Proc. of the 21st IFIP TC7 Conference on System Modeling and Optimization
Sophia Antipolis, July 21-25, 2003 (submitted)

ON THE MODELING AND CONTROL OF DELAMINATION PROCESSES

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Abstract This paper is motivated by problem of optimal shape design of laminated elastic bodies. We use a recently introduced model of delamination, based on minimization of potential energy which includes the free (Gibbs-type) energy and (pseudo)potential of dissipative forces, to introduce and analyze a special mathematical program with equilibrium constraints. The equilibrium is governed by a finite sequence of coupled mathematical programs that have to be solved one after another in the direction of increasing time. We derive optimality conditions for the control problem and illustrate them on an academic example.

Keywords: Inelastic damage, mathematical program with equilibrium constraints, evolution equilibrium, hemivariational inequality

1. Introduction

The design of crashworthy vehicles depends upon developing structures capable of absorbing large amounts of crash energy. Composite materials have been shown to have energy absorbing properties superior to conventional metallic structures. With the goal of designing crash elements (structural elements with high energy absorption by crash), we consider laminated structures. The energy is absorbed by *delamination*

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of such structures. Mathematical simulation of vehicle crash requires, first of all, finding a reliable mathematical model. In this paper, we use a recently introduced model of delamination, based on minimization of potential energy which includes the free (Gibbs-type) energy and (pseudo)potential of dissipative forces ([9]). Based on this model, we introduce and analyze an evolution control problem with the final goal of designing optimal shape of crash elements.

Delamination is a progressive separation of bonded laminate and, simultaneously, degradation of the used adhesive. The mechanism of delamination is very complex and involves phenomena like debonding and unilateral contact with nonmonotone friction. In the recent literature, the modeling of the delamination problem is generally approached either by using fracture mechanics (see, e.g., [3, 20]) or by introducing special constitutive laws for the interface material in the spirit of damage mechanics, or simply quasistatically. In the second approach, delamination is described by a *damage variable* reflecting the destruction of the bonds in the a-priori known delamination surface (see, e.g., [5, 17]).

Another, static approach was proposed by Panagiotopoulos [16] who formulated the problem of equilibrium positions as a hemivariational inequality (HVI), a generalization of variational inequality for nonmonotone operators; see also [2]. Thus, this method has limited applications only in processes with simple time–dependent loadings. After discretization by the finite elements method, this approach results in a nonsmooth and nonconvex optimization problem. The variable of this problem are the elements of the discretized displacement vector.

In the model introduced in [9], delamination is considered as a fracture-like process that can run along a-priori known surfaces between homogeneous isotropic elastic bodies that are in frictionless unilateral contact. It is an *activated and rate-independent process*, based on the philosophy that a specific energy is needed to cut the macromolecular structure of the adhesive, no matter how fast or slow this process is. This model is supported by a rigorous analysis based on the apparatus recently developed for rate-independent processes in, e.g., [10–11]. In this paper, we will refer to this model as *RI model*. After discretization in time and space, the RI model results in a sequence of smooth nonconvex optimization problems. Compared to the static HVI model, the dimension of one problem increases by the number of damage parameters.

Assume that the discretized RI model contains parameters, the values of which should be optimized with respect to an (upper-level) objective. In this way, we arrive at a special mathematical program with equilibrium constraints (MPEC) in which the underlying equilibrium has evolution nature. From the viewpoint of optimality conditions, similar

problems were investigated in [21]. There, however, the equilibrium is governed by a standard optimal control problem (i.e., the optimization is performed over the whole time interval). In our case, we have to do with a finite sequence of coupled mathematical programs that have to be solved one after another in the direction of increasing time. This difference is naturally reflected in the character of the resulting optimality conditions.

The paper is organized as follows: In the next section, we introduce the RI model of [9] and compare it the the static HVI model. After that, we present a conceptual MPEC with the discretized RI delamination process as equilibrium constraint. Section 3 is devoted to necessary optimality conditions for this MPEC. As a workhorse we use the generalized differential calculus of B. Mordukhovich ([13, 12]) which proved to be an efficient tool in the treatment of various equilibria. The resulting conditions are illustrated by means of an academic example introduced in Section 2.

The following notation is employed: If f is a differentiable function of two variables, then $\nabla_1 f$ and $\nabla_2 f$ denote the partial derivatives with respect to the first and the second variable, respectively. $\mathbb{B}$ is the unit ball and for a multifunction $Q[\mathbb{R}^n \rightsquigarrow \mathbb{R}^m], Gph\, Q := \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^m \,|\, y \in Q(x)\}$. To describe the local properties of sets, multifunctions and real-valued functions, we make use of suitable concepts from the generalized differential calculus of B. Mordukhovich ([13],[12]). So, $N_\Omega(x)$ denotes the limiting normal cone to the set Ω at $x \in cl\Omega, D^*Q(x, y)(\cdot)$ denotes the coderivative of the multifunction Q at $(x, y) \in cl\, Gph\, Q$ and $\partial f(x)$ is the limiting subdifferential of a real-valued function f at $x \in dom f$.

For the reader's convenience, we close this section with a useful stability concept for multifunctions which plays an important role in Section 3.

Definition 1 ([19]) *A multifunction $Q[\mathbb{R}^n \rightsquigarrow \mathbb{R}^m]$ is* calm *at $(\bar{x}, \bar{y}) \in Gph\, Q$ provided there is a constant $\kappa \in \mathbb{R}_+$ along with neighborhoods $\mathcal{U}$ of $\bar{x}$ and $\mathcal{V}$ of $\bar{y}$ such that*

$$Q(x) \cap \mathcal{V} \subset Q(\bar{x}) + \kappa \|x - \bar{x}\| \mathbb{B} \text{ for all } x \in \mathcal{U}.$$

2. Delamination process

In this section we recall the rate-independent model of the delamination process, as recently introduced in [9]. In this model, after a (time and space) discretization, one has to solve in each time step a smooth nonconvex optimization problem. We further propose a conceptual optimization problem in which the discretized delamination process arises as a constraint.

2.1 Modeling

For simplicity of notation, we only consider laminates consisting of two elastic bodies Ω_1 and Ω_2 with an interface boundary denoted by Γ_{12}; see Fig. 1. The two bodies are in unilateral contact along Γ_{12}; further they are glued along Γ_{12} by an adhesive. The matrix $b : \Gamma_{12} \to \mathbb{R}^{2\times 2}$ reflects the elastic properties of the adhesive. We adopt, in fact, a dimensional reduction of the two-dimensional adhesive layer to an one-dimensional surface Γ_{12}.

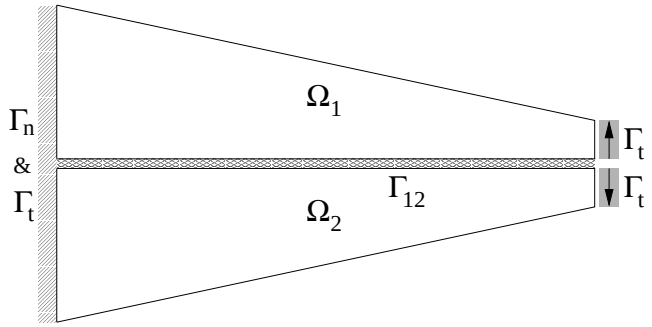

Figure 1.

The state of the system will be considered as $y = (u_1, u_2, \zeta)$ where $u_i : \Omega_i \to \mathbb{R}^2$ is the (small) displacement in the domain Ω_i, $i = 1, 2$, and $\zeta : \Gamma_{12} \to [0, 1]$ is a *damage parameter* indicating how much of the adhesive is effective: 1 means 100% of the adhesive glues at $x \in \Gamma_{12}$, 0 means that the surface is completely delaminated at the current point $x \in \Gamma_{12}$, and $0 < \zeta(x) < 1$ means that some portion of macromolecules of the adhesive is already cut while the rest is still effective.

A rate-independent delamination model has recently been introduced in [9]. This model is based on the minimization of the elastic stored energy and the dissipation potential subject to several constraints. The constraints reflect

- the unilateral contact of the two elastic bodies;
- the time-dependent Dirichlet loading by a "hard device";
- the irreversibility (in time) of the delamination of the adhesive.

The resulting minimization problem is first discretized in the time variable and further in the space variable by the standard finite element method. Below we present the fully discretized problem that will be further studied in the subsequent sections.

We use the same finite element mesh for both variables, u and ζ. In order to allow for the separation (delamination) of the elastic bodies, the joint boundary Γ_{12} is discretized by N pairs of nodes, say $(n_{1,j}, n_{2,j})$, $j = 1, \ldots, N$, with $n_{i,j} \in \Omega_i$, $i = 1, 2$. At the beginning of the delamination process the nodes $n_{1,j}, n_{2,j}$ have the same positions for all $j = 1, \ldots, N$.

Let A_1, A_2 be the stiffness matrices of the elastic bodies Ω_1, Ω_2, respectively. The discretized elastic stored energy becomes

$$V(u,\zeta) = \sum_{i=1}^{2} u_i^T A_i u_i + \sum_{j=1}^{N} \omega_j \zeta_j \, (u_{1,j} - u_{2,j})^\top b(n_j)(u_{1,j} - u_{2,j})$$

where ω_j are integration weights. Similarly, the discretized dissipation potential is

$$R(\zeta) = \sum_{j=1}^{N} -\omega_j d(n_j)\zeta_j.$$

Here $d(x)$ is a phenomenological parameter having the meaning of a specific energy needed to delaminate the surface Γ_{12} at a point $x \in \Gamma_{12}$, i.e., the energy needed to switch $\zeta(x)$ from 1 to 0. This energy is irreversibly dissipated to the structural change of the adhesive. The case $R(\zeta) = +\infty$ will be respected by a corresponding linear constraint.

We assume that the laminate is loaded by time-depended unilateral Dirichlet loading ("hard-device") on parts of the boundaries of Ω_1, Ω_2. The load vector (prescribed displacements) at a time step i is denoted by $\overline{u}^i$. Let L_1 be a rectangular matrix selecting the "loaded" boundary components from the whole vector u. Finally, denote by L_2 a rectangular matrix that takes care of the nonpenetration of Ω_1 and Ω_2 on Γ_{12}.

The discrete version of the delamination problem in time step i is then (we omit the current time step index for simplicity)

$$\begin{aligned} \text{minimize} \quad & V(u,\zeta) + R(\zeta - \zeta^{i-1}) \\ \text{subject to} \quad & L_1 u \geq \overline{u}^i \\ & L_2 u \leq 0 \\ & \zeta^{i-1} \geq \zeta \geq 0 \quad \text{componentwise.} \end{aligned} \tag{1}$$

Here the index $i-1$ refers to the previous time step. The irreversibility of the dissipation process is guaranteed by the left-hand side of the last constraint.

As we are only interested in the components of the displacement vector lying on the boundary Γ_{12}, we can eliminate all components corresponding to the interior nodes. This reduces the number of variables in (1) to

the number of interface boundary nodes times five (two times two components of the displacement vector plus the components of ζ) plus the number of boundary nodes with prescribed non-zero Dirichlet condition (loaded nodes) times two. In [9] it was shown that (1) can be efficiently solved by state-of-the-art optimization software and that the proposed modeling of the delamination process delivers reasonable results.

2.2 Relation to the HVI model

Let us briefly show the relation of the RI model described above to the HVI model, introduced by Panagiotopoulos and numerically solved in [2].

The hemivariational inequality model of the static delamination problem amounts to first-order optimality condition of the following nonsmooth nonconvex optimization problem (we use the same notation as in the previous section):

$$\begin{aligned} \text{minimize} & \sum_{i=1}^{2} u_i^T A_i u_i + \sum_{j=1}^{N} \omega_j \min\{(u_{1,j}-u_{2,j})^\top b(n_j)(u_{1,j}-u_{2,j}), d(n_j)\} \\ \text{subject to} & \quad L_1 u \geq \overline{u}^i \\ & \quad L_2 u \leq 0\,. \end{aligned} \tag{2}$$

Recall the simple fact that, for smooth convex functions f and g, the set of (Clarke) stationary points of the (nonsmooth) pointwise minimum function $\min\{f(x), g(x)\}$ is equal to the set of x-components of stationary points of the (smooth) mathematical program $\alpha f(x) + (1-\alpha)g(x)$, $\alpha \in [0,1]$ in variables x, α. Hence the (Clarke) stationary points of problem (2) are just the u-components of stationary points of the smooth problem (1), assuming that $\zeta^{i-1} \equiv 1$. In other words, solving the static HVI model "is the same" as solving the RI model for the first time step, starting from the non-delaminated state (of course, one has to take into account that different algorithms may find different stationary points of these two nonconvex problems). The static model tries to "jump" directly into the solution at the terminal time—the time discretization is reduced to only one interval. The HVI results may then only be reliable for monotone (in time) loadings and simple geometries, contrary to the RI model that allows for general nonmonotone loading (and unloading). The difference between the two models, even for monotone loading and simple problems, is clearly seen when solving the optimal control problems; see, in particular, Example 2 in Section 4.

2.3 Control

Our second goal is to control the (discretized) RI delamination process by certain parameters. The aim is to find such parameters that an objective function depending on the terminal state is minimized. For instance, having in mind our motivation from the Introduction, we want to find such a shape of the boundaries of Ω_1, Ω_2 that, at the terminal time, as much energy is dissipated as possible.

This optimal control problem can thus be written as the following "conceptual" MPEC

$$\begin{array}{ll} \text{minimize} & \varphi(x,y) \\ \text{subject to} & x \in U_{ad}, \\ & y \text{ is the terminal state of the delamination process} \\ & \quad \text{depending on parameter } x, \end{array} \tag{3}$$

where $U_{ad} \subset \mathbb{R}^n$ is the set of admissible controls. The detailed formulation of the problem is given in the next section.

Before going on, let us introduce a simplified example that demonstrates the difficulties connected with the control of the delamination process.

EXAMPLE 1 Consider the four-string example as shown in Figure 2. In reality, the strings are at the same horizontal position, here they are plotted with some gap for presentation reasons. The elasticity modulae of the strings are $e_1, \ldots, e_4$. Assume that $e_3 = e_4$ and denote it by e. The end-nodes of the strings are denoted n_0, n_1, n_2. The vertical displacements at the nodes are u_0, u_1, u_2. Node n_0 is fixed ($u_0 = 0$), node n_2 is subjected to nonzero Dirichlet boundary condition (prescribed displacements) $u_2 = \overline{u}$.

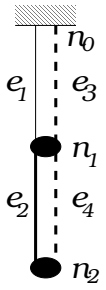

Figure 2.

The left-hand strings are elastic and do "never" break—they simulate the elastic bodies. The right-hand strings simulate the adhesive: they are also elastic but can break when the relative displacement reaches a certain value.

The Dirichlet condition $\overline{u}$ depends on time. The equilibrium state in the i-th time interval is obtained by solving the optimization problem

$$\begin{aligned} &\min_{u_1,u_2,\zeta_1,\zeta_2} \mathcal{E} := \sum_{j=1}^{2} \Big(e_j(u_j - u_{j-1})^2 + \zeta_j e (u_j - u_{j-1})^2 + (\zeta_j^{i-1} - \zeta_j) e d \Big) \\ &\text{subject to} \\ &\quad u_2 \geq \overline{u}^i \\ &\quad u_j - u_{j-1} \geq 0, \quad j = 1, 2 \\ &\quad \zeta^{i-1} \geq \zeta \geq 0 \end{aligned} \tag{4}$$

The first term under the sum is the strain energy of the elastic strings 1 and 2. The second term is the strain energy of the breakable strings 3 and 4 (the "adhesive"). The third term is the dissipation energy. Number d is the energy dissipated by breaking one string (this is given in our case).

In the MPEC, the control variables are e_1 and e_2. The goal is to find such design that, at the terminal time k, as much energy is dissipated as possible:

$$\begin{aligned} &\max_{e_1,e_2,u_1,u_2,\zeta_1,\zeta_2} \varphi := \zeta_1^k + \zeta_2^k \\ &\text{subject to} \\ &\quad e_1 + e_2 = 2 \\ &\quad (u_1, u_2, \zeta_1, \zeta_2) \text{ solves (4) at time } k. \end{aligned} \tag{5}$$

Assume the following problem data:

$d = 1 \cdot 10^{-6}$ (dissipation parameter)

$\overline{u}^k = 0.007$ (final prescribed displacement)

$e = 10.$

The optimal solution is

$e_1 = 1, \quad e_2 = 1,$

$\zeta_1^k = \zeta_2^k = 0, \quad u_1^k = 0.0035, \quad u_2^k = 0.007,$

$\varphi = 2, \quad \mathcal{E} = 4.45 \cdot 10^{-5},$

when both strings 3 and 4 break. However, there may be more solutions to (5) within some neighborhood of 1 that also lead to the break of both strings. One such solution is

$$e_1 = 1.05, \quad e_2 = 0.95,$$
$$\zeta_1^k = \zeta_2^k = 0, \quad u_1^k = 0.003325, \quad u_2^k = 0.007,$$
$$\varphi = 2, \quad \mathcal{E} = 4.44388 \cdot 10^{-5}.$$

Obviously, everything within the interval $e_1 \in (0.95, 1.05)$, $e_2 = 2 - e_1$ is a solution to (5).

Note that, for instance, $(e_1 = 1.1,\ e_2 = 0.9)$ is not an optimal control of the MPEC (5) any more, because it gives $\zeta_1^k = 1,\ \zeta_2^k = 0$ as a solution of the state problem (4). That means, only one string breaks and the corresponding upper-level criterium is only $\varphi = 1$.

Next two sections are devoted to necessary optimality conditions for MPECs of the type (3).

3. Optimality conditions

The discretized delamination model, introduced and discussed in the previous section, can be generally written down in the form of a finite sequence of coupled optimization problems

$$\begin{array}{rl} \text{minimize} & f^i(y^{i-1}, y^i) \\ \text{subject to} & y^i \in \Gamma^i(y^{i-1}),\ i = 1, 2, \ldots, k \\ & y^0 \text{ given}, \end{array} \tag{6}$$

where $y^{i-1} \in \mathbb{R}^m$ is the parameter, $y^i \in \mathbb{R}^m$ is the unknown variable, $f^i(y^{i-1}, \cdot)$ is the objective and the multifunction $\Gamma^i[\mathbb{R}^m \rightsquigarrow \mathbb{R}^m]$ specifies the feasible set. This sequence of optimization problems has to be solved starting from the initial "state" y^0, in the direction of the increasing time index. In this way, one obtains eventually the whole *trajectory* $y^1, y^2, \ldots, y^k$. The aim of this section is to analyze MPECs with equilibria governed by such a sequence of coupled optimization problems. In each of them, additionally, a control variable $x \in \mathbb{R}^n$ arises so that the ith problem attains the "controlled" form

$$\begin{array}{rl} \text{minimize} & f^i(x, y^{i-1}, y^i) \\ \text{subject to} & y^i \in \Gamma^i(x, y^{i-1}). \end{array} \tag{7}$$

Because our attention is paid to necessary optimality conditions for MPECs with such equilibria, we can replace the single problems (7)

by the respective 1st-order necessary optimality conditions. Assuming that all objectives $f^i(x, y^{i-1}, \cdot)$ are continuously differentiable for each pair (x, y^{i-1}), these conditions can be written down in the form

$$0 \in \nabla_3 f^i(x, y^{i-1}, y^i) + N_{\Gamma(x,y^{i-1})}(y^i),\ i = 1, 2, \ldots, k. \tag{8}$$

Instead of the sequence of relations (7), we can now consider the sequence of coupled generalized equations (GEs)

$$0 \in F^i(x, y^{i-1}, y^i) + Q^i(x, y^{i-1}, y^i),\ \ i = 1, 2, \ldots, k, \tag{9}$$

where $F^i[\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m]$, $Q^i[\mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m \rightsquigarrow \mathbb{R}^m]$ represent the single-valued and the multi-valued part, respectively. This generalization enlarges our applicability area also to equilibria governed, e.g., by a finite sequence of coupled complementarity problems or variational inequalities. In this way, we have arrived at a hopefully useful paradigm describing a specific time evolution of a fairly large class of equilibrium problems.

On the respective MPEC we impose the following simplifying assumptions:

(i) The (upper-level) objective depends only on x and y^k;

(ii) The state variables $y^1, y^2, \ldots, y^k$ are not subject to any constraints;

(iii) All function F^i are continuously differentiable and all maps Q^i have closed graphs.

The first two assumptions are not essential and can be removed. In the MPECs associated with the delamination process, however, they are fulfilled and so we decided to simplify the statement of the next theorem by imposing them from the very beginning. We thus have to deal with the following MPEC:

$$\begin{array}{rl} \text{minimize} & \varphi(x, y^k) \\ \text{subject to} & 0 \in F^i(x, y^{i-1}, y^i) + Q^i(x, y^{i-1}, y^i),\ \ i = 1, 2, \ldots, k \\ & y^0 \text{ given} \\ & x \in U_{ad}, \end{array} \tag{10}$$

where $\varphi[\mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}]$ is an (upper-level) objective and $U_{ad} \subset \mathbb{R}^n$ is as before the set of admissible controls. Throughout the rest of the paper it is assumed that φ is locally Lipschitz and U_{ad} is nonempty and closed. By y we denote the trajectory $(y^1, y^2, \ldots, y^k)$ and $\overline{m} := km$.

THEOREM 2 *Let $(\widehat{x},\widehat{y})$ be a (local) solution of MPEC (10). Denote $\widehat{z}^i = -F^i(\widehat{x},\widehat{y}^{i-1},\widehat{y}^i), i = 1,2,\ldots,k$, and define the multifunction $\Xi[\mathbb{R}^{\overline{m}} \rightsquigarrow \mathbb{R}^n \times \mathbb{R}^{\overline{m}}]$ by*

$$\begin{aligned}\Xi(\xi^1,\xi^2,\ldots,\xi^k)\\ := \left\{(x,y) \in U_{ad} \times \mathbb{R}^{\overline{m}} | \xi^i \in F^i(x,y^{i-1},y^i) + Q^i(x,y^{i-1},y^i),\right.\\ \left. i = 1,2,\ldots,k\right\}.\end{aligned}$$

Assume that Ξ is calm at $(0,\widehat{x},\widehat{y})$. Then there exist four sequences of adjoint vectors $p^1,p^2,\ldots,p^k,q^1,q^2,\ldots,q^k,v^1,v^2,\ldots,v^k,w^1,w^2,\ldots,w^k$ and subgradients $(\kappa,\eta) \in \partial\varphi(\widehat{x},\widehat{y}^k)$ such that (with $\hat{y}^0 = y^0$)

$$(p^i,q^i,v^i) \in D^*Q^i(\widehat{x},\widehat{y}^{i-1},\widehat{y}^i,\widehat{z}^i)(w^i), i = 1,2,\ldots,k \tag{11}$$

and the adjoint equation system

$$\left.\begin{aligned}0 &= \eta + (\nabla_3 F^k(\widehat{x},\widehat{y}^{k-1},\widehat{y}^k))^T w^k + v^k\\ 0 &= (\nabla_3 F^{k-1}(\widehat{x},\widehat{y}^{k-2},\widehat{y}^{k-1}))^T w^{k-1} + v^{k-1}\\ &\quad + (\nabla_2 F^k(\widehat{x},\widehat{y}^{k-1},\widehat{y}^k))^T w^k + q^k\\ &\cdots\cdots\\ 0 &= (\nabla_3 F^1(\widehat{x},y^0,\widehat{y}^1))^T w^1 + v^1 + (\nabla_2 F^2(\widehat{x},\widehat{y}^1,\widehat{y}^2))^T w^2 + q^2\end{aligned}\right\} \tag{12}$$

is fulfilled. Moreover, one has

$$0 \in \kappa + \sum_{i=1}^{k} \left[\left(\nabla_1 F^i(\widehat{x},\widehat{y}^{i-1},\widehat{y}^i)\right)^T w^i + p^i\right] + N_{U_{ad}}(\widehat{x}). \tag{13}$$

Proof. The constraints in (10) can be written down in the form

$$0 \in \Phi(x,y) + \Lambda,\ x \in U_{ad},$$

where

$$\Phi(x,y) = -\begin{bmatrix} x \\ y^0 \\ y^1 \\ -F^1(x,y^0,y^1) \\ x \\ y^1 \\ y^2 \\ -F^2(x,y^1,y^2) \\ \cdots\cdots \\ x \\ y^{k-1} \\ y^k \\ -F^k(x,y^{k-1},y^k) \end{bmatrix} \qquad \text{and} \quad \Lambda = X_{i=1}^k GphQ^i$$

Due to the imposed calmness assumption, one can invoke [14, Thm.2.4] which yields the existence of a Karush-Kuhn-Tucker (KKT) vector

$$b = (p^1, q^1, v^1, -w^1, p^2, q^2, v^2, -w^2, \ldots, p^k, q^k, v^k, -w^k,) \in N_\Lambda(-\Phi(\widehat{x},\widehat{y}))$$

and subgradients $(\kappa,\eta) \in \partial\varphi(\widehat{x},\widehat{y}^k)$ such that

$$0 \in \begin{bmatrix} \kappa \\ 0 \\ \vdots \\ 0 \\ \eta \end{bmatrix} - (\nabla\Phi(\widehat{x},\widehat{y}))^T b + \begin{bmatrix} N_{U_{ad}}(\widehat{x}) \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{14}$$

Because $N_\Lambda(-\Phi(\widehat{x},\widehat{y})) = X_{i=1}^k N_{GphQ^i}(\widehat{x},\widehat{y}^{i-1},\widehat{y}^i,\widehat{z}^i)$ see [13, Prop.1.6], it follows that $(p^i,q^i,v^i,-w^i) \in N_{GphQ^i}(\widehat{x},\widehat{y}^{i-1},\widehat{y}^i,\widehat{z}^i), i = 1,2,\ldots,k$. In this way relations (11) have been established. The first line of (14) leads now directly to relation (13), whereas the remaining k lines generate the adjoint system (12). ∎

The calmness assumption is automatically fulfilled provided U_{ad} is convex polyhedral, all function F^i are affine and all sets $GphQ^i$ are unions of finitely many convex polyhedral sets. Indeed, in such a case, $Gph\Xi$ is also a union of finitely many convex polyhedral sets and Ξ is locally upper Lipschitz around 0, cf. [18]. This is, however, a stronger property than the required calmness at $(0,\widehat{x},\widehat{y})$. Another possibility is to ensure the Aubin property of Ξ around $(0,\widehat{x},\widehat{y})$, which is also stronger than the required calmness condition. This can be done by the following Mangasarian-Fromowitz constraint qualification.

THEOREM 3 *Assume that the system*

$$
\begin{aligned}
0 &= (\nabla_3 F^k(\widehat{x}, \widehat{y}^{k-1}, \widehat{y}^k))^T w^k + v^k \\
0 &= (\nabla_3 F^{k-1}(\widehat{x}, \widehat{y}^{k-2}, \widehat{y}^{k-1}))^T w^{k-1} + v^{k-1} + (\nabla_2 F^k(\widehat{x}, \widehat{y}^{k-1}, \widehat{y}^k))^T w^k + q^k \\
&\cdots\cdots \\
0 &= (\nabla_3 F^1(\widehat{x}, y^0, \widehat{y}^1))^T w^1 + v^1 + (\nabla_2 F^2(\widehat{x}, \widehat{y}^1, \widehat{y}^2))^T w^2 + q^2 \\
0 &\in \sum_{i=1}^{k} \left[\left(\nabla_1 F^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i)\right)^T w^i + p^i \right] + N_{U_{ad}}(\widehat{x})
\end{aligned}
$$

with $(p^i, q^i, v^i) \in D^*Q^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i, \widehat{z}^i)(w^i), i = 1, 2, \ldots, k$, *possesses only the trivial solution* $p^1 = p^2 = \ldots = p^k = 0, q^2 = q^3 = \ldots = q^k = 0, v^1 = v^2 = \ldots = v^k = 0$ *and* $w^1 = w^2 = \ldots w^k = 0$. *Then* Ξ *has the Aubin property around* $(0, \widehat{x}, \widehat{y})$.

The statement follows from the Mordukhovich characterization of the Aubin property ([19, Thm.9.40]) and standard rules of the coderivative calculus [12]. As shown in [14], the above condition is automatically fulfilled, provided the multifunctions Q^i do not depend on the control and the multifunction $\Delta[\mathbb{R}^{\overline{m}} \rightsquigarrow \mathbb{R}^{\overline{m}}]$, defined by

$$
\begin{aligned}
\Delta(\xi) = \{\, y \in \mathbb{R}^{\overline{m}} \,|\, \xi^i \in\ & F^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i) \\
& + \nabla_2 F^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i)(y^{i-1} - \widehat{y}^{i-1}) \\
& + \nabla_3 F^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i)(y^i - \widehat{y}^i) \\
& + Q^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i), i = 1, 2, \ldots, k \,\},
\end{aligned}
$$

is locally single-valued and Lipschitz around $(0, \widehat{y})$ (Robinson's strong regularity). This is, however, not the case if we deal with the delamination model of Section 2. The optimality conditions of Theorem 2 can be substantially simplified provided the maps Q^i do not depend on x or y^{i-1}. This is expressed in the following corollaries.

COROLLARY 4 *Let all assumptions of Theorem 2 be fulfilled and assume that the maps* $Q^i, i = 1, 2, \ldots, k$, *do not depend on* x. *Then there exist three sequences of adjoint vectors* $q^1, q^2, \ldots, q^k$, $v^1, v^2, \ldots, v^k$, $w^1, w^2, \ldots, w^k$ *and subgradients* $(\kappa, \eta) \in \partial\varphi(\widehat{x}, \widehat{y}^k)$ *such that*

$$
(q^i, v^i) \in D^*Q^i(\widehat{y}^{i-1}, \widehat{y}^i, \widehat{z}^i)(w^i),\ i = 1, 2, \ldots, k,
$$

the adjoint equation system (12) is satisfied, and

$$
0 \in \kappa + \sum_{i=1}^{k} \left(\nabla_1 F^i(\widehat{x}, \widehat{y}^{i-1}, \widehat{y}^i)\right)^T w^i + N_{U_{ad}}(\widehat{x}). \tag{15}
$$

COROLLARY 5 *Let all assumptions of Theorem 2 be fulfilled and assume that for $i = 1, 2, \ldots, k$ the maps Q^i depend exclusively on variables y^i, respectively. Then there exist two sequences of adjoint vectors $v^1, v^2, \ldots, v^k$, $w^1, w^2, \ldots, w^k$ and subgradients $(\kappa, \eta) \in \partial\varphi(\widehat{x}, \widehat{y}^k)$ such that*

$$v^i \in D^* Q^i(\widehat{y}^i, \widehat{z}^i)(w^i), \ i = 1, 2, \ldots, k$$

and the adjoint equation system

$$\left.\begin{aligned} 0 &= \eta + (\nabla_3 F^k(\widehat{x}, \widehat{y}^{k-1}, \widehat{y}^k))^T w^k + v^k \\ 0 &= (\nabla_3 F^{k-1}(\widehat{x}, \widehat{y}^{k-2}, \widehat{y}^{k-1}))^T w^{k-1} + v^{k-1} \\ &\quad + (\nabla_2 F^k(\widehat{x}, \widehat{y}^{k-1}, \widehat{y}^k))^T w^k \\ &\ldots\ldots \\ 0 &= (\nabla_3 F^1(\widehat{x}, y^0, \widehat{y}^1))^T w^1 + v^1 + (\nabla_2 F^2(\widehat{x}, \widehat{y}^1, \widehat{y}^2))^T w^2 \end{aligned}\right\} \qquad (16)$$

is fulfilled. Moreover, relation (15) holds true.

REMARK As in the classic discrete-time optimal control problems [8], the adjoint systems (12),(16) have to be solved backwards starting from the terminal condition. Together with the GEs (9) they represent a special two-point boundary value problem.

4. Optimization of delamination processes

The aim of this section is to apply the preceding theory to an MPEC, where the equilibrium is governed by a sequence of optimization problems (7) with the data (functions f^i and multifunctions Γ^i) specified in Section 2. Without giving the structure of f^i in detail, the ith problem attains the form

$$\begin{aligned} \text{minimize} \quad & f(x, \zeta^{i-1}, u^i, \zeta^i) \\ \text{subject to} \quad & L_1 u^i \geq \bar{u}^i \\ & L_2 u^i \leq 0 \\ & \zeta^i \geq 0 \\ & \zeta^i \leq \zeta^{i-1}, \end{aligned} \qquad (17)$$

where the control x arises only in the objective, all other variables were described in Section 2 and also the problem data $f, L_1 L_2$ were defined there. The next step consists in the construction of such optimality conditions for (17) that will facilitate a subsequent application of Theorem 2 as much as possible. To this purpose, we introduce the polyhedral sets

$$\Omega^i := \left\{(u^i, \zeta^i) \,|\, L_1 u^i \geq \bar{u}^i, \zeta^i \geq 0\right\},$$

consisting (due to the structure of L_1) only of lower bounds for some variables.

THEOREM 6 *Let $x = \tilde{x}$ and $\zeta^{i-1} = \tilde{\zeta}^{i-1}$ be given and $(\tilde{u}, \tilde{\zeta}^i)$ be a solution of the respective problem (17). Then there exists a KKT vector $\tilde{\lambda}^i$ such that*

$$\begin{aligned} 0 &\in \nabla_{3,4} f(\tilde{x}, \tilde{\zeta}^{i-1}, \tilde{u}^i, \tilde{\zeta}^i) + (\nabla_{2,3} G(\tilde{\zeta}^{i-1}, \tilde{u}^i, \tilde{\zeta}^i))^T \tilde{\lambda}^i + N_{\Omega^i}(\tilde{u}^i, \tilde{\zeta}^i) \\ 0 &\in -G(\tilde{\zeta}^{i-1}, \tilde{u}^i, \tilde{\zeta}^i) + N_{\mathbb{R}^l_+}(\tilde{\lambda}^i), \end{aligned} \tag{18}$$

where

$$G(\zeta^{i-1}, u^i, \zeta^i) := \begin{bmatrix} L_2 u^i \\ \zeta^i - \zeta^{i-1} \end{bmatrix}$$

and l is the dimension of the image space of G.

Note that in the above optimality conditions we do not need any constraint qualification, because all functions arising in the constraints are affine. The GE (18) is already in the required form (9); it suffices to put

$$\begin{aligned} y^i &:= (u^i, \zeta^i, \lambda^i), \\ F(x, y^{i-1}, y^i) &:= \begin{bmatrix} \nabla_{3,4} f(x, \zeta^{i-1}, u^i, \zeta^i) + (\nabla_{2,3} G(\zeta^{i-1}, u^i, \zeta^i))^T \lambda^i \\ -G(\zeta^{i-1}, u^i, \zeta^i) \end{bmatrix} \end{aligned}$$

and

$$Q^i(y^i) := \begin{bmatrix} N_{\Omega^i}(u^i, \zeta^i) \\ N_{\mathbb{R}^l_+}(\lambda^i) \end{bmatrix}.$$

Since the sets Ω^i are translated nonnegative orthants, the coderivatives of the maps Q^i can easily be computed on the basis of [15, Lemma 2.1]. Moreover, F is affine and all sets $Gph Q^i$ are unions of a finite number of convex polyhedral sets ([18]). Hence, we do not need to take care about the calmness condition in Theorem 2, whenever U_{ad} is convex polyhedral.

We now illustrate the application of Corollary 5 and the form of the resulting optimality conditions by means of an MPEC generated on the basis of the academic equilibrium from Example 1.

EXAMPLE 2 Consider the four-string problem from Example 1, where we set $x_j = e_j$ for $j = 1, 2$. The respective problem (17) thus attains the

form

$$\begin{aligned} &\text{minimize } (x_1+e\zeta_1^i)(u_1^i)^2 + (x_2+e\zeta_2^i)(u_2^i-u_1^i)^2 - \sum_{j=1}^{2} ed\ (\zeta_j^i-\zeta_j^{i-1}) \\ &\text{subject to} \quad \begin{array}{l} u_1^i - u_2^i \le 0 \\ \zeta_1^i - \zeta_1^{i-1} \le 0 \\ \zeta_2^i - \zeta_2^{i-1} \le 0 \\ (u_1^i, u_2^i, \zeta_1^i, \zeta_2^i) \in \Omega^i, \end{array} \end{aligned} \tag{19}$$

where $\Omega^i = \left\{u_1^i, u_2^i, \zeta_1^i, \zeta_2^i \mid u_1^i \ge 0, u_2^i \ge \bar{u}^i, \zeta_1^i \ge 0, \zeta_2^i \ge 0\right\}$. The aim is to maximize the energy dissipated until the terminal time k so that

$$\varphi(x, y^k) = \zeta_1^k + \zeta_2^k.$$

Finally,

$$U_{ad} = \{x \in \mathbb{R}^2 \mid x_1 + x_2 = 2\}$$

and $\zeta_1^0 = \zeta_2^0 = 1$ (the remaining initial values are not needed). The application of Theorem 6 to (19) yields the following GE:

$$\begin{aligned} 0 \in &\begin{bmatrix} 2x_1u_1^i - 2x_2(u_2^i - u_1^i) + 2\zeta_1^i e u_1^i - 2\zeta_2^i e(u_2^i - u_1^i) + \lambda_1^i \\ 2x_2(u_2^i - u_1^i) + 2\zeta_2^i e(u_2^i - u_1^i) - \lambda_1^i \\ e(u_1^i)^2 - de + \lambda_2^i \\ e(u_2^i - u_1^i)^2 - de + \lambda_3^i \end{bmatrix} \\ &+ N_{\Omega^i}(u_1^i, u_2^i, \zeta_1^i, \zeta_2^i) \end{aligned} \tag{20}$$

$$0 \in \begin{bmatrix} u_2^i & - & u_1^i \\ \zeta_1^{i-1} & - & \zeta_1^i \\ \zeta_2^{i-1} & - & \zeta_2^i \end{bmatrix} + N_{\mathbb{R}^3_+}(\lambda_1^i, \lambda_2^i, \lambda_3^i).$$

Hence, even in this simple academic example, one has $m = 7, n = 2$ and $l = 3$. It is clear that each vector $(\widehat{x}, \widehat{u}^1, \ldots, \widehat{u}^k, \widehat{\zeta}^1, \ldots, \widehat{\zeta}^k)$, where $\widehat{x} \in U_{ad}, (\widehat{u}^i, \widehat{\zeta}^i) \in \mathbb{R}^2 \times \mathbb{R}^2$ is a solution of (19) with $x = \widehat{x}, \zeta^{i-1} = \widehat{\zeta}^{i-1}$ for $i = 1, 2, \ldots, k$ and $\widehat{\zeta}_1^k = \widehat{\zeta}_2^k = 0$ generates a global solution of the above MPEC. As explained in Example 1, for the data given there, it is possible to construct such a vector on the basis of physical consideration; in the case $k = 2$ we obtain, e.g., $\widehat{x}_1 = \widehat{x}_2 = 1, \widehat{u}_1^1 = 0.0032, \widehat{u}_2^1 = 0.0035, \widehat{u}_1^2 = 0.0035, \widehat{u}_2^2 = 0.007, \widehat{\zeta}_1^1 = 0, \widehat{\zeta}_2^1 = 1, \widehat{\zeta}_1^2 = \widehat{\zeta}_2^2 = 0$. The optimality conditions (20) are fulfilled with $\widehat{\lambda}_1^1 = \widehat{\lambda}_2^1 = 0, \widehat{\lambda}_3^1 = 10^{-6}, \widehat{\lambda}_1^2 = \widehat{\lambda}_2^2 = \widehat{\lambda}_3^2 = 0$ and the vectors $\widehat{z}^i \in N_{\Omega^1}(\widehat{u}_1^i, \widehat{u}_2^i, \widehat{\zeta}_1^i, \widehat{\zeta}_2^i) \times N_{\mathbb{R}^3_+}(\widehat{\lambda}_1^i, \widehat{\lambda}_2^i, \widehat{\lambda}_3^i)$,

$i = 1, 2$, equal to

$$\begin{aligned} \widehat{z}^1 &= (0, -0.0064, -10^{-5}, 0, -0.0003, -1, 0)^T \\ \widehat{z}^2 &= (0, -0.007, -0.0001, -0.0001, -0.0035, 0, -1)^T. \end{aligned}$$

To evaluate the coderivatives of the multivalued part in (20), we invoke, as already mentioned, [15, Lemma 2.1]. It follows that

$$v_1^1 = v_4^1 = v_7^1 = 0, \;\; w_2^1 = w_3^1 = w_5^1 = w_6^1 = 0$$

and

$$v_1^2 = 0, \;\; w_2^2 = w_3^2 = w_4^2 = w_5^2 = w_7^2 = 0.$$

Only the adjoint variables v_6^2 and w_6^2 are related in a more complicated way, because the respective constraint violates the strict complementarity. One has either $v_6^2 \; w_6^2 = 0$ or $v_6^2 < 0, w_6^2 < 0$. The respective adjoint equation system (16) can thus be substantially simplified and attains the form

$$0 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 4 & 0 \\ -2 & 0 \\ 0.07 & -1 \\ -0,07 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} w_1^2 \\ w_6^2 \end{bmatrix} + \begin{bmatrix} 0 \\ v_2^2 \\ v_3^2 \\ v_4^2 \\ v_5^2 \\ v_6^2 \\ v_7^2 \end{bmatrix}$$

$$0 = \begin{bmatrix} 24 & -0.006 & 0 \\ -22 & 0.006 & 0 \\ 0.064 & 0 & 0 \\ -0.006 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} w_1^1 \\ w_4^1 \\ w_7^1 \end{bmatrix} + \begin{bmatrix} 0 \\ v_2^1 \\ v_3^1 \\ 0 \\ v_5^1 \\ v_6^1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ w_6^2 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

This equation system in variables (v^1, v^2, w^1, w^2) possesses a solution in which $(w^1, w^2) = 0$. Because $\kappa = 0$, relation (15) holds true and the optimality conditions of Corollary 5 have been verified.

5. Conclusion

The optimality condition derived in Section 3 can be used to test the stationarity of approximate solutions to considered MPECs computed by available numerical methods [1],[4]. The complexity of these MPECs and the respective optimality conditions increases naturally with the number

of time levels (k). On the other hand, as explained in Section 2.1, in modeling of the delamination processes, a fine time discretization is really needed to compute a physically acceptable equilibrium. In MPECs associated with such equilibria, the need of a large k may be even stronger, because the (upper-level) objective may force the equilibrium to attain physically unacceptable values. For instance, in the illustrative four-string problem, the choice $k = 2$ is definitely to small to solve the associated MPEC (Example 2) by an SQP code. As soon as the starting point is not extremely close to a solution, the procedure terminates at a physically unacceptable equilibrium. The choice of k is thus a certain trade-off between the complexity of the problem (and the associated optimality conditions) and our effort to arrive at a physically acceptable equilibrium.

Acknowledgments

This research was supported by grant A1075005 of the Grant Agency of the Academy of Sciences of the Czech Republic and by BMBF project 03ZOM3ER.

References

[1] M. Anitescu. On solving mathematical programs with complementarity constraints as nonlinear programs. Preprint ANL/MCS-P864-1200, Argonne National Laboratory, Argonne, IL, 2000.

[2] C. C. Baniotopoulos, J. Haslinger, and Z. Morávková. Mathematical modeling of delamination and nonmonotone friction problems by hemivariational inequalities. Technical report, Charles Univesity, Prague, 2002.

[3] B. D. Davidson. An analytical investigation of delamination front curvature in double cantilever beam specimens. *J. Compos. Mater.*, 24:1124–1137, 1990.

[4] R. Fletcher and S. Leyffer. Numerical experience with solving MPECs as NLPs. Report NA\210, University of Dundee, 2002.

[5] M. Frémond. Dissipation dans l'adhrence des solides. *C. R. Acad. Sci., Paris, Sr. II*, 300:709–714, 1985.

[6] M. Frémond. Contact with adhesion. In J. J. Moreau, G. Panagiotopoulos, and G. Strang, editors, *Topics in Nonsmooth Mechanics*. Birkhäuser, 1988.

[7] H. Guidouche and N. Point. Unilateral contact with adherence. In A. Bossavit, A. Damlamian, and M. Frémond, editors, *Free boundary problems: applications and theory IV*, pages 340–346. Pitman Res. Notes Math. 121, 1985.

[8] H. Halkin. *Optimal Control for Systems Described by Difference Equations*. Academic Press, New York, 1964.

[9] M. Kočvara, A. Mielke, and T. Roubíček. Rate-independent approach to the delamination problem. Preprint 2003/29, SFB 404 "Mehrfeldprobleme in der Kontinuumsmechanik", Universität Sttutgart, 2003.

[10] A. Mielke and F. Theil. A mathematical model for rate-independent phase transformations with hysteresis. In H.-D. Alder, R. Balean, and R. Farwig, editors, *Models of continuum mechanics in analysis and engineering*, pages 117–129. Shaker Ver., Aachen, 1999.

[11] A. Mielke, F. Theil, and V. I. Levitas. A variational formulation of rate-independent phase transformations using an extremum principle. *Archive Rat. Mech. Anal.*, 162:137–177, 2002.

[12] B. S. Mordukhovich. Generalized differential calculus for nonsmooth and set-valued mappings. *J. Math. Anal. Appl.*, 183:250–288, 1994.

[13] B.S. Mordukhovich. *Approximation Methods in Problems of Optimization and Control*. Nauka, Moscow, 1988. In Russian.

[14] J. Outrata. A generalized mathematical program with equilibrium constraints. *SIAM J. Control. Optim.*, 38:1623–1638, 2000.

[15] J. V. Outrata. Optimality conditions for a class of mathematical programs with equilibrium constraints. *Math. Oper. Res.*, 24:627–644, 1999.

[16] P. D. Panagiotopoulos. *Inequality problems in mechanics and applications, convex and nonconvex energy functions*. Birkhäuser, Basel, 1985.

[17] N. Point and E. Sacco. A delamination model for laminated composites. *Int. J. Solids Structures*, 33:483–509, 1996.

[18] S. M. Robinson. Some continuity properties of polyhedral multifunctions. *Mathematical Programming Study*, 14:206–214, 1981.

[19] R. T. Rockafellar and R. Wets. *Variational Analysis*. Springer Verlag, Berlin, 1998.

[20] H. L. Schreyer, D. L. Sulsky, and S.-J. Zhou. Modelling delamination as strong discontinuity with the material point method. *Comput. Methods Appl. Mech. Engrg.*, 191:2483–2507, 2002.

[21] J. J. Ye. Necessary optimality conditions for bilevel dynamic problems. In *Proc. of the 36th Conference on Decision & Control, San Diego*, pages 1405–1410. IEEE, 1997.