}} > 0$ and $\mathbb{R}^{d\times d}_{\text{dev}} := \{A \in \mathbb{R}^{d\times d};\; A = A^\top,\; \text{tr}\, A = 0\}$, and δ_A stands for an indicator function of a convex set A and δ_A^* of its conjugate. Typically, S a ball, which makes both δ_S^* and K_1 of the 'ice-cream-type'.

A combination of the preceding case with a general polyhedral set K_0 is also possible. This combination allows for some applications in identification of parameters of some phenomenological models of phase transformations in certain ferroic materials as shape-memory alloys where K_0 forms constraints on an internal variable like p in (21) and may be considered polyhedral, cf. the polycrystalic models in [28,29], possibly also in combination with plasticity like that one in (21), cf. [30,31].

5. Adhesive contact problem and its identification

We illustrate the above abstract identification problem (3) on an unilateral adhesive-contact problem for a linear elastic body at small strains. We consider $\Omega \subset \mathbb{R}^2$ a Lipschitz domain with $\Gamma_{\text{C}} \subset \partial\Omega$ and $\Gamma_{\text{D}} \subset \partial\Omega$ disjoint parts of the boundary $\partial\Omega$, where the delamination is undergoing and time-varying Dirichlet boundary condition where $w_{\text{D}}(t)$ is prescribed, respectively. Now, $u : \Omega \to \mathbb{R}^2$ is the displacement and $z : \Gamma_{\text{C}} \to [0, 1]$ is a delamination parameter having the meaning of the portion of bonds of the adhesive which are not debonded. With $\mathbb{C}$ the tensor of elastic moduli, $h : [0, 1] \to \mathbb{R}$ a convex adhesive-stored-energy function, and with $e(u)$ denoting the small-strain tensor, i.e. $[e(u)]_{ij} = \frac{1}{2}\frac{\partial u_i}{\partial x_j} + \frac{1}{2}\frac{\partial u_j}{\partial x_i}$, we will consider the boundary-value problem

$$\text{div}\, \mathbb{C}e(u) = 0 \qquad \text{in } [0, T] \times \Omega, \tag{22a}$$

$$\mathbb{C}e(u)\vec{n} = 0 \qquad \text{on } [0, T] \times (\Gamma \backslash (\Gamma_{\text{C}} \cup \Gamma_{\text{D}})), \tag{22b}$$

$$u|_{\Gamma_{\text{D}}} = w_{\text{D}}(t, \cdot) \qquad \text{on } [0, T] \times \Gamma_{\text{D}}, \tag{22c}$$

$$\left.\begin{array}{l} u_{\text{N}} \geq 0, \quad z\kappa_{\text{N}} u_{\text{N}} + \vec{n}^\top \mathbb{C}e(u)\vec{n} \geq 0, \\ \big(z\kappa_{\text{N}} u_{\text{N}} + \vec{n}^\top \mathbb{C}e(u)\vec{n}\big) u_{\text{N}} = 0 \\ \dot{z} \leq 0, \quad \xi + \alpha_{\text{F}} \geq 0, \quad \dot{z}(\xi + \alpha_{\text{F}}) = 0, \\ \xi + h'(z) + \frac{1}{2}(\kappa_{\text{N}} u_{\text{N}}^2 + \kappa_{\text{T}} u_{\text{T}}^2) - \varepsilon \text{div}_{\text{S}} \nabla_{\text{S}} z \geq 0, \quad z \geq 0, \\ \big(\xi + h'(z) + \frac{1}{2}(\kappa_{\text{N}} u_{\text{N}}^2 + \kappa_{\text{T}} u_{\text{T}}^2) - \varepsilon \text{div}_{\text{S}} \nabla_{\text{S}} z\big)\, z = 0, \\ z\kappa_{\text{T}} u_{\text{T}} + \mathbb{C}e(u)\vec{n} - (\vec{n}^\top \mathbb{C}e(u)\vec{n})\vec{n} = 0, \end{array}\right\} \text{on } [0, T] \times \Gamma_{\text{C}}, \tag{22d}$$

where we used the decomposition of the trace of displacement $u = u_{\rm N}\vec{n} + u_{\rm T}$ with $u_{\rm N}$ being the normal displacement defined as $u \cdot \vec{n}$ and $u_{\rm T}$ being the tangential displacement on $\Gamma_{\rm C}$, and where $\nabla_{\rm S}$ denotes a 'surface gradient', i.e. the tangential derivative defined as $\nabla_{\rm S} z = \nabla z - (\nabla z{\cdot}\vec{n})\vec{n}$ for z defined around $\Gamma_{\rm C}$. Alternatively, pursuing the concept of fields defined exclusively on $\Gamma_{\rm C}$, we can consider $z : \Gamma_{\rm C} \to \mathbb{R}$ and extend it to a neighbourhood of $\Gamma_{\rm C}$ and then again define $\nabla_{\rm S} z := (\nabla z)P$ with $P = \mathbb{I} - \vec{n} \otimes \vec{n}$ onto a tangent space, which, in fact, does not depend on the particular extension. Moreover, ${\rm div}_{\rm S} := {\rm tr}\, \nabla_{\rm S}$. Then ${\rm div}_{\rm S} \nabla_{\rm S}$ is the so-called Laplace-Beltrami operator.

Let us remark that (22a) is the force equilibrium, (22b) prescribes the zero-traction (i.e. free surface) on $\Gamma \backslash (\Gamma_{\rm C} \cup \Gamma_{\rm D})$. The condition (22d) combines three complementarity problems related, respectively, to the Signorini unilateral contact for the displacement u, the non-negativity constraint for z, and the unidirectionality constraint (i.e. the non-positivity constraint on $\dot{z}$), and eventually the equilibrium of tangential stress. More in detail, the last two mentioned complementarity problems write in the classical formulation as the inclusion $\partial\delta^*_{[-\alpha_{\rm F},\infty)}(\dot{z}) \ni \xi$ with the admissible driving force fulfilling the inclusion $\xi \in -\partial_z \mathscr{E}(t, \pi, u, z) = \varepsilon {\rm div}_{\rm S} \nabla_{\rm S} z - h'(z) - \frac{1}{2}(\kappa_{\rm N} u_{\rm N}^2 + \kappa_{\rm T} u_{\rm T}^2) - {\rm N}_{[0,\infty)}(z)$.

Referring to the abstract problem (1), the boundary-value problem (22) corresponds to the stored and the dissipation energies

$$\mathscr{E}(t, \pi, u, z) := \begin{cases} \displaystyle\int_{\Gamma_{\rm C}} \frac{1}{2} z\big(\kappa_{\rm N} u_{\rm N}^2 + \kappa_{\rm T} u_{\rm T}^2\big) + h(z) + \frac{1}{2}\varepsilon \nabla_{\rm S} z{\cdot}\nabla_{\rm S} z \,{\rm d}S & \\ \qquad\qquad + \displaystyle\int_{\Omega} \frac{1}{2} \mathbb{C} e(u) \colon e(u)\,{\rm d}x & \text{if } u|_{\Gamma_{\rm D}} = w_{\rm D}(t,\cdot) \text{ on } \Gamma_{\rm D} \text{ and} \\ & u|_{\Gamma_{\rm C}}{\cdot}\vec{n} \geq 0 \text{ and } z \geq 0 \text{ on } \Gamma_{\rm C}, \\ \infty & \text{otherwise,} \end{cases} \tag{23a}$$

$$\mathscr{R}_1 \equiv 0, \quad \mathscr{R}_2(\dot{z}) := \begin{cases} \displaystyle\int_{\Gamma_{\rm C}} \alpha_{\rm F} |\dot{z}|\,{\rm d}S & \text{if } \dot{z} \leq 0 \text{ a.e. on } \Gamma_{\rm C}, \\ \infty & \text{otherwise,} \end{cases} \qquad \text{with } \pi = (\alpha_{\rm F}, \kappa_{\rm N}, \kappa_{\rm T}), \tag{23b}$$

Note that $\mathscr{E}(t, \pi, \cdot, \cdot)$ is not convex but it is separately convex and, if $\Gamma_{\rm D}$ is non-empty and h is strictly convex, it is separately strictly convex, complying with our assumption (A1)–(A2). Considering h quadratic, this leads, after a suitable spatial discretization of (4), to recursive alternating strictly convex *Quadratic-Programming* (QP) which can be solved by efficient prefabricated software packages.

The (distributed) parameters to be identified will be the fracture toughness $\alpha_{\rm F}$ and the elasticity-moduli of the adhesive $\kappa_{\rm N}$ and $\kappa_{\rm T}$, i.e. we have considered simply $\pi = (\alpha_{\rm F}, \kappa_{\rm N}, \kappa_{\rm T})$ as outlined in (23b). This choice has a certain motivation in engineering where, in contrast to essentially all the bulk material properties, these parameters are largely unknown and have to be set up in a rather ad-hoc way to fit at least roughly some experiments, cf. e.g. [32,33] based on experiments from [34]. Actually, the models of adhesive contacts used in engineering may be more complicated; typically they distinguish modes of delamination (opening vs shear) and/or may involve friction. Identification of friction/adhesive contacts may have interesting applications in geophysics where such contact surfaces (called faults) are deep in lithosphere and not accessible to direct investigations although a lot of indirect data from earthquakes are usually available; a popular rate-and-state friction model involves one internal parameter (called ageing) which is analogous to the delamination parameter used here, cf. [35] for a survey or also e.g. [36]. Other models that may lead to a recursive QP have been mentioned in Remark 2, in contrast to problems from Remark 3 that would lead to a recursive Second-Order Cone Programming (SOCP) for which efficient codes do exist, cf. [37].

We prescribe some initial conditions $u_0 \in H^1(\Omega)$ and $z_0 \in H^1(\Gamma_\mathrm{C})$, $0 \le z_0 \le 1$; note that then $0 \le z \le 1$ is satisfied during the whole evolution process. We further consider a fixed time horizon $T > 0$ and assume that we have some given desired response $(u_\mathrm{d}, z_\mathrm{d})$ corresponding, e.g. to some experimentally obtained measurements, and we want to identify parameters π such that the response $(u, z) = S(\pi)$ is as close to $(u_\mathrm{d}, z_\mathrm{d})$ as possible, i.e. we want to minimize the objective

$$\int_0^T \Big[\int_\Omega \frac{\zeta}{2} \big|u - u_\mathrm{d}\big|^2 \,\mathrm{d}x + \int_{\Gamma_\mathrm{C}} \frac{1}{2} \big|z - z_\mathrm{d}\big|^2 \,\mathrm{d}S \Big] \,\mathrm{d}t, \tag{23c}$$

where ζ is a fixed weight balancing both parts of the objective function.

After the semi-implicit time discretization, the whole problem (23) reads as

$$\begin{aligned} &\text{Minimize } \tau \sum_{k=1}^{K} \Big[\int_\Omega \frac{\zeta}{2} \big|u^k - u_\mathrm{d}^k\big|^2 \,\mathrm{d}x + \int_{\Gamma_\mathrm{C}} \frac{1}{2} \big|z^k - z_\mathrm{d}^k\big|^2 \,\mathrm{d}S \Big] \\ &\text{subject to } (u^k, z^k) = S^k(\pi, u^{k-1}, z^{k-1}), \quad k = 1, \dots, K, \quad \text{and} \\ &\qquad\qquad \pi = (\alpha_\mathrm{F}, \kappa_\mathrm{N}, \kappa_\mathrm{T}) \in \Pi, \end{aligned} \tag{24a}$$

where the solution map $S^k : (\pi, u^{k-1}, z^{k-1}) \mapsto (u^k, z^k)$ for a particular time instant is now defined by the alternating recursive system: given $\pi = (\alpha_\mathrm{F}, \kappa_\mathrm{N}, \kappa_\mathrm{T})$ and previous values (u^{k-1}, z^{k-1}), the first one is solved for u^k and the second one for z^k recursively for $k = 1, \dots, K$:

$$\begin{aligned} &\underset{u \in H^1(\Omega, \mathbb{R}^d)}{\text{Minimize}} \int_\Omega \frac{1}{2} \mathbb{C} e(u) \colon e(u) \,\mathrm{d}x + \int_{\Gamma_\mathrm{C}} \frac{1}{2} z^{k-1} \big(\kappa_\mathrm{N} u_\mathrm{N}^2 + \kappa_\mathrm{T} u_\mathrm{T}^2\big) \,\mathrm{d}S \\ &\text{subject to} \quad u|_{\Gamma_\mathrm{D}} = w_\mathrm{D}^k := w_\mathrm{D}(k\tau, \cdot) \quad \text{and} \quad u|_{\Gamma_\mathrm{C}} \cdot \vec{n} \ge 0, \end{aligned} \tag{24b}$$

$$\begin{aligned} &\underset{z \in H^1(\Gamma_\mathrm{C}) \cap L^\infty(\Gamma_\mathrm{C})}{\text{Minimize}} \int_{\Gamma_\mathrm{C}} \Big[h(z) + \frac{\varepsilon}{2} \nabla_\mathrm{S} z \cdot \nabla_\mathrm{S} z + \Big(\frac{1}{2} \big(\kappa_\mathrm{N} (u_\mathrm{N}^k)^2 + \kappa_\mathrm{T} (u_\mathrm{T}^k)^2\big) - \alpha_\mathrm{F} \Big) z \Big] \,\mathrm{d}S \\ &\text{subject to} \qquad 0 \le z \le z^{k-1}. \end{aligned} \tag{24c}$$

Discretizing system (24b) via finite elements, we obtain

$$\begin{aligned} &\underset{u = (u_\mathrm{C}, u_\mathrm{F}, u_\mathrm{D})}{\text{Minimize}} \ \frac{1}{2} u^\top A(\pi, z^{k-1}) u \\ &\text{subject to} \quad u_\mathrm{C} \in \Lambda_0 := \{u \,|\, u \cdot \vec{n} \ge 0\} \quad \text{and} \quad u_\mathrm{D} = w_\mathrm{D}^k, \end{aligned} \tag{25}$$

where the components of $u = (u_\mathrm{C}, u_\mathrm{F}, u_\mathrm{D})$ correspond to the displacement on contact boundary Γ_C, in free nodes (interior and Neumann) in $\bar{\Omega} \setminus (\Gamma_\mathrm{C} \cup \Gamma_\mathrm{D})$, and on Dirichlet boundary Γ_D, respectively. Matrix A has the following form

$$A(\pi, z^{k-1}) = \begin{pmatrix} A_\mathrm{CC} & A_\mathrm{CF} & A_\mathrm{CD} \\ A_\mathrm{FC} & A_\mathrm{CF} & A_\mathrm{FD} \\ A_\mathrm{DC} & A_\mathrm{DF} & A_\mathrm{DD} \end{pmatrix} + \begin{pmatrix} \tilde{A}(\pi, z^{k-1}) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where the first part corresponds to the discretization of the first part of the objective in (24b) and similarly for the second part. Using simple calculus, discretized problem (25) can be written as

$$\begin{aligned}&\underset{u_{\mathrm{C}}}{\text{Minimize}}\ \frac{1}{2}u_{\mathrm{C}}^\top(A_\alpha+\tilde{A}(\pi,z^{k-1}))u_{\mathrm{C}}+(A_\beta w_{\mathrm{D}}^k)^\top u_{\mathrm{C}}\\&\text{subject to } u_{\mathrm{C}}\in\Lambda_0,\end{aligned}\tag{26a}$$

where we have defined

$$\begin{aligned}A_\alpha&:=A_{\mathrm{CC}}-A_{\mathrm{CF}}A_{\mathrm{FF}}^{-1}A_{\mathrm{FC}}, &\qquad A_\gamma&:=-A_{\mathrm{FF}}^{-1}A_{\mathrm{FC}},\\A_\beta&:=A_{\mathrm{CD}}-A_{\mathrm{CF}}A_{\mathrm{FF}}^{-1}A_{\mathrm{FD}}, &\qquad A_\delta&:=-A_{\mathrm{FF}}^{-1}A_{\mathrm{FD}}.\end{aligned}$$

Similarly, when discretizing (24c), we obtain the following problem

$$\begin{aligned}&\underset{z}{\text{Minimize}}\ \frac{1}{2}z^\top Bz+b(\pi,u^k)^\top z\\&\text{subject to } 0\le z\le z^{k-1}.\end{aligned}\tag{26b}$$

Since both problems in (26) are quadratic, we can pass to their necessary optimality conditions and the whole optimization problem (8) reads as

$$\begin{aligned}&\underset{\pi,u_{\mathrm{C}},z}{\text{Minimize}}\ \tau\sum_{k=1}^K\left[\frac{\zeta}{2}\left|u_{\mathrm{C}}^k-[u_{\mathrm{d}}]_{\mathrm{C}}^k\right|^2+\frac{\zeta}{2}\left|A_\gamma u_{\mathrm{C}}^k+A_\delta w_{\mathrm{D}}^k-[u_{\mathrm{d}}]_{\mathrm{F}}^k\right|^2+\frac{1}{2}\left|z^k-z_{\mathrm{d}}^k\right|^2\right]\\&\text{subject to } 0\in(A_\alpha+\tilde{A}(\pi,z^{k-1}))u_{\mathrm{C}}^k+A_\beta w_{\mathrm{D}}^k+\mathrm{N}_{\Lambda_0}(u_{\mathrm{C}}^k),\ \ k=1,\dots,K,\ \ u^0=u_0,\\&\qquad\qquad 0\in Bz^k+b(\pi,u^k)+\mathrm{N}_{[0,z^{k-1}]}(z^k),\qquad k=1,\dots,K,\qquad z^0=z_0,\\&\qquad\qquad \pi\in\Pi.\end{aligned}\tag{27}$$

By passing from u^k to u_{C}^k we have managed to reduce the number of parameters in (24b) from the number of all nodes to the number of contact nodes only. This is especially powerful because the first inclusion in (27) will be solved many times during the parameter identification procedure while it is sufficient to compute matrices A_α, A_β, A_γ and A_δ only once.

To be able to use Theorem 4.5, we need to check whether assumptions (A1)–(A4) are satisfied. But this amounts to showing that matrices $A_\alpha+\tilde{A}(\pi,z^{k-1})$ and B are positive definite. Since A_α is Schur complement of A_{CC} in $\hat{A}:=\begin{pmatrix}A_{\mathrm{CC}}A_{\mathrm{CF}}\\A_{\mathrm{FC}}A_{\mathrm{FF}}\end{pmatrix}$, it is positive definite if $\hat{A}$ is positive definite. But the positive definiteness of $\hat{A}$ follows from the conformal FEM via positive definiteness of $\mathbb{C}$ together with the Korn inequality using Dirichlet boundary conditions on Γ_{D}. More precisely, the FEM may also involve some numerical integration (which in fact has been used for our implementation, too).

Remark 4 (Boundary-element method) Note that (26a) is the optimization problem on Γ_{C} because we eliminated the values u_{D} and u_{F}. This is the philosophy of the *boundary-integral method* and $(A_\beta w_{\mathrm{D}}^k)^\top$ in (26a) is in the position of the (discretized) Poincaré-Steklov operator transferring Dirichlet boundary conditions on Γ_{C} to traction forces on Γ_{C}.

The discretization then leads to the celebrated *Boundary-Element Method* (BEM). One option for this discretization is FEM, cf. e.g. [38], which is in fact what we used here and

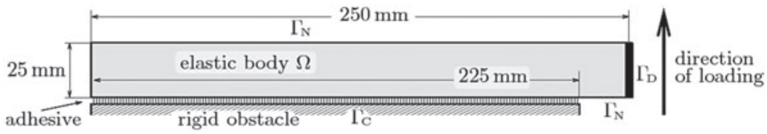

Figure 2. Geometry and boundary conditions of the two-dimensional problem used for calculation.

such BEM represents a noteworthy interpretation of (26a). Other options are based on a direct discretization of the Poincaré-Steklov operator using the approximate evaluation of the so-called Somigliana identity based on the underlying integral Green operators, cf. e.g. [33,39–41].

Remark 5 (Variants of the adhesive model) The contribution $h(z)$ in (23a) has the meaning of a stored energy deposited in the adhesive bonds and, during delamination, this energy naturally increases. If a reversible damage (called healing) were allowed, cf. Remark 2 above, $h'(z)$ would give a driving force for it. Strict convexity of h represents certain *cohesive effects*: when delamination is tended to be complete, still more and more energy is needed for complete delamination. Cohesive effects can also be modelled by letting κ_N and κ_T dependent on z so that $z \mapsto z\kappa_N(z)$ and $z \mapsto z\kappa_T(z)$ are convex. This however does not guarantee strict convexity of $\mathscr{E}(t, \pi, u, \cdot)$. Other option complying with a purely adhesive contact (e.g. $h = 0$) would be to consider a small, linear *viscosity* in z, i.e. $\mathscr{R}_2$ strictly convex and quadratic. Then the usual concept of weak solution can be used again together with the semi-implicit fractional-step-type time discretization. Yet, such problem becomes computational difficult if the viscosity is small, as often considered with the goal to approximate so-called vanishing-viscosity solution in the rate-independent inviscid limit, cf. [42].

6. Numerical experiments

In this section, we illustrate usage and efficiency of the theory developed in Section 4 and later specified in Section 5 on a two-dimensional problem where an elastic body glued along the x-axis and pulled in the direction of the y-axis by the time-varying loading w_D, cf. Figure 2. Considering the parameters α_F, κ_N, and κ_T to be unknown, the main goal is to identify them via an inverse problem. Following the delamination example in [24,42], we considered the isotropic material in the bulk with the tensor of elastic moduli

$$\mathbb{C}_{ijkl} := \frac{\nu E}{(1+\nu)(1-2\nu)}\delta_{ij}\delta_{kl} + \frac{E}{2(1+\nu)}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

with the Young modulus $E = 70$ GPa and the Poisson ratio $\nu = 0.35$. Concerning the adhesive-stored-energy and the gradient terms in (23a), we used $h(z) = \frac{1}{2}z^2 - z$ and $\varepsilon = 1$ J, while the weight ζ was chosen as $10^{10}\mathrm{m}^{-2}$. For the space discretization we employed a mesh with 14×20 nodes and the equidistant time discretization used 40 time instants. The contact boundary consists of 12 nodes. As already said, there are three parameters to be identified: α_F, κ_N, and κ_T. Moreover, we assume that the values of these parameters are not

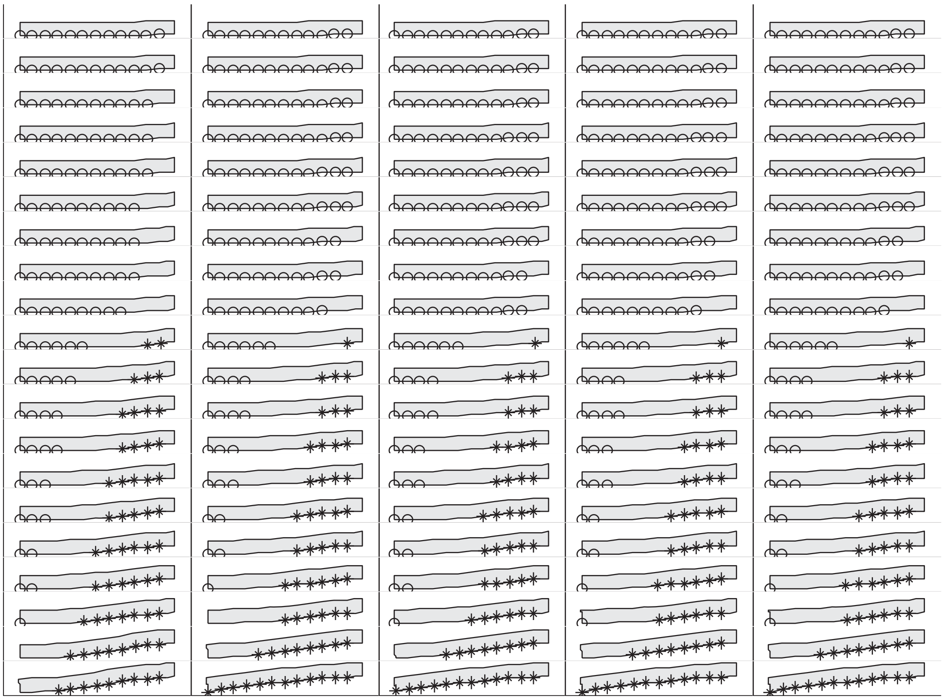

Figure 3. Evolution of the deformed specimen with distribution of the delamination parameter z along Γ_C (only values 1 or 0 are displayed) at 17 selected time instances. Displacements depicted as magnified by factor 50×.

constant along the contact boundary, but it may have different values in every contact node. This leads to a total number of $3 \times 12 = 36$ parameters to be identified.

We fixed these 36 values, to be more specific the mean of α_F, κ_N, and κ_T was 187.5 J/m^2, 150 GPa/m and 75 GPa/m, respectively. The difference between the smallest and largest value of α_F was approximately 10% and similarly for κ_N and κ_T. Next, we randomly generated some (with time increasing) dragging loading w_D, computed the corresponding (u_d, z_d), and plugged them into the upper level of problem (27). Since there was no perturbation of (u_d, z_d) present, the optimal objective value was zero, which allows numerical testing of the efficiency of the optimization algorithm.

The computation of problem (27) was performed in Matlab. To compute u^k from the first inclusion in (27), we modified and used the already written code.[43] Since a direct application of a gradient algorithm to whole problem (27) lead to rather inferior results, we had to find another way to solve (27), specifically we used a combination of three optimization algorithms. The first was PSwarm,[44] which combines pattern search with genetic algorithm particle swarm, the second one standard Matlab function `fminunc` and the last one a nonsmooth modification of BFGS algorithm [45] with its implementation.[46]

The optimization process was run in four phases. For the first phase, we simplified the problem and assumed that the parameters are constant along the contact boundary. This reduced the number of parameters from 36 to 3. To this problem, the algorithm PSwarm was used, however, we did not let it converge to the optimal solution but it was interrupted when

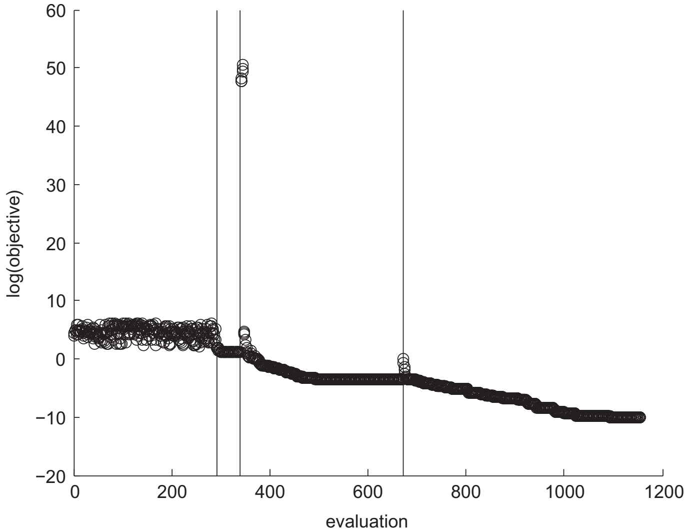

Figure 4. Development of the objective value during particular iterations of the optimization algorithms used during the four phases of our optimization: phase 1 used a global optimization algorithm (PSwarm), whereas phases 2–4 used a (sub)gradient algorithm with subsequently refined discretization of Γ_C.

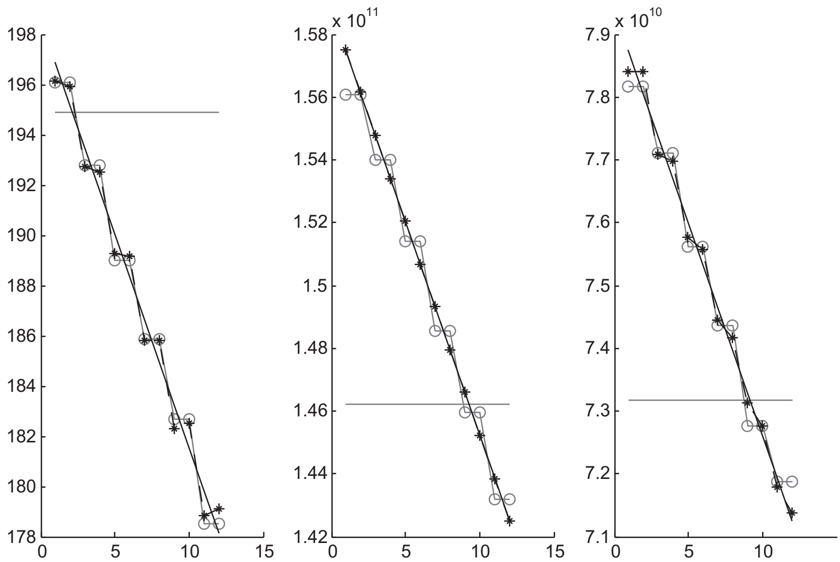

Figure 5. Parameter distribution along the contact boundary, graphs depicting form left to right α_F, κ_N and κ_T resulting after particular phases of the optimization algorithm.

the problem reached a priori given threshold or when the optimal value did not improve much in several successive iterations. In other words, the goal of the first phase was to find an estimate of the solution. Since PSwarm works rather with populations instead of single points, multiple initial points had to be chosen. These points were generated randomly from the following intervals

$$\alpha_\mathrm{F} \in \left[100\ \mathrm{J/m^2}, 500\ \mathrm{J/m^2}\right], \qquad \kappa_\mathrm{N}, \kappa_\mathrm{T} \in \left[10\ \mathrm{GPa/m}, 1000\ \mathrm{GPa/m}\right].$$

In the second phase, the reduced problem was still considered but this time, an algorithm using a gradient information was used. Similarly to the first phase, we did not let the it converge and interrupted it prematurely. Because of this interruption, non-regular points were usually evaded and it was possible to use `fminunc`, even though it is designed for smooth functions.

While in the first two phases, the values of parameters were constant on the contact boundary, this no longer holds true for the last two phases. In the third one, we considered the state in which one parameter corresponds to two nodes on the contact boundary, while in the fourth phase every parameter corresponded to only one node. This means that there were 18 parameters in the third phase and 36 in the last one. The evolution of the optimal value can be seen in Figure 4. Note that on the y axis the logarithm of the objective value is depicted and that the vertical lines separate the four phases.

The following table summarizes the values of parameters and of the objective function for all phases. The first column presents the best point in the initial population of PSwarm. The next four columns show the optimal solutions and values of all four phases. Finally, the last column corresponds to the actual values of parameters. Since there were multiple values distributed along the boundary for the last three columns, we show only their mean in such cases.

	Starting	Phase 1	Phase 2	Phase 3	Optimal	Desired
α_F	203.934	190.405	194.877	187.489	187.512	187.5
κ_N	$0.822{\cdot}10^{11}$	$1.586{\cdot}10^{11}$	$1.462{\cdot}10^{11}$	$1.499{\cdot}10^{11}$	$1.500{\cdot}10^{11}$	$1.5{\cdot}10^{11}$
κ_T	$47.251{\cdot}10^{10}$	$2.326{\cdot}10^{10}$	$7.317{\cdot}10^{10}$	$7.498{\cdot}10^{10}$	$7.499{\cdot}10^{10}$	$7.5{\cdot}10^{10}$
Objective	3138.97	70.503	14.184	$3.573{\cdot}10^{-4}$	$7.538{\cdot}10^{-11}$	0

In Figure 3, we show the the displacement u (magnified by factor 50) corresponding to one of the random initial points used for PSwarm and solution of the four phases. A circle on the contact boundary mean that no delamination has taken place yet at the corresponding node while an asterisk means that the corresponding node has been completely delaminated. No symbol being present indicates that only a partial delamination took place. Since the contact boundary is shorter than the length of the body, there are no symbols at the bottom right corner.

In Figure 5, we show the distribution of the elastic adhesive moduli κ_N and κ_T as well as the fracture toughness α_F along the contact boundary Γ_C. Four lines corresponding to the actual parameters and to the terminal points of phases 2, 3 and 4 are depicted. The horizontal line without any symbols corresponds to phase 2, the line with circles corresponds to line 3 and the line with asterisks corresponds to phase 4, which means that it depicts the parameters identified by the algorithm. The last line without any symbols (which coincides with the line with asterisks for κ_N) depicts the actual parameters. We see that while the result of phase 3 provided a good estimate for the actual parameters. Phase 4 provided only a slight improvement for κ_T while it managed to identify the values of κ_N completely.

7. Concluding remarks

The optimality conditions stated in Theorem 4.5 are in the MPEC literature called M-stationarity conditions because they are based exclusively on notions from the Mordukhovich subdifferential calculus. They are relatively sharp and can very well be used, e.g. for testing this type of stationarity at points computed via ImP. It would be a great challenge to derive suitable optimality conditions also for the original continuous MPEEC (3). Unfortunately, this problem is formulated over non-Asplund spaces (with a possible exception of the space for the variable π) which are not amenable for a treatment via the Mordukhovich calculus.

If function $\mathscr{R}_2$ in (4) happens to be Non-differentiable as in Remarks 2–3, then in the generalized equation system defining S one has to do with sums of multifunctions. Such situations occur in the so-called Stampacchia variational inequalities, whose sensitivity and stability analysis represents a great open problem. One possible way to overcome this hurdle could be a smoothening of $\mathscr{R}_2$ or a smooth penalization of the constraint.

In this paper, apart from some particular cases like that mentioned in Remark 1, the main peculiarity consists in the fact that the original continuous problem in (3) (whose parameters π are to be identified) does not need to have a unique response. To control (or identify) such systems is, from very fundamental reasons, very doubtful. Therefore, one should interpret the approach used in this article carefully, counting only with a response of (1) that can be approximated by a particular numerical method (4) and being aware that possibly some other responses might exist and give even more accurate results. This is the best one can do and assume in identification of system of the type (1) which may cover very general situation, e.g. sudden ruptures which are naturally very difficult to be controlled (or identified).

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