

# On the Control of Time Discretized Dynamical Contact Problems

Georg Müller\* and Anton Schiela†

Chair of Applied Mathematics, University of Bayreuth

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We consider optimal control problems with distributed control that involve a time-stepping formulation of dynamical one body contact problems as constraints. We link the continuous and the time-stepping formulation by a nonconforming finite element discretization, and derive existence of optimal solutions and strong stationarity conditions. We use this information for a steepest descent type optimization scheme based on the resulting adjoint scheme and implement its numerical application.

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## 1 Introduction

The following work concerns the optimal control of time discretized, dynamical contact problems of a linearly viscoelastic body with a rigid obstacle in the absence of friction, where a linearized non-penetration condition is employed. This condition is also referred to as the Signorini condition, after first being introduced by Signorini in [33] in the statical one body context.

Contact problems have a multitude of applications in mechanics, engineering and medicine, and are pretty well understood in the statical context nowadays. They are closely related to obstacle problems and both are modeled through structurally similar, elliptic variational inequalities. Their theoretical properties can therefore oftentimes be examined simultaneously. There are, however, two main additional complications concerning contact problems. While obstacle problems are scalar problems that extend the Poisson problem, contact problems are vector-valued problems, extending linear elasticity. Furthermore, while the constraints in the obstacle problem are formulated on the reference domain, the non-penetration condition in contact problems is imposed on part of the reference boundary.

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\*phone: +49 921 55 3282, email: georg.mueller@uni-bayreuth.de

†phone: +49 921 55 3281, email: anton.schiela@uni-bayreuth.de

In [28], Lions and Stampacchia were the first to show the existence of a generally nonlinear but Lipschitz continuous solution operator to these variational inequalities and from Mignot's work in [29], we know the solution operator to even be directionally differentiable in case the admissible set is polyhedral at a solution with respect to the contact forces. Existence of solutions and first order optimality conditions for optimal control problems of variational inequalities and complementarity constrained problems have been investigated, e.g., in [29, 37], and in [39], optimization algorithms for optimal control of statical contact problems are considered in a medical optimal design application.

Numerically, statical contact problems can be solved, e.g., with optimal complexity by the multi-grid techniques developed in [16, 25] or alternatively by a combination of regularization and semi-smooth Newton [34, 20, 36].

Dynamical contact problems, unfortunately, are not as well understood as their statical counterparts are. To the best of our knowledge, only the authors in [2] investigate the existence of possibly non-unique solutions to viscoelastical, frictionless, dynamical contact problems, by studying weak convergence of a time-discretization scheme. However, some crucial steps in the proofs are implausible to us. Consequently, the theoretical framework, in which dynamical contact problems should be considered, currently admits some ambiguity.

Algorithmically, however, there are several time-stepping schemes, that are based on the Newmark scheme which was introduced in [30] and which include reasonable adaptations for the contact constrained case. We restrict our examinations to time-stepping formulations of the dynamical contact problems. Often, solvers for static contact problems are employed for the step computation in those time-stepping schemes. The thesis [22] deals with the adaptive integration of dynamical contact problems and gives a detailed overview over the possible approaches and modifications based on the Newmark scheme. For our purposes, the energy dissipative, contact implicit modification by Kane et al. in [21] seems to be best suited since it is relatable to a temporal finite element discretization of the continuous problem. This allows for a consistent derivation of an adjoint scheme in the optimal control context. In the context of spatial finite element discretization, a couple of modifications have been proposed and analyzed [9, 18, 26, 23, 24, 10]. These variants mostly coincide with [21] in the spatially continuous case.

So although information on a control-to-state operator on the continuous level is still missing, reasonable time-stepping schemes are available, which motivates the consideration of optimal control of dynamical contact problems in a time-discretized, spatially continuous setting.

The aims of this work are thus the following: For the optimal control of dynamic contact problems, we first derive a discontinuous finite element formulation in time that yields a slightly modified version of [21], concerning external forces and applied controls. Then, we deduce basic results for the time-discretized optimal control problem, such as existence of optimal solutions and strong stationarity conditions. These results are used to obtain a backwards in time scheme for the computation of an adjoint state, which is in turn the basis for a gradient-like method used for the numerical solution of the optimal control problem. In this method, the forward problem is solved by a variant of [21], using a monotone multigrid solver [16] for the computation of steps.

**Structure.** Section 2 gives an introduction into the modeling of one body contact problems. A reformulation of the usual second order hyperbolic variational inequality is used to convert the fully continuous optimal control problem into a system of first order. The subsequent Section 3 depicts a finite element semi-discretization of the underlying functional spaces to the aforementioned first order system, that results in a time-stepping formulation of the contact problem which closely resembles the contact implicit Newmark scheme for contact problems. Section 4 deals with the optimal control of the semi-discretized system and includes the existence of a Lipschitz continuous solution operator to the state equation, i.e. the time-stepping scheme. We can therefore show the existence of minimizers to the optimal control problem under standard assumptions. This operator is shown to be directionally differentiable in case the set of admissible states is polyhedral with respect to the solution and the residual to the variational inequality. Using this differentiability, we provide a rigorously derived system of first order necessary optimality conditions in the polyhedral

case. The information on the adjoint state will be used in a preconditioned, steepest decent type optimization algorithm in Section 5, where the optimization algorithm is applied in a numerical example. Finally, Section 6 concludes the paper with an outlook on possible extensions of the presented framework.

**Notation and Preliminaries.** We work on a bounded time interval  $I = [0, T] \subset \mathbb{R}$ , where  $T > 0$ , and two or three dimensional spatial domains denoted by  $\Omega \subset \mathbb{R}^n$ ,  $n \in \{2, 3\}$  with Lipschitz boundary  $\Gamma = \partial\Omega \in C^{0,1}$ , as defined in [19, Def. 1.13].

For any set  $X \subset \mathbb{R}^{\tilde{n}}$ ,  $\tilde{n} \in \mathbb{N}$  and a Banach space  $Y$ , we write  $L^2(X, Y)$  for the Bochner-Lebesgue spaces of square integrable functions,  $C(X, Y)$  for the space of continuous functions and  $H^s(X, Y)$ , for Bochner-Sobolev spaces with  $s > 0$ . We always consider measurability in the Lebesgue measure, which we denote  $\zeta_X = \zeta_{X_1} \times \zeta_{X_2}$  for product spaces  $X = X_1 \times X_2 \subset \mathbb{R}^{\tilde{n}}$ . We denote a property to hold almost everywhere (a.e.), if it is violated only on sets of measure 0 and quasi everywhere (q.e.), if it is violated only on sets of capacity 0. See, e.g., [38, Appendix A] for an excellent overview on those aspects of capacity theory that are relevant for variational inequalities.

Whenever  $X = \Omega$ ,  $Y = \mathbb{R}^n$  we omit the arguments to the Lebesgue and Sobolev spaces and abbreviate  $\mathbf{L}^2 := L^2(\Omega, \mathbb{R}^n)$ ,  $\mathbf{H}^1 := H^1(\Omega, \mathbb{R}^n)$ .

For the treatment of weak time differentiation, we also utilize the space  $W([0, T]) := W^{1,2}(I, \mathbf{L}^2, \mathbf{H}^1)$ , cf. [42, Sec. 23.6], and we denote the weak time derivative of  $y \in W([0, T])$  by  $\dot{y} \in L^2(I, (\mathbf{H}^1)^*)$ . Furthermore, whenever we have an  $\mathbf{H}^1$ -function which we want to identify with an  $(\mathbf{H}^1)^*$ -functional, we always consider the mapping  $\mathcal{E}^* \circ \mathcal{R}_{\mathbf{L}^2} \circ \mathcal{E}: \mathbf{H}^1 \mapsto (\mathbf{H}^1)^*$ , where  $\mathcal{E}: \mathbf{H}^1 \mapsto \mathbf{L}^2$  is the usual, compact Sobolev embedding and  $\mathcal{R}_{\mathbf{L}^2}: \mathbf{L}^2 \mapsto (\mathbf{L}^2)^*$  the  $\mathbf{L}^2$ -Riesz isomorphism.

We have assumed the boundary  $\Gamma$  to be  $C^{0,1}$ -regular, so for  $\Gamma$  and a measurable subset  $\tilde{\Gamma} \subset \Gamma$  there exist linear and bounded trace operators

$$\tau: \mathbf{H}^1 \mapsto L^2(\Gamma, \mathbb{R}^n), \quad \tau_{\tilde{\Gamma}}: \mathbf{H}^1 \mapsto L^2(\tilde{\Gamma}, \mathbb{R}^n),$$

associated with the boundary  $\Gamma$  or boundary segment  $\tilde{\Gamma} \subset \Gamma$ .

For the sake of brevity, we will notationally suppress trace operators if no ambiguity is possible. On the boundary segment  $\tilde{\Gamma}$ , we consider the standard surface measure, denoted as  $\zeta_{\tilde{\Gamma}}$ .

We write the scalar product on a Hilbert space  $X$  as  $(\cdot, \cdot)_X: X \times X \rightarrow \mathbb{R}$  and for a reflexive Banach space  $Y$  and its dual space  $Y^*$  we denote the dual pairing by  $\langle \cdot, \cdot \rangle_Y: Y^* \times Y \rightarrow \mathbb{R}$ . Thus, for a Hilbert space  $X$  (which is a reflexive Banach space) we distinguish between the scalar product  $(\cdot, \cdot)_X$  and the dual pairing  $\langle \cdot, \cdot \rangle_X$ . Further, we define the polar cone and annihilator for subsets  $K_1 \subset Y$ ,  $K_2 \subset Y^*$  as

$$\begin{aligned} K_1^\circ &= \{f \in Y^* : \langle f, y \rangle_Y \leq 0 \text{ for all } y \in K_1\}, & K_1^\perp &= \{f \in Y^* : \langle f, y \rangle_Y = 0 \text{ for all } y \in K_1\}, \\ K_2^\circ &= \{y \in Y : \langle f, y \rangle_Y \leq 0 \text{ for all } f \in K_2\}, & K_2^\perp &= \{y \in Y : \langle f, y \rangle_Y = 0 \text{ for all } f \in K_2\}, \end{aligned}$$

and denote the adjoint operator to an operator  $A: X \mapsto Y$  by  $A^*: Y^* \mapsto X^*$ .

For a convex subset  $K \subset Y$ , we write the reachable cone and tangent cone to  $K$  at  $y \in K$  as

$$R_K(y) = \bigcup_{\lambda > 0} \lambda(K - y), \quad T_K(y) = \text{cl}(R_K(y)),$$

cf. [37], where  $\text{cl}(\cdot)$  is the norm closure of a set and we denote  $\text{int}(\cdot)$  for the interior of a set. For  $y \in K$ ,  $r \in T_K(y)^\circ$ , we denote the critical cone to  $K$  with respect to  $(y, r)$  as

$$\mathcal{K}_K(y, r) = T_K(y) \cap \{r\}^\perp.$$

The components of a vector  $y \in \mathbb{R}^n$  or a vector valued function  $y: \Omega \mapsto \mathbb{R}^n$  are denoted by  $y_{(k)}$ ,  $k = 1 \dots n$  and we denote the positive and negative part  $y^+$  and  $y^-$  respectively.

## 2 Dynamic One Body Contact

This paper focuses on optimal control problems with a weak formulation of dynamical, viscoelastic contact problems as side constraints and the following section is dedicated to the presentation of the configuration of interest. The initial modeling of the physical setting is followed by a short overview of the reasoning behind the chosen approach and the limitations of linear contact conditions in general. The modeling will result in the well known second order, hyperbolic variational inequality which describes the contact problem. The second order form will be rewritten as a system of first order and embedded into an optimal control problem on the continuous level.

### 2.1 Modeling and Contact Condition

We model a linearly viscoelastic body on the time interval  $I \subset \mathbb{R}$ , that comes into contact with a rigid obstacle in the absence of friction. The undeformed reference state of the body is described by the domain  $\Omega$  and on it, we seek displacements  $y: I \times \Omega \mapsto \mathbb{R}^n$  describing the constrained deformation of the body when external forces act on parts of its boundary and interior.

To this end, we identify three disjoint parts  $\Gamma_D, \Gamma_N, \Gamma_C \subset \Gamma$  on the boundary, with  $\Gamma_D \cup \Gamma_N \cup \Gamma_C = \Gamma$ , where the body is clamped with Dirichlet conditions, can experience boundary forces by Neumann conditions or where we consider contact to potentially occur, respectively.

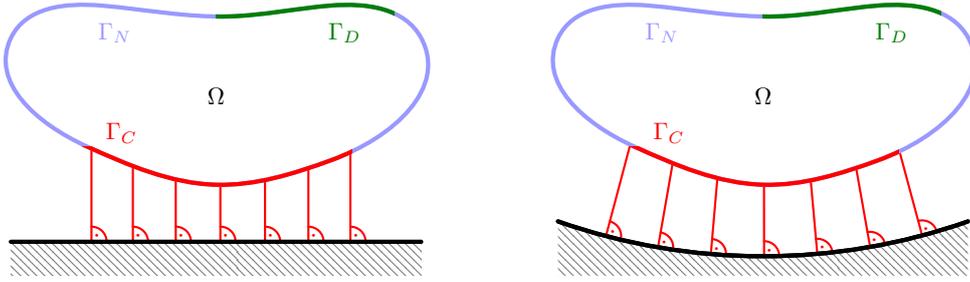


Fig. 1 Reference configurations of one body contact problems

The elastic and viscose properties of the material are described by the respective of the two bounded, coercive bilinear forms

$$a, b: \mathbf{H}^1 \times \mathbf{H}^1 \mapsto \mathbb{R},$$

which are assumed to be of the form

$$a(y, v) = \int_{\Omega} \sum_{i,j,k,l=1}^n E_{ijkl} \partial_j y_i \partial_l v_k d\omega, \quad b(y, v) = \int_{\Omega} \sum_{i,j,k,l=1}^n V_{ijkl} \partial_j y_i \partial_l v_k d\omega \quad (2.1)$$

for sufficiently smooth tensors  $E$  and  $V$ . More details can be found, e.g., in [22]. For the time dependent problem, we define

$$a_I, b_I: L^2(I, \mathbf{H}^1) \times L^2(I, \mathbf{H}^1) \mapsto \mathbb{R},$$

where

$$a_I(y, v) = \int_0^T a(y(t), v(t)) dt, \quad b_I(y, v) = \int_0^T b(y(t), v(t)) dt. \quad (2.2)$$

As usual, homogeneous Dirichlet boundary conditions are incorporated into the state space and we denote

$$\mathbf{H}_D^1 = \{y \in \mathbf{H}^1 \mid y = 0 \text{ a.e. on } \Gamma_D\}$$

accordingly, with a.e. meaning the surface measure sense. Furthermore, the external forces are composed of boundary and volume forces and are modeled by  $f_{ext} \in L^2(I, \mathbf{H}^1)^*$  with

$$f_\Omega \in L^2(I, \mathbf{L}^2), \quad f_N \in L^2(I, L^2(\Gamma_C))$$

$$\langle f_{ext}, y \rangle_{L^2(I, \mathbf{H}^1)} = \int_0^T \int_\Omega f_\Omega y \, d\omega + \int_{\Gamma_N} f_N y \, ds dt.$$

We choose the state space for possible displacements to be

$$Y = \{y \in C(I, \mathbf{H}_D^1) \cap W([0, T]) \mid \dot{y} \in W([0, T])\}.$$

and the rigid obstacle will be modeled by a set of admissible states. The obstacle is described by the set  $\mathcal{O} \subset \mathbb{R}^n$  and contact with it is modeled in a linear manner. To this end, we assume the existence of a *contact mapping*  $\Phi: \Gamma_C \mapsto \partial\mathcal{O}$ , mapping all points on the contact boundary to an associated point on the boundary of the obstacle. This allows for the definition of a contact normal on the contact boundary  $\Gamma_C$  of the viscoelastic body, namely

$$\nu_\Phi: \Gamma_C \mapsto \mathbb{R}^n, \quad \nu_\Phi(\omega) = \begin{cases} \frac{\Phi(\omega) - \omega}{\|\Phi(\omega) - \omega\|} & \omega \neq \Phi(\omega) \\ \nu(\omega) & \omega = \Phi(\omega) \end{cases},$$

where  $\nu: \Gamma_C \mapsto \mathbb{R}^n$  denotes the geometric outer normal on the contact boundary of the body in the reference configuration. We assume  $\nu_\Phi$  to be measurable in the surface measure sense and call the mapping  $\psi: \omega \mapsto \|\omega - \Phi(\omega)\|$  the initial gap function on the contact boundary of the reference configuration, which is assumed to be measurable as well. In the case of the one body problem with linearized contact condition, the set of admissible states can then be described by

$$\bar{K} = \{y \in C(I, \mathbf{H}_D^1) \mid y \cdot \nu_\Phi \leq \psi \text{ a.e. on } I \times \Gamma_C\}, \quad (2.3)$$

where a.e. means the time-surface sense. The contact condition describes that the contact boundary of the body may not move into a certain direction further than its initial distance from the obstacle.

Lastly, we point out that the continuous embedding of  $W([0, T]) \hookrightarrow C(I, \mathbf{L}^2)$  and the restriction of the state space to  $C(I, \mathbf{H}_D^1)$  functions with  $W([0, T])$  time derivatives allow for a reasonable definition of initial values  $(y_{ini}, v_{ini}) \in \mathbf{H}_D^1 \times \mathbf{L}^2$  and we have now described all modeling aspects to the setting and will focus on a mathematical formulation next.

**Remark 2.1.** *The general condition (2.3) has to be used with some care from the point of view of physical modeling. By definition, we attempt to model an obstacle by restricting displacements in a given direction. It is, however, not guaranteed that these restrictions always correspond to a physically meaningful obstacle. Some simple, well understood situations are the pure detachment problem of Signorini, where  $\nu_\Phi = \nu$  and  $y \cdot \nu \leq 0$ , and the horizontal plane as an obstacle.*

## 2.2 Second Order Dynamics

With the preparation of Section 2.1 in mind, we can now establish the mathematical model for the optimal control of dynamic contact. The time continuous, viscoelastical contact problem comes to finding a  $y \in Y \cap \bar{K}$  with  $y(0) = y_{ini}$ ,  $\dot{y}(0) = v_{ini}$  for which the hyperbolic variational inequality

$$\langle \ddot{y}, v - y \rangle_{L^2(I, \mathbf{H}^1)} + a_I(y, v - y) + b_I(\dot{y}, v - y) - \langle f_{ext}, v - y \rangle_{L^2(I, \mathbf{H}^1)} \geq 0 \quad \forall v \in \bar{K}$$

holds. This can be stated in a more compact way using the normal cone  $T_{\bar{K}}(y)^\circ$  to  $\bar{K}$  at  $y$ , so that the entire problem then reads as

$$y \in \bar{K} \quad (2.4a)$$

$$\langle f_{ext} - \ddot{y}, \cdot \rangle_{L^2(I, \mathbf{H}^1)} - a_I(y, \cdot) + b_I(\dot{y}, \cdot) \in T_{\bar{K}}(y)^\circ \quad (2.4b)$$

$$y(0) = y_{ini}, \quad \dot{y}(0) = v_{ini}. \quad (2.4c)$$

In order to keep notation compact, we define the set  $K$  and the test space  $P$  by

$$K = \bar{K} \times \mathbf{L}^2 \times \mathbf{L}^2, \quad P = C(I, \mathbf{H}_D^1) \times \mathbf{L}^2 \times \mathbf{L}^2,$$

where the time dependent test functions are dense in  $L^2(I, \mathbf{H}_D^1)$ . For  $y \in L^2(I, \mathbf{H}^1)$  the mapping  $p \mapsto \int_0^T a(y(t), p(t)) dt$  defines a bounded, linear functional on  $L^2(I, \mathbf{H}^1)$  because:

$$\left| \int_0^T a(y(t), p(t)) dt \right| \leq \int_0^T M_a \|y(t)\|_{\mathbf{H}^1} \|p(t)\|_{\mathbf{H}^1} dt \leq M_a \left( \int_0^T \|y(t)\|_{\mathbf{H}^1}^2 dt \right)^{\frac{1}{2}} \left( \int_0^T \|p(t)\|_{\mathbf{H}^1}^2 dt \right)^{\frac{1}{2}}$$

for all  $p \in L^2(I, \mathbf{H}^1)$ , since  $\|y(\cdot)\|_{\mathbf{H}^1}, \|p(\cdot)\|_{\mathbf{H}^1}$  are square integrable over time. The same holds for  $b$ . We also consider the operators  $A: Y \mapsto P^*, f \in P^*$  with

$$\begin{aligned} \langle Ay, (p, p_0, q_0) \rangle_P &= \langle \ddot{y}, p \rangle_{L^2(I, \mathbf{H}^1)} + a_I(y, p) + b_I(\dot{y}, p) + (y(0), q_0)_{\mathbf{L}^2} + (\dot{y}(0), p_0)_{\mathbf{L}^2} \\ \langle f, (p, p_0, q_0) \rangle_P &= \langle f_{ext}, p \rangle_{L^2(I, \mathbf{H}^1)} + (y_{ini}, q_0)_{\mathbf{L}^2} + (v_{ini}, p_0)_{\mathbf{L}^2}, \end{aligned}$$

which finally allows us to rewrite the continuous problem (2.4) in a more compact way as

$$(y, y(0), \dot{y}(0)) \in K \tag{2.5a}$$

$$f - Ay \in T_K(y, y(0), \dot{y}(0))^\circ, \tag{2.5b}$$

Here, (2.5b) represents the variational inclusion (2.4b) and enforces the initial values (2.4c) as well, because it splits up into

$$\begin{aligned} \ddot{y} + a_I(y, \cdot) + b_I(\dot{y}, \cdot) - f_{ext} &\in -T_{\bar{K}}(y)^\circ && \text{in } (C(I, \mathbf{H}_D^1))^* \\ (y(0) - y_{ini}, q_0)_{\mathbf{L}^2} &= 0 && \forall q_0 \in \mathbf{L}^2 \\ (\dot{y}(0) - v_{ini}, p_0)_{\mathbf{L}^2} &= 0 && \forall p_0 \in \mathbf{L}^2. \end{aligned}$$

The last two lines in this ensure the initial values in the  $\mathbf{L}^2$ -sense and therefore in the  $\mathbf{H}^1$ -sense in the case of  $y(0)$  and  $y_0$  since the weak derivative is unique and  $y_{ini} \in \mathbf{H}_D^1$ . Therefore, the two inclusions (2.5a)-(2.5b) represent the entire contact problem.

### 2.3 First Order Dynamics

As mentioned above, Section 3 will include a time discretization that can be interpreted as a Newmark type scheme. We will elaborate on this in the appropriate section. In order to describe this time-stepping procedure by a finite element discretization, the time continuous framework with second order dynamics needs to be modified beforehand to obtain a system of first order. We redefine some of the sets in the previous subsection and fix

$$V = W([0, T]), \quad P = C(I, \mathbf{H}_D^1) \times L^2(I, \mathbf{H}^1) \times \mathbf{L}^2 \times \mathbf{L}^2, \quad K = \bar{K} \times L^2(I, \mathbf{H}^1) \times \mathbf{L}^2 \times \mathbf{L}^2,$$

as well as the modified operators  $A: Y \times V \mapsto P^*, f \in (P)^*$  to read

$$\begin{aligned} \langle A(y, v), (p, q, p_0, q_0) \rangle_P &= \langle \dot{v}, p \rangle_{L^2(I, \mathbf{H}^1)} + a_I(y, p) + b_I(\dot{y}, p) \\ &\quad + \langle v, q \rangle_{L^2(I, \mathbf{H}^1)} - \langle \dot{y}, q \rangle_{L^2(I, \mathbf{H}^1)} \\ &\quad + (y(0), q_0)_{\mathbf{L}^2} + (v(0), p_0)_{\mathbf{L}^2} \\ \langle f, (p, q, p_0, q_0) \rangle_P &= \langle f_{ext}, p \rangle_{L^2(I, \mathbf{H}^1)} + (y_{ini}, q_0)_{\mathbf{L}^2} + (v_{ini}, p_0)_{\mathbf{L}^2}. \end{aligned}$$

this leads to the first order reformulation of the contact problem

$$(y, v, y(0), v(0)) \in K \tag{2.6a}$$

$$f - A(y, v) \in T_K(y, v, y(0), v(0))^\circ. \tag{2.6b}$$

Here, (2.6b) splits up into

$$\dot{v} + a_I(y, \cdot) + b_I(\dot{y}, \cdot) - f_{ext} \in -T_{\bar{K}}(y)^\circ \quad \text{in } C(I, \mathbf{H}_D^1)^* \quad (2.7a)$$

$$\langle v - \dot{y}, q \rangle_{L^2(I, \mathbf{H}^1)} = 0 \quad \forall q \in L^2(I, \mathbf{H}^1) \quad (2.7b)$$

$$(y(0) - y_{ini}, q_0)_{\mathbf{L}^2} = 0 \quad \forall q_0 \in \mathbf{L}^2 \quad (2.7c)$$

$$(v(0) - v_{ini}, p_0)_{\mathbf{L}^2} = 0 \quad \forall p_0 \in \mathbf{L}^2. \quad (2.7d)$$

The second line ensures that the velocity and the time derivative of the displacement coincide in the  $L^2(I, \mathbf{H}^1)^*$ -sense.

Since  $v, \dot{y} \in W([0, T])$  and the weak time derivative is unique, they coincide in the  $W([0, T])$ -sense as well. Finally, the first line is only a restatement of the variational inclusion (2.4b) and the initial values have been adapted to fit the first order system.

Note, that the variational inclusion (2.7a) can equivalently be expressed with the help of a multiplier  $\lambda \in T_{\bar{K}}(y)^\circ \subset M(I, (\mathbf{H}_D^1)^*)$  so that

$$\dot{v} + a_I(y, \cdot) + b_I(\dot{y}, \cdot) - f_{ext} + \lambda = 0 \quad (2.8)$$

holds in  $C(I, \mathbf{H}_D^1)^* \doteq M(I, (\mathbf{H}_D^1)^*)$ . The multiplier  $\lambda$  can be interpreted as the contact forces acting upon the area of active contact when the unconstrained movement of the body is disrupted by the obstacle.

## 2.4 Continuous Optimal Control Problem

Based on the first order reformulation, we consider the continuous optimal control problem, with the dynamic contact problem as constraints as well as distributed control  $u \in U = L^2(I, \mathbf{L}^2)$ . With the operator

$$B: U \mapsto P^*, \quad \langle Bu, (p, q, p_0, q_0) \rangle_P = (u, p)_{L^2(I, \mathbf{L}^2)}$$

and given a cost functional  $J: Y \times V \times U \mapsto \mathbb{R}$ , this amounts to

$$\min J(y, v, u) \quad (2.9a)$$

$$s.t. (y, v, u) \in Y \times V \times U \quad (2.9b)$$

$$(y, v, y(0), v(0)) \in K \quad (2.9c)$$

$$Bu + f - A(y, v) \in T_K(y, v, y(0), v(0))^\circ \quad (2.9d)$$

which is an optimal control problem with a dynamical contact problem as constraints, where the states are controlled in a distributed manner by the forces in the state system.

## 3 Semi-Discretization of the Contact Problem

In this section, we present a finite element time discretization of the optimization problem (2.9), where the resulting discretized constraints correspond to the application of the contact implicit Newmark scheme, proposed by Kane et al. in [21], to the constrained formulation of second order. The advantage of the contact implicit scheme over the classical Newmark scheme is better stability in the constrained case, whereas there is no difference to the classic scheme, when no constraints are active, cf. also [22]. The finite element framework allows for the consistent derivation of an adjoint time-stepping scheme, which will be presented in Section 4.5 and leads to an optimal control problem with semi-discretized dynamic contact as constraints.

### 3.1 Finite Element Discretization

In order to handle the inequality structure in (2.9), we begin by introducing the multiplier  $\lambda \in T_{\bar{K}}(y)^\circ$ , mentioned in (2.8), so the the set of constraints (2.5a)-(2.5b) can equivalently be expressed by the system

$$y \in \bar{K}, \lambda \in T_{\bar{K}}(y)^\circ \quad (3.10a)$$

$$\langle \dot{v}, p \rangle_{L^2(I, \mathbf{H}^1)} + a_I(y, p) + b_I(v, p) - (u, p)_{L^2(I, \mathbf{L}^2)} + \langle \lambda - f_{ext}, p \rangle_{L^2(I, \mathbf{H}^1)} = 0 \quad \forall p \in C(I, \mathbf{H}_D^1) \quad (3.10b)$$

$$\langle v - \dot{y}, q \rangle_{L^2(I, \mathbf{H}^1)} = 0 \quad \forall q \in L^2(I, \mathbf{H}^1) \quad (3.10c)$$

$$(y(0) - y_{ini}, q_0)_{\mathbf{L}^2} = 0 \quad \forall q_0 \in \mathbf{L}^2 \quad (3.10d)$$

$$(v(0) - v_{ini}, p_0)_{\mathbf{L}^2} = 0 \quad \forall p_0 \in \mathbf{L}^2 \quad (3.10e)$$

The semi-discretization follows the temporal part of the Petrov-Galerkin discretization presented in [27], where the authors investigate optimal control problems with control constraints for the wave equation. The discretization consists of dividing the temporal domain  $I = [0, T]$  into

$$0 = t_0 < t_1 < \dots < t_N = T, \quad I_k = (t_{k-1}, t_k], \quad k = 1 \dots N \in \mathbb{N}$$

and we restrict ourselves to the equidistant case here, assuming  $|I_k| = \tau$  to be constant. The displacements, velocities, forces, controls, test functions and multipliers are then chosen from finite element spaces in the following way:

$$\begin{aligned} y \in \mathcal{A}_{1, \mathbf{H}_D^1} &= \{y \in C(I, \mathbf{H}_D^1) \mid y|_{I_k} \in \mathcal{P}_1(I_k, \mathbf{H}_D^1)\} \\ v \in \mathcal{A}_{1, \mathbf{H}^1} &= \{v \in C(I, \mathbf{H}^1) \mid v|_{I_k} \in \mathcal{P}_1(I_k, \mathbf{H}^1)\} \\ u, f_{ext} \in \mathcal{A}_{0, \mathbf{L}^2} &= \{u \in L^2(I, \mathbf{L}^2) \mid u|_{I_k} \in \mathcal{P}_0(I_k, \mathbf{L}^2), u(0) = u(t_1)\} \\ p \in \mathcal{T}_{0, \mathbf{H}_D^1} &= \{p \in L^2(I, \mathbf{H}_D^1) \mid p|_{I_k} \in \mathcal{P}_0(I_k, \mathbf{H}_D^1), p(0) = p(t_1)\} \\ q \in \mathcal{T}_{0, \mathbf{H}^1} &= \{q \in L^2(I, \mathbf{H}^1) \mid q|_{I_k} \in \mathcal{P}_0(I_k, \mathbf{H}^1), q(0) = q(t_1)\} \\ \lambda \in \mathcal{A}_\delta &= \{\lambda \in M(I, (\mathbf{H}_D^1)^*) \mid \lambda \in \text{lin}_{(\mathbf{H}_D^1)^*}(\delta_{t_k}, k = 1 \dots N)\}. \end{aligned}$$

The discretization is nonconforming with respect to the test functions  $p$ , which are discretized discontinuously. Also the velocity, which is assumed to be the derivative of the piecewise linear state, is assumed piecewise linear itself. This leads to a symmetric averaging of implicit and explicit information when the states are updated from the velocities in the time-stepping scheme.

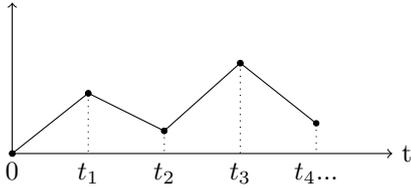


Fig. 2 Continuous ansatz spaces

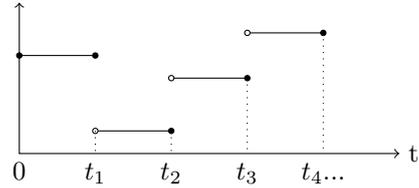


Fig. 3 Discontinuous test/control spaces

All in all, we have piecewise linear and continuous states and velocities, as well as forces and test functions that are piecewise constant and continuous from the left. Further, the multiplier to the contact condition is a linear combination of vector Dirac measures acting at the subinterval endpoints.

For the respective parts in (3.10b), we obtain:

$$\int_0^T a(y, p) dt = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} a(y, p) dt = \sum_{k=0}^{N-1} \frac{\tau}{2} (a(y_{k+1}, p_{k+1}) + a(y_k, p_{k+1})) \quad (3.11a)$$

$$\int_0^T b(\dot{y}, p) dt = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} b(v, p) dt = \sum_{k=0}^{N-1} \frac{\tau}{2} (b(v_{k+1}, p_{k+1}) + b(v_k, p_{k+1})) \quad (3.11b)$$

$$\int_0^T (u, p)_{\mathbf{L}^2} dt = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} (u, p)_{\mathbf{L}^2} dt = \sum_{k=0}^{N-1} \tau (u_{k+1}, p_{k+1})_{\mathbf{L}^2} \quad (3.11c)$$

$$\langle f_{ext}, p \rangle_{L^2(I, \mathbf{H}^1)} = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \langle f_{ext}, p \rangle_{\mathbf{H}^1} dt = \sum_{k=0}^{N-1} \tau \langle f_{ext k+1}, p_{k+1} \rangle_{\mathbf{H}^1} \quad (3.11d)$$

$$\langle \dot{v}, p \rangle_{L^2(I, \mathbf{H}^1)} = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \langle \dot{v}, p \rangle_{\mathbf{H}^1} dt = \sum_{k=0}^{N-1} (v_{k+1}, p_{k+1})_{\mathbf{L}^2} - (v_k, p_{k+1})_{\mathbf{L}^2} \quad (3.11e)$$

$$\langle \lambda, p \rangle_{C(I, \mathbf{H}^1)} = \sum_{k=0}^{N-1} \langle \lambda_{k+1}, p_{k+1} \rangle_{\mathbf{H}^1} \quad (3.11f)$$

This decouples w.r.t. the test functions' values due to the discontinuous form of the test space and yields a time-stepping scheme. The velocity update (3.10c) in the discretized form reads

$$\sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \langle \dot{y} - v, q \rangle_{\mathbf{H}^1} dt = \sum_{k=0}^{N-1} (y_{k+1} - y_k, q_{k+1})_{\mathbf{L}^2} - \frac{\tau}{2} (v_{k+1} + v_k, q_{k+1})_{\mathbf{L}^2} = 0. \quad (3.12)$$

Equations (3.11a)-(3.11b) follow because the argument is linear on each subinterval, while equations (3.11c) - (3.11e) follow because of the constant arguments. The system remains unchanged if in (3.11b)  $\dot{y}$  is considered instead of  $v$  because the velocity coupling (3.12) then leads to the same outcome.

Recall the comment in the preliminaries, stating that we identify  $\mathbf{H}^1$ -functions with  $(\mathbf{H}^1)^*$ -functionals by use of the  $\mathbf{L}^2$ -Riesz isomorphism instead of the  $\mathbf{H}^1$ -isomorphism. Therefore, the dual pairings resolve into the  $\mathbf{L}^2$ -terms seen in (3.11d)-(3.11e) and (3.12).

Since the initial values do not require any time discretization, only the state and multiplier constraints in (3.10a) are left to be discussed. To this end, recall the definition of the set

$$\bar{K}_\tau = \{y \in \mathbf{H}_D^1 \mid y \cdot \nu_\Phi \leq \psi \text{ a.e. on } \Gamma_C\}. \quad (3.13)$$

and consider the following Lemma 3.1, which gives alternative characterizations of admissible displacements.

**Lemma 3.1** (Admissible Displacements). *For  $y \in Y$  the following conditions are equivalent:*

1.  $y \in \bar{K} = \{y \in C(I, \mathbf{H}_D^1) \mid y \cdot \nu_\Phi \leq \psi \text{ a.e. on } I \times \Gamma_C\}$
2.  $y \in \{y \in C(I, \mathbf{H}_D^1) \mid y(\cdot) \cdot \nu_\Phi \leq \psi \text{ a.e. on } \Gamma_C \text{ holds a.e. on } I\}$
3.  $y(t) \in \bar{K}_\tau \forall t \in I$

*Proof.* Note that 2 can equivalently be written as  $y \in \{y \in C(I, \mathbf{H}_D^1) \mid y(t) \in \bar{K}_\tau \text{ a.e. on } I\}$ .

1  $\Leftrightarrow$  2 Since  $(y \cdot \nu_\Phi) - \psi$  is  $\zeta_{I \times \Gamma_C}$ -measurable, we can deduce from Fubini's theorem, cf. [12, Thm. 2.6.2]:

$$\zeta_{I \times \Gamma_C}((y \cdot \nu_\Phi - \psi)^{-1}(0, \infty)) = \int_I \zeta_{\Gamma_C}(\{\omega \in \Gamma_C \mid y(t, \omega) \cdot \nu_\Phi(\omega) > \psi(\omega)\}) dt$$

providing the equivalence of the two conditions.

2  $\Leftarrow$  3: This is obvious, since the condition of 2 is not only satisfied up to a set of measure zero, but everywhere.

2  $\Rightarrow$  3:

This follows indirectly by  $\neg 3 \Rightarrow \neg 2$  since  $\mathbf{H}_D^1 \setminus \bar{K}_\tau$  is an open set and  $y$  is continuous. So for any  $t \in I$  with  $y(t) \notin \bar{K}_\tau$  there exists an entire interval with positive measure of states outside the set of admissible displacements.  $\square$

The pointwise state constraint formulation 3 in Lemma 3.1 for a continuous, piecewise linear state with  $y_k = y(t_k)$ ,  $k = 0 \dots N$  then reduces to  $y_k \in \bar{K}_\tau$ ,  $k = 0 \dots N$  due to the convexity of the set  $\bar{K}_\tau$ . The multiplier constraint  $\lambda \in T_{\bar{K}}(y)^\circ$  for  $y \in \bar{K}$  results in

$$\langle \lambda, \varphi - y \rangle_{C(I, \mathbf{H}^1)} = \sum_{k=1}^N \langle \lambda_k, \varphi_k - y_k \rangle_{\mathbf{H}^1} \leq 0 \quad \forall \varphi \in \bar{K}. \quad (3.14)$$

The variation over  $\varphi$  includes the choice  $\varphi_i = y_i \in \bar{K}_\tau$ ,  $i = 1 \dots N$ ,  $i \neq k$ , therefore (3.14) decouples and leaves us with the componentwise condition

$$\langle \lambda_k, \varphi_k - y_k \rangle_{\mathbf{H}^1} \leq 0 \quad \forall \varphi_k \in \bar{K}_\tau, \quad k = 1 \dots N$$

and therefore the inclusions

$$\lambda_k \in T_{\bar{K}_\tau}(y_k)^\circ, \quad k = 1 \dots N. \quad (3.15)$$

### 3.2 Time-Stepping Scheme

The discontinuity of the test functions in the discretization of (3.10) leads to a set of equations, that is decoupled with respect to the test functions' degrees of freedom and yields a modified Crank-Nicolson time-stepping scheme in the values  $(y_k, v_k) \in \mathbf{H}_D^1 \times \mathbf{H}^1$ ,  $k = 0 \dots N$ , i.e.:

$$(y_0, \psi_0)_{\mathbf{L}^2} = (y_{ini}, \psi_0)_{\mathbf{L}^2} \quad \forall \psi_0 \in \mathbf{H}^1 \quad (3.16a)$$

$$(v_0, \varphi_0)_{\mathbf{L}^2} = (v_{ini}, \varphi_0)_{\mathbf{L}^2} \quad \forall \varphi_0 \in \mathbf{H}^1 \quad (3.16b)$$

$$(y_{k+1}, \psi)_{\mathbf{L}^2} = (y_k, \psi)_{\mathbf{L}^2} + \frac{\tau}{2} (v_{k+1} + v_k, \psi)_{\mathbf{L}^2} \quad \forall \psi \in \mathbf{H}^1 \quad (3.16c)$$

$$(v_{k+1}, \varphi)_{\mathbf{L}^2} = (v_k, \varphi)_{\mathbf{L}^2} - \frac{\tau}{2} (a(y_{k+1}, \varphi) + a(y_k, \varphi) + b(v_{k+1}, \varphi) + b(v_k, \varphi)) \\ + \tau \langle f_{extk+1}, \varphi \rangle_{\mathbf{H}_D^1} + \tau (u_{k+1}, \varphi)_{\mathbf{L}^2} + \langle \lambda_{k+1}, \varphi \rangle_{\mathbf{H}^1} \quad \forall \varphi \in \mathbf{H}_D^1 \quad (3.16d)$$

$$y_{k+1} \in \bar{K}_\tau, \quad \lambda_{k+1} \in T_{\bar{K}_\tau}(y_{k+1})^\circ \quad (3.16e)$$

The Crank-Nicolson scheme for an equivalent system of first order is well known to be equivalent to the symmetric ( $2\beta = \tau = 0.5$ ) classical Newmark scheme applied to the corresponding form of a second order ordinary differential equation. The modifications in (3.16) lie in the purely implicit treatment of the contact forces  $\lambda_k$  and the volume forces  $u_k, f_{extk}$ .

In the case of the contact forces, this is the desired modification, first presented in [21], to the classical scheme, guaranteeing energy dissipativity in the appropriate situation.

The implicit treatment of external forces in the time-stepping scheme is due to the discretization of the volume forces as piecewise constant in time, whereas a piecewise linear continuous discretization would yield an averaged input of current and future forces. This step is justified physically, since there is no apparent reason for the system to be influenced in a continuous manner only. Algorithmically, this discretization is sound as well, as we will see in the optimization Section 4, where we employ an adjoint based minimization technique and need test functions and controls (volume forces) to be contained in the same space in order to be able to add the computed corrections to the iterates without changing the search space.

This implicit treatment of the external forces does not spoil the advantage of energy dissipativity gained by the implicit treatment of the contact condition because this only holds for constant external forces anyway. The proof of energy dissipativity of the modified Newmark scheme due to Kane et al. in the viscoelastic framework can be obtained by modification of [9, Thm. 2.1] and its extension in [22, Thm. 2.4.2] and is shortly stated for the readers convenience.

**Theorem 3.2** (Energy Dissipativity of the Time-Stepping Scheme). *Let the external forces  $f_{ext}(\cdot, \varphi) + u(\cdot, \varphi) \equiv f(\varphi) \forall \varphi \in \mathbf{L}^2$  be constant in time, then the time-stepping scheme (3.16) is energy conserving in the absence of contact but can be dissipative when contact occurs.*

*Proof.* The energy gained in a time step  $y_k \rightarrow y_{k+1}$  amounts to

$$\begin{aligned} \Delta \mathcal{E}_{k+1} &= \mathcal{E}(y_{k+1}, v_{k+1}) - \mathcal{E}(y_k, v_k) + \tau \mathcal{E}_{visc} \left( \frac{y_{k+1} - y_k}{\tau} \right) \\ \text{with } \mathcal{E}(y, v) &= \mathcal{E}_{kin}(v) + \mathcal{E}_{el}(y) + \mathcal{E}_w(y) = \frac{1}{2}(v, v)_{\mathbf{L}^2} + \frac{1}{2}a(y, y) - \langle f, y \rangle_{\mathbf{H}^1} \\ \mathcal{E}_{visc}(v) &= b(v, v). \end{aligned}$$

Rearranging (3.16c), (3.16d) leads to

$$\begin{aligned} v_{k+1} + v_k &= \frac{2}{\tau}(y_{k+1} - y_k) \\ v_{k+1} - v_k &= -\frac{\tau}{2}(a(y_{k+1} + y_k, \cdot) + b(v_{k+1} + v_k, \cdot)) + \tau \langle f_{k+1}, \cdot \rangle_{\mathbf{H}^1} - \langle \lambda_{k+1}, \cdot \rangle_{\mathbf{H}^1} \end{aligned}$$

from which we obtain

$$\begin{aligned} \mathcal{E}_{kin}(v_{k+1}) - \mathcal{E}_{kin}(v_k) &= \frac{1}{2}(v_{k+1} - v_k, v_{k+1} + v_k)_{\mathbf{L}^2} \\ &= -\frac{1}{2}a(y_{k+1} + y_k, y_{k+1} - y_k) - \frac{1}{2}b(v_{k+1} + v_k, y_{k+1} - y_k) \\ &\quad - \frac{1}{2\tau} \langle \lambda_{k+1}, y_{k+1} - y_k \rangle_{\mathbf{H}^1} + \langle f_{k+1}, y_{k+1} - y_k \rangle_{\mathbf{H}^1} \\ &= -\frac{1}{2}(a(y_{k+1}, y_{k+1}) - a(y_k, y_k)) - \frac{1}{2}b(v_{k+1} + v_k, y_{k+1} - y_k) \\ &\quad - \frac{1}{2\tau} \langle \lambda_{k+1}, y_{k+1} - y_k \rangle_{\mathbf{H}^1} + \langle f_{k+1}, y_{k+1} \rangle_{\mathbf{H}^1} - \langle f_k, y_k \rangle_{\mathbf{H}^1} \\ &= -(\mathcal{E}_{el}(y_{k+1}) - \mathcal{E}_{el}(y_k) + \mathcal{E}_w(y_{k+1}) - \mathcal{E}_w(y_k)) \\ &\quad - \frac{1}{2}b(v_{k+1} + v_k, y_{k+1} - y_k) - \frac{1}{2\tau} \langle \lambda_{k+1}, y_{k+1} - y_k \rangle_{\mathbf{H}^1} \end{aligned}$$

as well as

$$\tau \mathcal{E}_{visc} \left( \frac{y_{k+1} - y_k}{\tau} \right) = \frac{1}{\tau} b(y_{k+1} - y_k, y_{k+1} - y_k) = \frac{1}{2} b(v_{k+1} + v_k, y_{k+1} - y_k)$$

and finally because  $\lambda_{k+1} \in T_{\bar{K}}(y_{k+1})^\circ$  we conclude the energy dissipativity

$$\Delta \mathcal{E}_{k+1} = -\frac{1}{2\tau} \langle \lambda_{k+1}, y_{k+1} - y_k \rangle_{\mathbf{H}^1} \leq 0$$

□

Our minor modification of the contact implicit Newmark scheme therefore retains stability and also corresponds to a finite element discretization of the time continuous contact problem.

**Discussion of the Modified Discretization.** In this subsection, we want to justify the particular choice of discretization. Specifically, the reason why the modifications to the temporal part of the Petrov-Galerkin discretization used in [27] were necessary. In the aforementioned paper, the authors present a nonconforming finite element discretization for the wave equation, that results in the Crank-Nicolson scheme.

The key differences between the case in [27] and our application are twofold. Firstly, we do not want to obtain a discretization that corresponds to the symmetric Newmark scheme, which is equivalent to the Crank-Nicolson scheme in that case, but instead we want to obtain the contact implicit Newmark scheme. This requirement is due to the poor stability properties of the symmetric Newmark scheme in the contact constrained case, see, e.g., [22, Sec. 2.1] and the reference therein. Secondly, we deal with a hyperbolic variational inequality instead of a hyperbolic partial differential equation. We want this variational inequality to be discretized in such a way, that it results in a set of  $N$  time independent variational inequalities in which the solutions to the variational inequalities are coupled sequentially and where the multiplier condition  $\lambda \in T_{\bar{K}}(y)^\circ$  decouples completely. By nature of the variational inequality, the multiplier condition (3.16e) in the continuous formulation is tested with a difference of two ansatz functions from the admissible set, meaning

$$\lambda \in T_{\bar{K}}(y)^\circ \Leftrightarrow \langle \lambda, \varphi - y \rangle_{\mathbf{H}^1} \leq 0 \quad \forall \varphi \in \bar{K} \quad (3.17)$$

Here,  $\varphi, y$  are chosen from  $\bar{K} \subset Y$  and as ansatz functions, they are discretized piecewise linear and continuous. This introduces a coupling in (3.17) unless the multiplier is chosen to act only on the time discretization points  $t_k$ ,  $k = 1 \dots N$ , which leaves the vector valued Dirac measures as the only viable option.

The discretization as a whole retains physical relevance because the behavior of realistic displacements and velocities needs to be modeled continuously, while forces may change instantly. Allowing the contact forces to only act locally at the times of discretization to respect the contact constraints at those specific times, is justified as well, due to the convex set of piecewise linear admissible states, which are admissible at all times, whenever they are admissible at all discretization time points, cf. Lemma 3.1.

## 4 Optimal Control of the Semi-Discretized Problem

Following the time discretization in the previous section, we will now focus on the optimal control framework for the semi-discretized dynamical contact problem. We shortly state the analytical setting that all of the results in this section will be based upon and which we will assume to be known in this section.

The discrete setting involves the discretized controls  $u_k$ ,  $k = 1 \dots N$ , and the discretized tuples of states and velocities  $(y_{ini}, v_{ini}), (y_k, v_k)$ ,  $k = 0 \dots N$ . First note the following observation, which allows for a more compact notation:

**Proposition 4.1.** *All velocities  $v_k \in \mathbf{H}^1$ , for  $k = 1 \dots N$  can be explicitly expressed in terms of  $v_{ini}, y_{ini}, y_1, \dots, y_k$  by*

$$v_k = (-1)^k v_{ini} + \frac{2}{\tau} \sum_{j=1}^k (-1)^{k+j} (y_j - y_{j-1}), \quad k = 1 \dots N$$

*and can therefore be eliminated from the semi-discretized system. The initial values  $(y_{ini}, v_{ini})$  can be considered as right hand side input, removing  $y_0$  from the unknowns.*

*Proof.* This immediately follows by a recursion argument for the velocity coupling (3.12) and by the correspondence between the initial values and the first states and velocities seen in (3.16a).  $\square$

The examinations in this chapter therefore build on the discretized state-, control- and test spaces

$$Y_\tau = (\mathbf{H}_D^1)^N, \quad U_\tau = (\mathbf{L}^2)^N, \quad P_\tau = (\mathbf{H}_D^1)^N.$$

Following proposition 4.1, we define the linear operator

$$\begin{aligned}\bar{v}_k &: Y_\tau \mapsto \mathbf{H}^1 \\ \bar{v}_k(y) &= \frac{2}{\tau} \left( (-1)^{k+1} y_1 + \sum_{j=2}^k (-1)^{k+j} (y_j - y_{j-1}) \right)\end{aligned}$$

and for the discretized operators, cf. (3.11), we define  $A_\tau: Y_\tau \mapsto P_\tau^*$  and  $B_\tau: U_\tau \mapsto P_\tau^*$  to read

$$\begin{aligned}\langle A_\tau y, p \rangle_{P_\tau} &= (y_1, p_1)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(y_1, p_1) + \frac{\tau}{2} b(y_1, p_1) + \\ &\quad \sum_{k=1}^{N-1} (y_{k+1} - y_k - \tau \bar{v}_k(y), p_{k+1}) + \frac{\tau^2}{4} (a(y_k, p_{k+1}) + a(y_{k+1}, p_{k+1})) + \\ &\quad \frac{\tau}{2} (b(y_{k+1}, p_{k+1}) - b(y_k, p_{k+1})) \\ \langle B_\tau u, p \rangle_{P_\tau} &= \frac{\tau^2}{2} \sum_{k=1}^N (u_k, p_k)_{\mathbf{L}^2}\end{aligned}$$

The right hand side  $f_\tau \in P_\tau^*$  is a result of all affine parts that influence the system, i.e. the (scaled) external forces  $f_{ext,\tau} \in P_\tau^*$  and the part involving all initial value influences, denoted  $f_{ini} \in P_\tau^*$ , where

$$\begin{aligned}\langle f_{ini}, p \rangle_{P_\tau} &= (y_{ini} + \tau v_{ini}, p_1)_{\mathbf{L}^2} - \frac{\tau^2}{4} a(y_{ini}, p_1) + \frac{\tau}{2} b(y_{ini}, p_1) \\ &\quad + \tau \sum_{k=1}^{N-1} (-1)^k (v_{ini}, p_{k+1})_{\mathbf{L}^2} + 2 \sum_{k=1}^{N-1} (-1)^k (y_{ini}, p_{k+1})_{\mathbf{L}^2}\end{aligned}$$

and

$$f_\tau = f_{ext,\tau} + f_{ini}$$

We assume an appropriate representation of the discretized cost functional  $J: Y \times V \times U \mapsto \mathbb{R}$  to be given as  $J_\tau: Y_\tau \times U_\tau \mapsto \mathbb{R}$  and define the set of admissible displacements as

$$K_\tau = \bar{K}_\tau^N.$$

This leads to the semi-discretized optimization problem

$$\min J_\tau(y, u) \tag{4.18a}$$

$$s.t. (y, u) \in Y_\tau \times U_\tau \tag{4.18b}$$

$$y \in K_\tau \tag{4.18c}$$

$$B_\tau u + f_\tau - A_\tau y \in T_{K_\tau}(y)^\circ \tag{4.18d}$$

where

$$\begin{aligned}\langle A_\tau y - B_\tau u - f_\tau, p \rangle_{P_\tau} &= \sum_{k=0}^{N-1} (y_{k+1} - y_k - \tau \bar{v}_k, p_{k+1})_{\mathbf{L}^2} \\ &\quad + \frac{\tau^2}{4} (a(y_{k+1}, p_{k+1}) + a(y_k, p_{k+1})) \\ &\quad + \frac{\tau}{2} (b(y_{k+1}, p_{k+1}) - b(y_k, p_{k+1})) \\ &\quad - (u_{k+1}, p_{k+1})_{\mathbf{L}^2} - \langle f_{ext_{k+1}}, p_{k+1} \rangle_{\mathbf{H}^1}\end{aligned} \tag{4.19}$$

for all  $p \in P_\tau$ . The optimal control problem (4.18) includes all of the discretized constraints since the velocity coupling and the initial values have been incorporated explicitly.

The reason for including the initial values in the right hand side directly, instead of enforcing the equality of  $y_0$  and  $y_{ini}$ , is a formal one. While the formulations are equivalent, the variational equation that enforces the equality of the initial values is not influenced by the control and we lose density of the image space of the operator  $B_\tau$  in  $P_\tau^*$ , which is needed later on. This also means that we need  $y_{ini} \in \bar{K}_\tau$ , which is a reasonable requirement.

In the following subsection, we will establish the existence of a solution operator to the variational inequality (4.18d) which allows us to show the existence of minimizers to the optimal control problem (4.18). We will show directional differentiability of the solution operator under the assumption of certain polyhedricity properties, cf. Definition 4.6, for the set of admissible states and we use the differentiability in order to derive optimality conditions of first order for the minimizers of (4.18).

## 4.1 Solutions of the State Problem

In this subsection, we will show the existence of a Lipschitz continuous solution operator to the variational inequality (4.18c)-(4.18d). The considerations are largely based on the time-stepping interpretation of the variational inequality.

We begin by establishing the existence of a solution operator to the variational inequalities in each time step of the discretized dynamical contact problem, that will be used in the representation of the solution operator to the complete variational inequality.

**Lemma 4.2** (Preliminaries). *We state preliminary results for the definition of the solution operator:*

1. *The linear operator*

$$\begin{aligned} D: \mathbf{H}_D^1 &\mapsto (\mathbf{H}_D^1)^* \\ y &\mapsto (Dy)(\cdot) := d(y, \cdot) \end{aligned}$$

*associated with the bilinear form*

$$\begin{aligned} d: \mathbf{H}_D^1 \times \mathbf{H}_D^1 &\mapsto \mathbb{R} \\ d(\cdot, \cdot) &= (\cdot, \cdot)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(\cdot, \cdot) + \frac{\tau}{2} b(\cdot, \cdot) \end{aligned} \tag{4.20}$$

*is an isomorphism.*

2. *There exists a Lipschitz continuous solution operator*

$$\begin{aligned} s: (\mathbf{H}_D^1)^* &\mapsto \bar{K}_\tau \\ l &\mapsto y \end{aligned}$$

*that maps any right hand side  $l \in (\mathbf{H}_D^1)^*$  to the solution  $y$  of the variational inequality*

$$\begin{aligned} y &\in \bar{K}_\tau \\ l - Dy &\in T_{\bar{K}_\tau}(y)^\circ. \end{aligned}$$

3. *For  $k < N$  and  $w = (w_1, \dots, w_N) \in P_\tau^*$  the operator*

$$\begin{aligned} l_{k+1}: (\mathbf{H}_D^1)^{k+1} \times P_\tau^* &\mapsto (\mathbf{H}_D^1)^* \\ l_{k+1}(y_0, \dots, y_k, w) &= (y_k + \tau(-1)^k v_{ini} + \frac{2}{\tau} \sum_{j=1}^k (-1)^{k+j} (y_j - y_{j-1}), \cdot)_{\mathbf{L}^2} \\ &\quad - \frac{\tau^2}{4} a(y_k, \cdot) + \frac{\tau}{2} b(y_k, \cdot) + \langle w_{k+1}, \cdot \rangle_{\mathbf{H}_D^1} + \langle f_{extk+1}, \cdot \rangle_{\mathbf{H}_D^1} \end{aligned}$$

*is well defined and Lipschitz continuous.*

*Proof.* The form  $d: \mathbf{H}_D^1 \times \mathbf{H}_D^1 \mapsto \mathbb{R}$  is obviously bilinear. Boundedness and coercivity with constants  $\underline{M}(\tau), \bar{M}(\tau) > 0$ , depending on the time discretization, follow by the same properties of the forms  $(\cdot, \cdot)_{\mathbf{L}^2}, a, b$ :

$$\begin{aligned} |d(y, v)| &= |(y, v)_{\mathbf{L}^2} + \frac{\tau^2}{4}a(y, v) + \frac{\tau}{2}b(y, v)| \leq \bar{M}(\tau)\|y\|_{\mathbf{H}^1}\|v\|_{\mathbf{H}^1} & \forall y, v \in \mathbf{H}_D^1 \\ d(y, y) &= (y, y)_{\mathbf{L}^2} + \frac{\tau^2}{4}a(y, y) + \frac{\tau}{2}b(y, y) \geq \underline{M}(\tau)\|y\|_{\mathbf{H}^1}^2 & \forall y \in \mathbf{H}_D^1 \end{aligned}$$

and the Lax-Milgram lemma yields the first proposition. Since  $\bar{K}_\tau$  is closed and convex, [28, Thm. 2.1] yields the existence of the Lipschitz continuous solution operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$ .

Furthermore, for  $w \in P_\tau^*$ , we denote  $z = (y_0, \dots, y_k, w) \in (\mathbf{H}_D^1)^{k+1} \times P_\tau^*$ . Then the operator  $l_{k+1}(z): \mathbf{H}_D^1 \mapsto \mathbb{R}$  is linear and because of

$$\begin{aligned} |\langle l_{k+1}(z), \varphi \rangle_{\mathbf{H}_D^1}| &\leq \|y_k\|_{\mathbf{L}^2}\|\varphi\|_{\mathbf{L}^2} + \tau\|v_k\|_{\mathbf{L}^2}\|\varphi\|_{\mathbf{L}^2} + \bar{M}_a\|y_k\|_{\mathbf{H}^1}\|\varphi\|_{\mathbf{H}^1} \\ &\quad + \bar{M}_b\|y_k\|_{\mathbf{H}^1}\|\varphi\|_{\mathbf{H}^1} + \|w_{k+1}\|_{(\mathbf{H}^1)^*}\|\varphi\|_{\mathbf{H}^1} + \|f_{ext, k+1}\|_{(\mathbf{H}^1)^*}\|\varphi\|_{\mathbf{H}^1} \\ &\leq M_{l_{k+1}}(\tau)\|\varphi\|_{\mathbf{H}^1}, \end{aligned}$$

for  $\varphi \in \mathbf{H}_D^1$  and constants  $\bar{M}_{a/b}, M_{l_{k+1}} > 0$ , it is continuous as well and therefore the operator  $l_{k+1}: (\mathbf{H}_D^1)^{k+1} \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  is well defined. The Lipschitz continuity of  $z \mapsto l_{k+1}(z)$  follows from the affine linear structure with bounded linear part.  $\square$

With the quantities from the previous lemma, we find the existence of a solution to the next time step in the time-stepping scheme.

**Lemma 4.3** (Solution of a Time Step). *Let  $w \in P_\tau^*$  be given. Under the assumptions of the discretized setting and assuming  $y_{ini} = y_0, y_1, \dots, y_k \in \bar{K}_\tau$  to be the solutions of the first  $k < N$  time steps of the discretized dynamical contact problem*

$$\begin{aligned} y &\in K_\tau \\ w - A_\tau y &\in T_{K_\tau}(y)^\circ, \end{aligned} \tag{4.21}$$

compare (4.18c)-(4.18d), there exists a unique time step solution  $y_{k+1} \in \bar{K}_\tau$ , which can be represented as  $y_{k+1} = s(l_{k+1}(y_0, \dots, y_k, w))$  where the operator  $l_{k+1}: (\mathbf{H}_D^1)^{k+1} \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  maps a right hand side for the time-stepping problem to a right hand side of the time step  $k+1$ .

*Proof.* For  $k = 0 \dots N-1$  a time step corresponds to solving the variational inclusion

$$y_{k+1} \in \bar{K}_\tau \tag{4.22a}$$

$$l_{k+1}(y_0, \dots, y_k, w) - Dy_{k+1} \in T_{\bar{K}_\tau}(y_{k+1})^\circ, \tag{4.22b}$$

which can be seen in the decoupling of (4.18d) with respect to the test functions, cf. (4.19). The operator  $l_{k+1}: (\mathbf{H}_D^1)^{k+1} \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  then maps the right hand side of the original time-stepping problem to the right hand side of time step  $k+1$  depending on the previously computed states. The existence of  $y_{k+1}$  follows from the solution operator to the variational inequality, see Lemma 4.2 (2).  $\square$

The solution to the entire variational inclusion (4.18d) naturally follows from the solutions of each time step.

**Theorem 4.4** (Solutions to the Variational Inclusion). *The discretized dynamical contact problem (4.18c)-(4.18d) in the optimal control problem allows for a Lipschitz continuous solution operator  $S: P_\tau^* \mapsto K_\tau$ .*

*Proof.* Let  $w \in P_\tau^*$ . We can recursively define the solution operator  $S$  to the state problem as

$$\begin{aligned} S: P_\tau^* &\mapsto K_\tau \\ w &\mapsto y = S(w) \end{aligned}$$

where  $y_k = S_k(w)$  with,

$$\begin{aligned} S_k: P_\tau^* &\mapsto \bar{K}_\tau \subset \mathbf{H}_D^1 \\ S_0(w) &= y_{ini} \\ S_k(w) &= s\left(\tilde{l}_k(w)\right), \quad k = 1 \dots N \end{aligned}$$

and

$$\begin{aligned} \tilde{l}: P_\tau^* &\mapsto (\mathbf{H}_D^1)^* \\ \tilde{l}_k(w) &= l_k(S_0(w), S_1(w), \dots, S_{k-1}(w), w). \end{aligned} \tag{4.23}$$

From Lemma 4.2, we know  $l_k: \mathbf{H}_D^1 \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  and from Lemma 4.3, we know  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  to be Lipschitz continuous. We recursively obtain the Lipschitz continuity of all  $S_k, k = 1 \dots N$  as the composition of Lipschitz continuous operators with

$$\begin{aligned} l_{k+1}(S_0(w), \dots, S_k(w), w) &= (S_k(w), \cdot)_{\mathbf{L}^2} + (\tau(-1)^k v_{ini} + 2 \sum_{j=1}^k (-1)^{k+j} (S_j(w) - S_{j-1}(w)), \cdot)_{\mathbf{L}^2} \\ &\quad - \frac{\tau^2}{4} a(S_k(w), \cdot) + \frac{\tau}{2} b(S_k(w), \cdot) + \langle w_{k+1}, \cdot \rangle_{\mathbf{H}_D^1} + \langle f_{ext_{k+1}}, \cdot \rangle_{\mathbf{H}_D^1}. \end{aligned}$$

Therefore, the Lipschitz continuity of  $S: P_\tau^* \mapsto K_\tau$  follows from the Lipschitz continuity of each component mapping  $S_k$ .  $\square$

This concludes the existence of a Lipschitz continuous solution operator associated with the discretized dynamical contact problem.

## 4.2 Existence of Optimal Controls

The control-to-state operator now allows for deriving the existence of minimizers to the optimization problem, which is stated in the following theorem.

**Theorem 4.5** (Existence of Minimizers). *Let  $J_\tau: Y_\tau \times U_\tau \mapsto \mathbb{R}$  be a lower semi-continuous functional that is weakly lower semi-continuous with respect to  $u$  and*

$$\lim_{\|(y,u)\| \rightarrow \infty} J_\tau(y, u) = \infty \tag{4.24}$$

*then the optimal control problem*

$$\min J_\tau(y, u) \tag{4.25a}$$

$$s.t. (y, u) \in Y_\tau \times U_\tau \tag{4.25b}$$

$$y \in K_\tau \tag{4.25c}$$

$$B_\tau u + f_\tau - A_\tau y \in T_{K_\tau}(y)^\circ \tag{4.25d}$$

*admits a solution  $(\bar{y}, \bar{u})$ .*

*Proof.* We follow the standard proof technique focusing on weak subsequential convergence of a minimizing sequence where compactness is supplied by the embedding of the  $\mathbf{L}^2$  controls into  $(\mathbf{H}^1)^*$ .

Let  $(u^{(i)})_{i \in \mathbb{N}}$  be a feasible minimizing sequence to  $J_\tau$ , so that  $J_\tau(S(u^{(i)}), u^{(i)}) \rightarrow \inf_{U_\tau} J_\tau(S(\cdot), \cdot)$ . Due to the coercivity of the functional  $J_\tau$ , the sequence  $(u^{(i)})_{i \in \mathbb{N}}$  is bounded in  $U_\tau$ , so from the reflexivity of  $\mathbf{H}^1$  and  $\mathbf{L}^2$  we obtain existence of a weakly convergent subsequence, which will also be denoted  $(u^{(i)})_{i \in \mathbb{N}}$ ,  $u^{(i)} \rightharpoonup u$ .

Weak convergence of  $B_\tau u^{(i)} + f_\tau \rightharpoonup B_\tau u + f_\tau$  in  $(\mathbf{L}^{2N})^*$  follows from Riesz's isomorphism. From application of Schauder's theorem to the embedding  $\mathbf{H}^1 \hookrightarrow \mathbf{L}^2$  one obtains the compact embedding of  $(\mathbf{L}^2)^* \hookrightarrow (\mathbf{H}^1)^*$  and we therefore obtain strong convergence

$$B_\tau u^{(i)} + f_\tau \rightarrow B_\tau u + f_\tau \text{ in } P_\tau^*$$

Therefore, we conclude  $S(B_\tau u^{(i)} + f_\tau) = y^{(i)} \rightarrow y = S(B_\tau u + f_\tau)$  from the continuity of  $S: P_\tau^* \mapsto Y_\tau$ .

Finally, due to the lower semicontinuity of  $J_\tau$  for  $y^{(i)} \rightarrow y$  and  $u^{(i)} \rightharpoonup u$  we obtain

$$\inf_{U_\tau} J_\tau(S(\cdot), \cdot) = \liminf_{i \rightarrow \infty} J_\tau(y^{(i)}, u^{(i)}) \geq J_\tau(y, u) \geq \inf_{U_\tau} J_\tau(S(\cdot), \cdot).$$

□

The assumptions in Theorem 4.5 hold, e.g., in the case of a tracking functional with quadratic regularization

$$J_\tau(y, u) = \frac{1}{2} \tau \sum_{k=1}^N \frac{1}{2} (\|y_{k-1} - y_{d,k-1}\|_{\mathbf{L}^2}^2 + \|y_k - y_{d,k}\|_{\mathbf{L}^2}^2) + \frac{\alpha}{2} \tau \sum_{k=1}^N \|u_k\|_{\mathbf{L}^2}^2 \quad (4.26)$$

for  $\alpha > 0$ , which is convex and continuous w.r.t. all arguments, and therefore weakly lower semicontinuous, cf. [11, P. 562], and the regularization part guarantees the coercivity (4.24). The state dependent part in (4.26) follows from an approximation of  $\|y - y_d\|_{L^2(I, \mathbf{L}^2)}$  by the trapezoidal rule.

### 4.3 Differentiability Properties of the Solution Operator

Before we can state optimality conditions for the minimizers, the differentiability properties of the solution operator need to be discussed. This subsection addresses these properties of the operator  $S: P_\tau^* \mapsto Y_\tau$ . We begin by examining the directional differentiability of the operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  in an abstract setting and extend the results to the solution operator  $S$ . We end this subsection with examples, in which the proposed conditions are satisfied.

#### 4.3.1 Directional Differentiability of $s$

This subsection focuses on the conditions, in which we can guarantee directional differentiability of the time-stepping operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$ . Our examination of the operator's differentiability properties is based on Mignot's central result in [29, Sec. 2], which uses the notion of polyhedricity of a set as a key property and we therefore recall:

**Definition 4.6** (Polyhedricity). A subset  $C \subset Y$  of a Banach space  $Y$  is called polyhedral w.r.t.  $(y, f) \in C \times Y^*$ , iff

$$\text{cl}(R_C(y) \cap \{f\}^\perp) = \text{cl}(R_C(y)) \cap \{f\}^\perp$$

holds.

The set, which we will examine with respect to polyhedricity, will be the set of admissible states. It is apparent that this is a property of the physical setup and its modeling. With the definition of polyhedricity in mind, Theorem 2.1 of the aforementioned paper states

**Theorem 4.7** ([29, Thm. 2.1]). *Let  $V$  be a Hilbert space,  $d: V \times V \mapsto \mathbb{R}$  be bilinear, bounded and coercive,  $K \subset V$  be a closed convex set and  $w \in V^*$ . Assume  $y = P_K^d(w)$  to be the  $d(\cdot, \cdot)$ -orthogonal projection of  $w$  onto  $K$  with respect to the norm induced by  $d$ . If  $K$  is polyhedral w.r.t.  $(y, d(y - w, \cdot))$ , then the projection operator  $P_K^d$  is directionally differentiable at  $w$  and the derivative at  $w$  in direction  $\delta w$  can be computed as the  $d(\cdot, \cdot)$ -orthogonal projection of  $\delta w$  onto the critical cone to  $K$  w.r.t.  $(y, d(y - w, \cdot))$ , namely  $\mathcal{K}_K(y, d(y - w, \cdot))$ .*

As stated in Lemma 4.2 (1), the operator  $D: \mathbf{H}_D^1 \mapsto (\mathbf{H}_D^1)^*$  has a continuous, linear inverse, therefore we can write the solution operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  as the  $d(\cdot, \cdot)$ -orthogonal projection of  $D^{-1}(\cdot)$  onto  $\bar{K}_\tau \subset \mathbf{H}_D^1$ , meaning  $s = P_{\bar{K}_\tau}^d \circ D^{-1}$ . Therefore, the previous theorem yields the directional differentiability of  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  together with an explicit expression for its derivative, as long as the polyhedricity assumption holds. The aim of this section is therefore to show polyhedricity of  $\bar{K}_\tau$  w.r.t.  $(y, Dy - l)$ .

In [29], the case of a simplified, “scalar” contact problem on an  $n$ -dimensional domain is studied as an example, where constraints are enforced solely on the boundary of the reference domain, but the unknown displacement is assumed to be a scalar function, modeling a displacement with respect to a prescribed direction. This results in the set of admissible displacements being

$$C = \{v \in H_D^1(\Omega, \mathbb{R}) \mid v \leq \psi \text{ a.e. on } \Gamma_C\},$$

for which polyhedricity w.r.t. the desired directions of the Theorem 4.7 is shown in settings, where  $(V, d)$  additionally form a Dirichlet space, cf. [29, Def. 3.1]. As a result, this yields the directional differentiability of the projection operator onto  $C$ .

For our setting of  $n$ -dimensional displacements on an  $n$ -dimensional domain, additional work is required in order to obtain polyhedricity. The additional difficulty is introduced, because the set  $C$  is replaced by a more complex set, involving the vector field  $\nu_\Phi$  on the contact boundary  $\Gamma_C$ , namely

$$\bar{K}_\tau = \{v \in \mathbf{H}_D^1 = H_D^1(\Omega, \mathbb{R}^n) \mid v \cdot \nu_\Phi \leq \psi \text{ a.e. on } \Gamma_C\}$$

The important case, where the contact normal coincides with the geometric normal on the contact boundary,  $\nu_\Phi \hat{=} \nu$ , has been considered by Betz in [7], where he extends Mignot’s proof of polyhedricity to this case and obtains polyhedricity of the admissible set in the sense of Theorem 4.7. For this special case, the assumptions of Theorem 4.7 are therefore satisfied and we obtain the directional differentiability of  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$ .

In the following, we will show polyhedricity of the set  $\bar{K}_\tau \subset \mathbf{H}^1 \hat{=} H^1(\Omega, \mathbb{R}^3)$  in more general frameworks. Our strategy will be to reduce the question of polyhedricity in the vector valued case to the scalar case, studied by Mignot. Our idea is to regard  $\bar{K}_\tau$  as the preimage of  $C$  under a linear operator. We will derive some abstract results on how polyhedricity is inherited by preimages, and then give examples, where these abstract conditions can be verified, at the end of the subsection.

To this end, let us fix the assumptions for a more general setting, in which we want to investigate polyhedricity.

**Assumption 4.8.** *Let*

(A4.8<sub>a</sub>)  $H, V$  be Hilbert spaces

(A4.8<sub>b</sub>)  $L: H \mapsto V$  be a surjective, linear and bounded mapping

(A4.8<sub>c</sub>)  $K \subset H$  and  $C \subset V$  with  $K = \{y \in H \mid Ly \in C\} = L^{-1}(C)$ .

Note, that the linear operator  $L$  is generally not injective, so it will have a nontrivial kernel. For a set  $R \subset H$ , the expression  $L^{-1}R$  in the following denotes the preimage of  $R$  in  $H$ . We begin with the following theorem on the commutativity of the preimage and the interior/closure operations of a set.

Due to the open mapping theorem by Banach and Schauder,  $L$  is also an open mapping. Note, that several of the following results do not rely on the Hilbert space structure of  $H, V$  and can be extended to hold in Banach spaces. We restrict ourselves to the Hilbert space case for simplicity.

**Lemma 4.9.** *Let the assumptions (A4.8<sub>a</sub>)-(A4.8<sub>b</sub>) hold and let  $R \subset H$  be an arbitrary subset. Then*

1.  $L^{-1}(\text{int}(R)) = \text{int}(L^{-1}(R))$
2.  $L^{-1}(\text{cl}(R)) = \text{cl}(L^{-1}(R))$

hold.

*Proof.* For the reader's convenience, we restate the proof from [35]:

$L$  is continuous, therefore  $L^{-1}(\text{int}(R))$  is open and also a subset of  $L^{-1}R$ . Thus,  $L^{-1}(\text{int}(R)) \subset \text{int}(L^{-1}(R))$  because  $\text{int}(L^{-1}(R))$  can be characterized as the union of all open subsets of  $L^{-1}R$ . Since  $L$  is an open map,  $L\text{int}(L^{-1}(R))$  is open and because  $L\text{int}(L^{-1}(R)) \subset R$ , the same characterization of  $\text{int}(R)$  yields  $L\text{int}(L^{-1}(R)) \subset \text{int}(R)$  and therefore  $L^{-1}(\text{int}(R)) \supset \text{int}(L^{-1}(R))$ , which concludes part 1.

Part 2 then follows from  $L^{-1}\text{cl}(R) = L^{-1}(V \setminus \text{int}(V \setminus R)) = H \setminus \text{int}(H \setminus L^{-1}R) = \text{cl}(L^{-1}R)$ .  $\square$

This allows us to formulate the following lemma, which gives some insight into how we can express the kernel of  $L$  and the tangent cone to  $K$  at  $y \in K$ .

**Lemma 4.10.** *In the setting of Assumption 4.8, we have the following additional information on the kernel of  $L$  as well as the reachable and tangent cones to  $K$  at a point  $y \in K$ :*

1.  $\ker(L) \subset R_K(y)$
2.  $R_K(y) + \ker(L) = R_K(y)$
3.  $R_K(y) = L^{-1}R_{LK}(Ly) = L^{-1}R_C(Ly)$
4.  $T_K(y) = L^{-1}T_{LK}(Ly) = L^{-1}T_C(Ly)$

*Proof.* Part 1 follows, because for  $y \in K$  and  $\delta y \in \ker(L)$  the equation  $Ly + \lambda L\delta y = Ly \in C$  holds for any  $\lambda \in \mathbb{R}$  and therefore  $\delta y \in R_K(y)$ .

For part 2, let  $\delta y \in R_K(y)$  and  $\tilde{\delta}y \in \ker(L)$ , then  $Ly + \lambda L\delta y \in C$  holds for a  $\lambda > 0$ . For the same  $\lambda$

$$Ly + \lambda L(\delta y + \tilde{\delta}y) = Ly + \lambda L\delta y \in C$$

holds, therefore  $\delta y + \tilde{\delta}y \in R_K(y)$ .

The relation

$$L^{-1}R_C(Ly) = L^{-1}R_{LK}(Ly) = L^{-1}LR_K(y) = R_K(y) + \ker(L) = R_K(y)$$

then implies part 3.

Part 4 follows directly from Lemma 4.9 (2) due to the commutation of preimage and closure:

$$T_K(y) = \text{cl}(R_K(y)) = \text{cl}(L^{-1}R_C(Ly)) = L^{-1}\text{cl}(R_C(Ly)) = L^{-1}T_C(Ly).$$

$\square$

In the next lemma, the adjoint operator to  $L$  will play a key role. Because  $L$  is surjective, the closed range theorem, cf. e.g. [40, Thm. III.4.5], states that  $L^*: V^* \mapsto H^*$  is injective and has closed range and therefore

$$\text{im}(L^*) = \ker(L)^\perp. \quad (4.27)$$

However,  $L^*$  generally is not surjective, so we may only consider a linear, bounded inverse operator on its image, meaning  $L^{-*}: \text{im}(L^*) \mapsto V^*$ . This explains one requirement of the following lemma.

**Lemma 4.11.** *In the setting of Assumption 4.8, let  $(y, r) \in K \times \text{im}(L^*)$  and assume the set  $C = L(K)$  is polyhedral w.r.t.  $(Ly, L^{-*}r)$ .*

*Then,  $\ker(L) \subset \{r\}^\perp$  and the set  $K \subset H$  is polyhedral w.r.t.  $(y, r)$ .*

*Proof.* The idea to this proof is, to rewrite the reachable set and annihilator in the polyhedricity Definition (Def. 4.6) with the help of the linear operator  $L$  and use the commutativity of the closure and preimage from Lemma 4.9. We will start by gathering the prerequisites for the actual proof.

By assumption, we know  $r \in \text{im}(L^*) = \ker(L)^\perp$  and we therefore directly obtain

$$\ker(L) \subset \{r\}^\perp$$

from duality. Due to Lemma 4.10, we additionally know  $R_K(y) = L^{-1}R_C(Ly)$  to hold.

Moreover, because  $\{r\}^\perp$  is a linear subspace, we have

$$\{r\}^\perp + \{r\}^\perp = \{r\}^\perp.$$

Consequently, the relation  $\{r\}^\perp = L^{-1}(L(\{r\}^\perp))$  is true because of

$$\{r\}^\perp \subset L^{-1}(L(\{r\}^\perp)) = \{r\}^\perp + \ker(L) \subset \{r\}^\perp + \{r\}^\perp = \{r\}^\perp.$$

Lastly,  $L(\{r\}^\perp) = \{L^{-*}r\}^\perp$  holds since for  $v \in L(\{r\}^\perp)$  there exists  $w \in \{r\}^\perp$  with  $Lw = v$  and

$$\langle L^{-*}r, v \rangle_V = \langle L^{-*}r, Lw \rangle_V = \langle L^*L^{-*}r, w \rangle_H = \langle r, w \rangle_H = 0$$

and for any  $v \in \{L^{-*}r\}^\perp$  and any  $w \in L^{-1}(\{v\})$

$$\langle r, w \rangle_H = \langle L^*L^{-*}r, w \rangle_H = \langle L^{-*}r, v \rangle_V = 0$$

holds.

Using the polyhedricity properties assumed on  $C$  the commutativity results in Lemma 4.9 - 4.10 lead to the proof of the initial claim:

$$\begin{aligned} \text{cl}(R_K(y) \cap \{r\}^\perp) &= \text{cl}(L^{-1}(R_C(Ly)) \cap L^{-1}(\{L^{-*}r\}^\perp)) = L^{-1}(\text{cl}(R_C(Ly) \cap \{L^{-*}r\}^\perp)) \\ &= L^{-1}(\text{cl}(R_C(Ly)) \cap \{L^{-*}r\}^\perp) = \text{cl}(R_K(y) \cap \{r\}^\perp). \end{aligned}$$

□

For the setting of interest, the requirement  $r \in \text{im} L^*$  in the previous lemma is fulfilled, as the following lemma states.

**Lemma 4.12.** *In the setting of Assumption 4.8, let  $D: H \mapsto H^*$  be a linear, bounded, coercive operator and  $f \in H^*$ .*

*Further, let  $y \in K$  be the unique solution of the variational inequality*

$$\begin{aligned} y &\in K \\ f - Dy &\in T_K(y)^\circ, \end{aligned}$$

*with the residual  $r := f - Dy$ , then*

1.  $\ker(L) \subset R_K(y) \cap \{r\}^\perp$
2.  $r \in \text{im}(L^*)$

holds.

*Proof.* From Lemma 4.10, we know that  $\ker(L) \subset R_K(y) \subset T_K(y)$  and therefore

$$T_K(y)^\circ \subset \ker(L)^\circ = \ker(L)^\perp$$

By nature of the variational inequality, we have  $r \in T_K(y)^\circ \subset \ker(L)^\perp$ , and consequently  $\ker(L) \subset \{r\}^\perp$ .

The second part follows, again, from the closed range theorem, cf. (4.27), because  $r \in \ker(L)^\perp = \text{cl}(\text{im}(L^*)) = \text{im}(L^*)$ .  $\square$

At this point, in order to show polyhedricity of the set  $K$  w.r.t.  $(y, r)$ , it suffices to give a linear mapping  $L: H \mapsto V$  so that  $L(K) = C$  where  $C$  is polyhedral w.r.t.  $(Ly, L^*r)$ . We will use Mignot's results on polyhedricity in the setting of metric projections in Dirichlet spaces.

The idea is to define a bilinear, bounded and coercive form  $d_E$  on  $V$  and a right hand side  $g \in V^*$ , such that  $Ly$  is the unique solution to the variational inequality associated with  $d_E$ ,  $g$  and the set  $C$ , where the residual coincides with  $L^*r$  and  $(V, d_E)$  forms a Dirichlet space. We give both abstract results and concrete examples for the technique.

The central task in our method is the construction of the quantities with their respective properties, which can be done on an abstract level. We base the definition of the bilinear form  $d_E$  on  $V$  on the original data, and for this we need an inverse mapping to the linear operator  $L$ . Recall, that  $L$  is generally not injective and therefore not invertible. It turns out, however, that for the following considerations, we only need a right inverse:

**Assumption 4.13.** Consider an operator  $E: V \mapsto H$  that is

(A4.13<sub>a</sub>) linear and bounded

(A4.13<sub>b</sub>) a right inverse to  $L$ , meaning:  $LE = \text{id}: V \mapsto V$

For an operator  $E$  satisfying 4.13, the composition  $EL: H \mapsto H$  is a projection because

$$(EL)^2y = E(LE)Ly = ELy \quad \forall y \in H$$

so that  $\text{im}(\text{id} - EL) = \ker L$  holds:

$$L(\text{id} - EL)y = Ly - (LE)Ly = 0 \quad \text{and} \quad y \in \ker(L) \Rightarrow (\text{id} - EL)y = y \Rightarrow y \in \text{im}(\text{id} - EL).$$

We use such an operator to pull back our variational inequality on  $K \subset H$  to a variational inequality on  $C \subset V$ .

**Theorem 4.14.** In the setting of Assumption 4.8, let  $D: H \mapsto H^*$  be a linear, bounded, coercive operator,  $f \in H^*$  and  $y \in K$  be the unique solution to the variational inequality

$$\begin{aligned} y &\in K \\ f - Dy &\in T_K(y)^\circ. \end{aligned}$$

Under the assumptions 4.13, the bilinear form

$$\begin{aligned} d_E: V \times V &\mapsto \mathbb{R} \\ d_E(v, w) &= d(Ev, Ew) \end{aligned}$$

is bounded and coercive with the associated operator  $D_E: V \mapsto V^*$ ,  $(D_E v)w = d_E(v, w)$ . For  $y_{\ker} = (I - EL)y$  the map

$$g: V \mapsto \mathbb{R} \\ \langle g, w \rangle_V := \langle f, Ew \rangle_H - d(y_{\ker}, Ew)$$

is linear and continuous. Furthermore,  $Ly \in C$  solves the variational inequality

$$v \in C \\ g - D_E v \in T_C(v)^\circ$$

with the well defined residual  $g - D_E Ly = L^{-*}(f - Dy)$ .

*Proof.* The operators  $d_E$  and  $g$  are obviously (bi)linear and well defined. The continuity of  $L$  implies

$$\|v\|_V = \|LEv\|_V \leq \|L\| \|Ev\|_H,$$

therefore the coercivity of  $d_E$  holds due to

$$d(Ev, Ev) \geq M_d \|Ev\|_H \|Ev\|_H \geq \frac{M_d}{\|L\|^2} \|v\|_V^2 \quad \forall v \in V$$

and the boundedness of  $d_E$  and  $g$  follows from the continuity of  $E$  since

$$|d(Ev, Ew)| \leq \bar{M}_d \|Ev\|_H \|Ew\|_H \leq \bar{M}_d \|E\|^2 \|v\|_V \|w\|_V \\ |\langle f, Ew \rangle_H - d(y_{\ker}, Ew)| \leq \|f\| \|Ew\|_H + \bar{M}_d \|y_{\ker}\|_H \|Ew\|_H \leq (\|f\| + \bar{M}_d \|y_{\ker}\|) \|E\| \|w\|_V$$

with the coercivity and bounding constants  $M, \bar{M}_d > 0$  to  $d: H \times H \mapsto \mathbb{R}$ .

Moreover, we have  $r = f - Dy \in \ker(L)^\perp$  due to Lemma 4.12 and by definition  $y_{\ker} \in \ker(L)$  as well as  $Ew \in K$  for all  $w \in C$ . Therefore,

$$d_E(Ly, w - Ly) - \langle g, w - Ly \rangle_H = d(ELy, Ew - ELy) - \langle f, Ew - ELy \rangle_H + d(y_{\ker}, Ew - ELy) \\ = d(y, Ew - ELy) - \langle f, Ew - ELy \rangle_H \\ = d(y, Ew - y) - \langle f, Ew - y \rangle_H \geq 0 \quad \forall w \in C$$

because  $y$  is the solution to the variational inclusion associated with  $D$  and  $f$ . Therefore,  $Ly$  solves the auxiliary variational inclusion. The residual has the form

$$\langle g, w \rangle_V - d_E(Ly, w) = \langle f, Ew \rangle_H - d(y_{\ker}, Ew) - d(ELy, Ew) = \langle f, Ew \rangle_H - d(y, Ew) \\ = \langle r, Ew \rangle_H = \langle L^* L^{-*} r, Ew \rangle_H = \langle L^{-*} r, LEw \rangle_V = \langle L^{-*} r, w \rangle_V.$$

□

With the construction in the previous theorem, we can use Mignot's results on the polyhedricity in the functional analytic setting, and we will therefore transfer to the more specific framework of  $V = H_D^1$  at this time.

**Theorem 4.15** (Polyhedricity in  $\mathbf{H}_D^1$ ). *Let  $\Omega_C \subset \mathbb{R}^n$  be a set with a boundary segment  $\Gamma_C$  as described in Section 2.1 and the assumptions of Theorem 4.14 hold with  $V = H_D^1(\Omega_C, \mathbb{R})$  and  $C = \{v \in V \mid v \leq \psi \text{ a.e. on } \Gamma_C\}$ . Additionally, assume*

$$d(Ev_+, Ev_-) \leq 0 \quad \forall v \in V, \tag{4.28}$$

then  $K$  is polyhedral w.r.t  $(y, f - Dy)$ .

*Proof.*  $C$  can be rewritten as  $C = \{v \in V \mid v \leq \Psi \text{ q.e. on } \Omega\}$  with

$$\Psi = \begin{cases} \psi & \text{on } \Gamma_C \\ \infty & \text{on } \Omega_C \setminus \Gamma_C, \end{cases}$$

cf. [29, Thm. 3.1 / P. 150 Ex. 2].

The operator  $d_E: V \times V \mapsto \mathbb{R}$  is bilinear, coercive and bounded with the additional property  $d_E(v_+, v_-) \leq 0 \forall v \in V = H_D^1(\Omega_C, \mathbb{R})$ . Further,  $H_D^1(\Omega_C, \mathbb{R})$  is continuously embedded into  $L^2(\Omega_C, \mathbb{R})$ . The intersection  $H_D^1(\Omega_C, \mathbb{R}) \cap C_0(\Omega_C, \mathbb{R})$  is dense in  $C_0(\Omega_C, \mathbb{R})$ , cf. [29, P. 148, Ex. 1] and from the additional assumption 4.28 on  $d: H \times H \mapsto \mathbb{R}$ , we therefore know  $(H_D^1(\Omega_C, \mathbb{R}), d_E)$  to form a Dirichlet space, cf. [29, Def. 3.1].

Theorem 4.14 yields that  $Ly$  solves the variational inequality associated with the set  $C$  and the operators  $d_E, g$  with residual  $L^{-*}(f - Dy)$ , therefore we have found a Dirichlet space, in which  $Ly$  is the metric projection of  $D_E^{-1}g$  with respect to the natural norm induced by  $d_E$  onto the set  $C$ . [29, Thm. 3.2] therefore yields the polyhedricity of  $C$  w.r.t.  $(Ly, L^{-*}(f - Dy))$  and Lemma 4.11 concludes the proof.  $\square$

The previous theorem is where Mignot's results find their application. The essential condition, which was added, is the inequality condition (4.28) for the positive and negative part of a  $H_D^1(\Omega_C, \mathbb{R})$ -function. This is not a trivial requirement, but the following corollary to Theorem 4.15 gives some insight into the one body case. The crucial observation is that (4.28) holds, when  $L$  and  $E$  are defined in a pointwise fashion and  $d$  involves only pointwise evaluations of the functions and their first derivatives.

**Corollary 4.16** (One Body Contact). *Let  $H = \mathbf{H}_D^1$ ,  $V = H_D^1(\Omega, \mathbb{R})$ ,  $f \in (\mathbf{H}^1)^*$  and  $d: \mathbf{H}_D^1 \times \mathbf{H}_D^1 \mapsto \mathbb{R}$  be the bilinear, bounded and coercive bilinear form in the time-stepping problems (4.20). Furthermore, let  $\bar{\nu}_\Phi \in W^{1,\infty}(\Omega, \mathbb{R}^n)$  with  $\|\bar{\nu}_\Phi(\omega)\| = 1$  a.e. on  $\Omega$ , for which the contact normal  $\nu_\Phi: \Gamma_C \mapsto \mathbb{R}^n$  results from  $\nu_\Phi = \tau_{\Gamma_C}(\bar{\nu}_\Phi)$ , and  $y$  the solution to the variational inequality*

$$\begin{aligned} y &\in \bar{K}_\tau \\ f - Dy &\in T_{\bar{K}_\tau}(y)^\circ, \end{aligned}$$

with

$$\bar{K}_\tau = \{y \in \mathbf{H}_D^1 \mid y \cdot \nu_\Phi \leq \psi \text{ a.e. on } \Gamma_C\}.$$

Then the set of admissible states  $\bar{K}_\tau$  is polyhedral with respect to  $(y, f - Dy)$

*Proof.* Like in the previous theorem, we define  $C = \{v \in H_D^1(\Omega, \mathbb{R}) \mid v \leq \psi \text{ a.e. on } \Gamma_C\}$  and

$$\begin{aligned} L: \mathbf{H}_D^1 &\mapsto H_D^1 \\ Ly &= y \cdot \bar{\nu}_\Phi \end{aligned}$$

First of all,  $L$  is well defined, because the pointwise product  $\omega \mapsto y_{(i)} \bar{\nu}_{\phi_2(i)}(\omega)$ ,  $i = 1 \dots d$  still lies in  $H^1$  due to the form of  $\bar{\nu}_\Phi$ . Further,  $L$  is linear and bounded and  $\bar{K}_\tau = \{y \in \mathbf{H}_D^1 \mid Ly \in C\}$  holds. We define the extension operator  $E$  as

$$\begin{aligned} E: H_D^1(\Omega, \mathbb{R}) &\mapsto \mathbf{H}_D^1 \\ Ev &= v \bar{\nu}_\Phi \end{aligned}$$

which is obviously linear and bounded as well, and due to the pointwise normalized extension  $\bar{\nu}_\Phi$  we have

$$LEv = v \bar{\nu}_\Phi \cdot \bar{\nu}_\Phi = v$$

for any  $v \in H_D^1(\Omega, \mathbb{R})$ , which also shows the surjectivity of  $L$ .

Moreover, the subset of  $\Omega$ , where  $v^+$  and  $v^-$  are both nonzero is a set of measure 0, meaning

$$\zeta(\{v^+ \neq 0\} \cap \{v^- \neq 0\}) = 0$$

holds. This pointwise condition transfers to  $Ev^+, Ev^-$ , and therefore

$$\zeta(\{(Ev^+)_{(i)} \neq 0\} \cap \{(Ev^-)_{(j)} \neq 0\}) = 0, \quad i, j = 1 \dots d.$$

The form of  $d$  in (4.20) then yields  $d(Ev^+, Ev^-) = 0$  and Theorem 4.15 concludes the proof.  $\square$

Note, that the previous corollary yields directional differentiability of  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  at any  $f \in (\mathbf{H}_D^1)^*$ , not just at specific points in  $(\mathbf{H}_D^1)^*$ .

**Remark 4.17.** *We have chosen to assume existence of  $\bar{\nu}_\Phi$  as a unit vector field on  $\Omega$  for simplicity of presentation. In applications,  $\nu_\Phi$  may be a given unit vector field, defined on  $\Gamma_C$  only. Then we have to extend  $\nu_\Phi$  to an appropriate subset  $\Omega_C \subset \Omega$ . To this end, one needs to establish, by techniques of differential geometry, a surjective  $C^1$  mapping  $\varphi: \Omega_C \rightarrow \Gamma_C$ . Then, we can define  $\bar{\nu}_\Phi(\omega) := \nu_\Phi(\varphi(\omega))$ .*

### 4.3.2 Hadamard Differentiability of $S$

Assuming, the time-stepping operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  is directionally differentiable, we can extend the differentiability to the time-stepping solution operator  $S: P_\tau^* \mapsto K_\tau$ . The structure of the right hand sides  $\tilde{l}_{k+1}(\cdot)$  in each time step results from the sequential nature of the time-stepping scheme, so the right hand side in a time step depends on the solutions of the previous steps. Since a chain rule generally does not hold for directionally differentiable operators, directional differentiability of the time-stepping solution operators  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  may not be sufficient for differentiability of the solution operator  $S: P_\tau^* \mapsto K_\tau$ .

The differentiability concept of Hadamard allows for an extension of the chain rule to the case of “tangential” directional differentiability and is recalled for the reader’s convenience.

**Definition 4.18** (Hadamard Differentiability). Let  $X, Y$  be Banach spaces. A functional  $F: X \mapsto Y$  is called directionally differentiable in the sense of Hadamard, or Hadamard differentiable for short, at  $x \in X$  in direction  $\delta x$  iff for all sequences  $\{\delta x_t\}_{t>0} \subset X$  with  $\frac{\delta x_t - t\delta x}{t} \xrightarrow{t \rightarrow 0} 0$

$$\lim_{t \rightarrow 0} \frac{F(x + \delta x_t) - F(x)}{t} = F'(x, \delta x) \in X$$

holds.  $F'(x, \delta x) \in X$  is called the directional derivative.

The essential properties of Hadamard differentiable functionals are stated in the following lemma.

**Lemma 4.19.** *Let  $X, Y, Z$  be Banach spaces,  $F: Y \mapsto Z$  and  $G: X \mapsto Y$  directionally differentiable functionals. Then it holds that:*

- *If  $F$  is additionally Lipschitz continuous, then  $F$  is Hadamard differentiable.*
- *If  $F$  is additionally Hadamard differentiable, then  $H = F \circ G: X \mapsto Z$  is directionally differentiable with*

$$H'(x, \delta x) = F'(G(x), G'(x, \delta x))$$

- *If both  $F$  and  $G$  are Hadamard differentiable, the composition  $H = F \circ G: X \mapsto Z$  is Hadamard differentiable as well.*

*Proof.* The computations are straightforward and included, e.g., in [32].  $\square$

We already know  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  to be Lipschitz continuous, so whenever it is directionally differentiable, it is Hadamard differentiable as well and the chain rule holds.

Therefore, the properties of the operators in the time steps transfer to the discretized contact problem, as it did in the previous section.

**Lemma 4.20** (Differentiability of  $S$ ). *Let  $w \in P_\tau^*$  be a right hand side and assume the time-stepping solution operator  $s: (\mathbf{H}_D^1)^* \mapsto \bar{K}_\tau$  from Lemma 4.3 to be directionally differentiable, as well as  $y = S(w)$ . Then  $S: P_\tau^* \mapsto Y_\tau$  is Hadamard differentiable at  $w$  and the derivative  $S'(w, \delta w)$  reads*

$$S'(w, \delta w) = \begin{pmatrix} S'_1(w, \delta w) \\ \vdots \\ S'_N(w, \delta w) \end{pmatrix} = \begin{pmatrix} s'(\tilde{l}_1(w), \tilde{l}'_1(w, \delta w)) \\ \vdots \\ s'(\tilde{l}_N(w), \tilde{l}'_N(w, \delta w)) \end{pmatrix}$$

with  $\tilde{l}_k: (\mathbf{H}_D^1)^k \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  defined as in (4.23). If  $\delta l \mapsto s'(l, \delta l)$  is Lipschitz continuous, then so is  $\delta w \mapsto S'(w, \delta w)$ .

*Proof.* This proof follows from induction. The operator  $\tilde{l}_1: P_\tau^* \mapsto (\mathbf{H}_D^1)^*$ , mapping the right hand side  $w \in P_\tau^*$  to the right hand side of the first time step, has the form

$$\tilde{l}_1(w) = \langle y_{ini} + \tau v_{ini}, \cdot \rangle_{\mathbf{H}_D^1} - \frac{\tau^2}{4} a(y_{ini}, \cdot) + \frac{\tau}{2} b(y_{ini}, \cdot) + \langle w_1, \cdot \rangle_{\mathbf{H}_D^1} + \langle f_{ext1}, \cdot \rangle_{\mathbf{H}_D^1}$$

which is affine linear with a bounded linear part. Therefore  $\tilde{l}_1$  is Fréchet differentiable, implying Hadamard differentiability with

$$\tilde{l}'_1(w, \delta w) = \langle \delta w_1, \cdot \rangle_{\mathbf{H}_D^1}. \quad (4.29)$$

Because  $s: (\mathbf{H}_D^1)^* \mapsto \mathbf{H}_D^1$  was assumed directionally differentiable and it is Lipschitz continuous, it is Hadamard differentiable. Lemma 4.19 then yields the Hadamard differentiability of  $S_1: P_\tau^* \mapsto \mathbf{H}_D^1$  with  $S'_1(w, \delta w) = s'(\tilde{l}_1(w), \tilde{l}'_1(w, \delta w))$ .

For  $1 < k \leq N$  this argument holds analogously. The mappings  $\tilde{l}_k(\cdot): P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  are compositions of the affine linear maps  $l_k: (\mathbf{H}_D^1)^k \times P_\tau^* \mapsto (\mathbf{H}_D^1)^*$  and the component mappings  $S_i: P_\tau^* \mapsto \mathbf{H}_D^1$ ,  $i = 1 \dots k-1$  of the solution operator  $S$ . The maps  $l_k$  have bounded linear part and are therefore Fréchet differentiable, while the component maps  $S_i$ ,  $i = 1 \dots k$ , are Hadamard differentiable. Therefore, Hadamard differentiability of the operator  $S_k: P_\tau^* \mapsto \bar{K}_\tau$  follows again due to the chain rule in Lemma 4.19, which also yields the representation of the directional derivative as

$$\begin{aligned} S'_k(w, \delta w) &= s'(\tilde{l}_k(w), \tilde{l}'_k(w, \delta w)) \\ \text{where } \tilde{l}'_k(w, \delta w) &= S'_{k-1}(w, \delta w) + 2 \sum_{j=1}^{k-1} (-1)^{k+j} (S'_j(w, \delta w) - S'_{j-1}(w, \delta w)) \\ &\quad - \frac{\tau^2}{4} a(S'_{k-1}(w, \delta w), \cdot) + \frac{\tau}{2} b(S'_{k-1}(w, \delta w), \cdot) + \langle \delta w_k, \cdot \rangle_{\mathbf{H}_D^1}. \end{aligned}$$

The Lipschitz continuity of  $\delta w \mapsto S'(w, \delta w)$  follows analogously to the Lipschitz continuity of the solution mapping  $S: P_\tau^* \mapsto K_\tau$  from the Lipschitz continuity of the component mappings  $\delta w \mapsto S_k(w, \delta w)$ , which follows from the same type of induction argument.

The mapping  $\delta w \mapsto \tilde{l}_1(w, \delta w)$  is obviously Lipschitz, cf. (4.29), since it is linear and bounded, therefore  $\delta w \mapsto S_1(w, \delta w)$  is Lipschitz continuous being the composition of  $S'_1(w, \cdot) = s'(\tilde{l}_1(w), \tilde{l}'_1(w, \cdot))$ . The mappings  $\delta w \mapsto \tilde{l}_k(w, \delta w)$  are again Lipschitz continuous as compositions of bounded, linear mappings with the mappings  $\delta w \mapsto S'_i(w, \delta w)$ ,  $i = 1 \dots k-1$ . By composition with  $s'(\tilde{l}_k(w), \cdot)$ , we have Lipschitz continuity of  $\delta w \mapsto S_k(w, \delta w)$ ,  $k = 1 \dots N$  and therefore for  $\delta w \mapsto S'(w, \delta w)$ .  $\square$

In the following theorem, we summarize the results of the previous subsections and specify the form of the derivatives in the cases where Mignot's results on polyhedricity can be used.

**Theorem 4.21** (Properties of the Variational Inclusion). *Let  $w \in P_\tau^*$ . The variational inclusion*

$$y \in K_\tau \tag{4.30a}$$

$$w - A_\tau y \in T_{K_\tau}(y)^\circ \tag{4.30b}$$

*allows for a unique solution operator*

$$S: P_\tau^* \mapsto K_\tau$$

$$w \mapsto y$$

*which is Lipschitz continuous. If  $\bar{K}_\tau$  is polyhedral w.r.t.  $(y_k, \tilde{l}_k(w) - Dy_k)$ ,  $k = 1 \dots N$ , then  $S$  is directionally differentiable in the sense of Hadamard and the map of directional derivatives  $\delta w \mapsto \delta y = S'(w, \delta w)$  is Lipschitz continuous w.r.t.  $\delta w$  and can be computed by solving the variational inequality*

$$\delta y \in \mathcal{K} \tag{4.31}$$

$$\delta w - A_\tau \delta y \in T_{\mathcal{K}}(\delta y)^\circ$$

*with the critical cone  $\mathcal{K} = \prod_{k=1}^N \mathcal{K}_{\bar{K}_\tau}(y_k, \tilde{l}_k(w) - Dy_k)$ .*

*Proof.* We have already seen the existence of the Lipschitz continuous solution operator in Section 4.1.

Due to the polyhedricity assumptions on  $\bar{K}_\tau$ , Theorem 4.7 yields the directional differentiability of  $s: (\mathbf{H}_D^1)^* \mapsto \mathbf{H}_D^1$  at all  $\tilde{l}_k(w)$ ,  $k = 1 \dots N$  with the directional derivative  $s'(\tilde{l}_k(w), \delta l)$  being the solution to the variational inclusion

$$\begin{aligned} \delta y &\in \mathcal{K}_{\bar{K}_\tau}(y_k, \tilde{l}_k(w) - Dy_k) \\ \delta l - D\delta y &\in T_{\mathcal{K}_{\bar{K}_\tau}(y_k, \tilde{l}_k(w) - Dy_k)}(\delta y)^\circ. \end{aligned}$$

Theorem 4.20 yields the differentiability of  $S: P_\tau^* \mapsto K_\tau$  with the derivative being

$$S'(w, \delta w) = \begin{pmatrix} S'_1(w, \delta w) \\ \vdots \\ S'_N(w, \delta w) \end{pmatrix} = \begin{pmatrix} s'(\tilde{l}_1(w), \tilde{l}'_1(w, \delta w)) \\ \vdots \\ s'(\tilde{l}_N(w), \tilde{l}'_N(w, \delta w)) \end{pmatrix}.$$

A straightforward calculation, using the particular form of the  $\tilde{l}_k$  and  $A_\tau$  yields the form (4.31) of the derivative.

The Lipschitz continuity of  $\delta l \mapsto s'(l, \delta l)$  is clear, because of the representation as the solution operator to the variational inclusion associated with the critical cone  $\mathcal{K}_{\bar{K}_\tau}(y_k, \tilde{l}_k(w) - Dy_k)$  and [28, Thm. 2.1]. therefore, we obtain the Lipschitz continuity of  $\delta w \mapsto S'(w, \delta w)$  by Theorem 4.20.  $\square$

At this point, we have a set of abstract conditions for existence and differentiability of the solution operator to the discretized variational inclusion level that need to be verified in the respective concrete settings.

### 4.3.3 Examples

A first canonical example for the applicability of our theory is one body unilateral contact with a rigid plane, for which we will verify the assumptions of Theorem 4.21.

**Example 4.22** (One Body Unilateral Contact with Plane). *The setting is the one, displayed on the left side of the illustration in figure 1. The plane may be tilted as well. The description then amounts to*

1. the spaces  $H = \mathbf{H}_D^1$  and  $V = H_D^1(\Omega, \mathbb{R})$ ,
2. the constant contact normal  $\nu_\Phi: \Gamma_C \mapsto \mathbb{R}^n$ ,
3. a measurable gap function  $\psi: \Gamma_C \mapsto \mathbb{R}^+$  and
4. the set of admissible states  $\bar{K}_\tau^N$  with  $\bar{K}_\tau = \{y \in \mathbf{H}_D^1 \mid y \cdot \nu_\Phi \leq \psi \text{ a.e. on } \Gamma_C\}$ .

The constant extension of  $\nu_\Phi$  to  $\bar{\nu}_\Phi: \Omega \mapsto \mathbb{R}^n$  yields a  $W^{1,\infty}$ -function that fulfills the requirements of Theorem 4.16, so  $\bar{K}_\tau$  is polyhedral in the sense of Theorem 4.21 and we obtain a Lipschitz continuous, Hadamard differentiable solution operator by the same theorem.

Even though we focus on one body contact problems in this paper, the techniques are applicable to two body problems as well, therefore we want to give a short outlook for the two body problems at this time. An overview on the specifics for modeling two body problems can be found in, e.g., [22].

**Example 4.23** (Symmetric Two Body Unilateral Contact). *Let  $\Omega_1, \Omega_2 \subset \mathbb{R}^n, \Omega = \Omega_1 \cup \Omega_2$  where  $\Omega_{1/2}$  are two spheres in  $\mathbb{R}^n$  with  $\text{dist}(\Omega_1, \Omega_2) > 0$  and a reflection*

$$\Phi: \Omega_1 \mapsto \Omega_2$$

being a smooth bijection with a smooth inverse and uniformly bounded Jacobian for which  $\frac{\Phi(\omega) - \omega}{|\Phi(\omega) - \omega|}$  is constant.

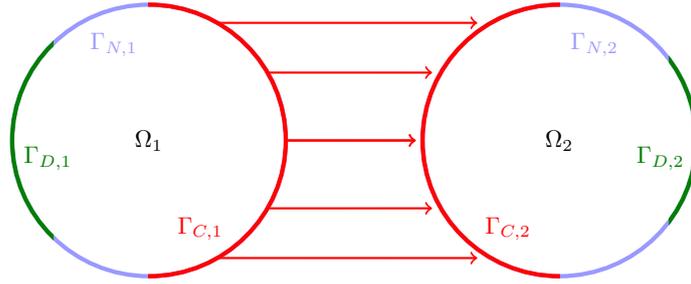


Fig. 4 Symmetric, unilateral two body contact problem

The description then amounts to

1. the spaces  $H = H_D^1(\Omega_1, \mathbb{R}^n) \times H_D^1(\Omega_2, \mathbb{R}^n)$ ,  $V = H_D^1(\Omega_1, \mathbb{R})$
2. the constant contact normal between the bodies

$$\bar{\nu}_\Phi: \Omega_1 \mapsto \mathbb{R}^n, \quad \bar{\nu}_\Phi(\omega) = \frac{\Phi(\omega) - \omega}{|\Phi(\omega) - \omega|}$$

3. the set of admissible displacements  $\bar{K}_\tau = \{y \in H \mid (y_1 - y_2 \circ \Phi) \cdot \bar{\nu}_\Phi \leq \psi \text{ a.e. on } \Gamma_{C,1}\}$ .

While Theorem 4.15 still holds in this section, we cannot rely on Corollary 4.16 to obtain the respective polyhedricity. Instead, we define

1.  $C = \{v \in V \mid v \leq \psi \text{ a.e. on } \Gamma_{C,1}\}$
2.  $L: H \mapsto V, \quad Ly = (y_1 - y_2 \circ \Phi) \cdot \bar{\nu}_\Phi$
3.  $E: V \mapsto H, \quad Ev = (y_1, y_2) := (\frac{1}{2}v \bar{\nu}_\Phi, -(\frac{1}{2}v \bar{\nu}_\Phi) \circ \Phi^{-1})$

to obtain an analogous result to the corollary. Both  $L$  and  $E$  are linear and bounded and

$$LEv = v \quad \forall v \in V,$$

which yields surjectivity of  $L$  and  $L\bar{K}_\tau = C$ .

The pointwise argument for the inequality condition (4.28) on the positive and negative part of a  $V$ -function can be carried over to this case and we therefore obtain all the requirements of Theorem 4.15, which yields polyhedricity with respect to the solution of a variational inclusion and its residual for the respective bilinear forms. By Theorem 4.21, we obtain the existence of a Hadamard differentiable and Lipschitz continuous solution operator to the time sequential variational inclusion.

#### 4.4 First Order Optimality Conditions

First note the following lemma.

**Lemma 4.24** (Density of Controls). *The image  $\text{im}(B_\tau)$  of the operator  $B_\tau: U_\tau \mapsto P_\tau^*$  is dense in  $P_\tau^*$ .*

*Proof.* Recall that  $U_\tau = (\mathbf{L}^2)^N$ ,  $P_\tau = (\mathbf{H}_D^1)^N$  and  $B(U_\tau) = ((\mathbf{L}^2)^N)^* \hat{=} (\mathbf{L}^2)^{*N}$  and that the embedding operator  $\mathcal{E}: \mathbf{H}^1 \mapsto \mathbf{L}^2$  has trivial kernel.

By identification of  $\mathbf{H}^1$  with its bidual, it follows that  $\mathcal{E}^{**}: (\mathbf{H}^1)^{**} \mapsto (\mathbf{L}^2)^{**}$  also has trivial kernel. Due to [40, Thm. III.4.5] applied to the adjoint  $\mathcal{E}^*: (\mathbf{L}^2)^* \mapsto (\mathbf{H}^1)^*$ , we know that  $\overline{\text{im } \mathcal{E}^*} = (\ker \mathcal{E}^{**})^\perp$  and the claim follows since

$$\begin{aligned} \overline{\text{im } \mathcal{E}^*} &= \overline{(\mathbf{L}^2)^*} \\ \ker \mathcal{E}^{**} &= \{0\}_{(\mathbf{H}^1)^{**}} \end{aligned}$$

This directly transfers to the product spaces as well.  $\square$

Following the same argument used in Wachsmuth's example [37, Sec. 5.1], we can now derive necessary conditions of first order, which are stated in Theorem 4.25, based on a linearization of the optimal control problem and a density argument. The following will include an adjoint state  $p \in (P_\tau)^{**}$  that can be identified with an element of the primal space  $\tilde{p} \in P_\tau$  due to the reflexivity of  $P_\tau$ , and we denote both by  $p$  without further differentiation.

**Theorem 4.25** (First Order Optimality Conditions). *Let  $J_\tau: Y_\tau \times U_\tau \mapsto \mathbb{R}$  be Fréchet differentiable and  $\bar{x} := (\bar{y}, \bar{u})$  be a local minimizer to the problem*

$$\min J_\tau(y, u) \tag{4.32a}$$

$$s.t. (y, u) \in Y_\tau \times U_\tau \tag{4.32b}$$

$$y \in K_\tau \tag{4.32c}$$

$$B_\tau u + f_\tau - A_\tau y \in T_{K_\tau}(y, v)^\circ \tag{4.32d}$$

If  $\bar{K}_\tau$  is polyhedral in the sense of Theorem 4.21, then there exist multipliers  $p \in P_\tau$ ,  $\mu \in P_\tau^*$  with

$$\partial_y J_\tau(\bar{x}) + \mu + A_\tau^* p = 0, \quad -p \in T_{K_\tau}(\bar{y}) \cap (B_\tau \bar{u} + f_\tau - A_\tau \bar{y})^\perp \tag{4.33}$$

$$\partial_u J_\tau(\bar{x}) - B_\tau^* p = 0, \quad \mu \in (T_{K_\tau}(\bar{y}) \cap (B_\tau \bar{u} + f_\tau - A_\tau \bar{y})^\perp)^\circ \tag{4.34}$$

*Proof.* Due to the polyhedricity assumptions, we have Hadamard differentiability of the solution operator and the optimality of  $(\bar{y}, \bar{u}) = (S\bar{u}, \bar{u})$  therefore implies

$$\partial_y J_\tau(\bar{x}) S'(B_\tau \bar{u} + f_\tau, B_\tau \delta u) + \partial_u J_\tau(\bar{x}) \delta u \geq 0 \quad \text{for all } \delta u \in U_\tau.$$

Testing the previous line with  $\pm\delta u$  as in [29, 37] yields the existence of  $M(\tau) > 0$  with

$$\begin{aligned} -\partial_u J_\tau(\bar{x})\delta u \leq \partial_y J_\tau(\bar{x})S'(B_\tau\bar{u} + f_\tau, \delta u) &\leq |\partial_y J_\tau(\bar{x})S'(B_\tau\bar{u} + f_\tau, B_\tau\delta u)| \\ &\leq \|\partial_y J_\tau(\bar{x})\| \|S'(B_\tau\bar{u} + f_\tau, B_\tau\delta u)\| \\ &\leq \|\partial_y J_\tau(\bar{x})\|_{L_{S'}} \|B_\tau\delta u\| = M(\tau) \|B_\tau\delta u\| \\ \partial_u J_\tau(\bar{x})\delta u \leq \partial_y J_\tau(\bar{x})S'(B_\tau\bar{u} + f_\tau, -\delta u) &\leq |\partial_y J_\tau(\bar{x})S'(B_\tau\bar{u} + f_\tau, -B_\tau\delta u)| \\ &\leq \|\partial_y J_\tau(\bar{x})\|_{L_{S'}} \|-B_\tau\delta u\| = M(\tau) \|B_\tau\delta u\| \end{aligned}$$

due to the fact that  $S'(B_\tau\bar{u} + f_\tau, \cdot): P_\tau^* \mapsto Y_\tau$  is Lipschitz continuous with constant  $L_{S'}$  and  $S'(B_\tau\bar{u} + f_\tau, 0) = 0$ . Consequently, there exists a constant  $M > 0$  with

$$|\partial_u J_\tau(\bar{x})\delta u| \leq M \|B_\tau\delta u\|$$

and therefore  $B_\tau\delta u \mapsto \partial_u J_\tau(\bar{x})\delta u$  defines a bounded functional and can be extended to a functional  $p \in (P_\tau)^{**} \doteq P_\tau$ , where  $\partial_u J_\tau(\bar{x}) = B_\tau^*p$ , see [37]. The density of  $\text{im}(B_\tau)$  in  $P_\tau^*$  yields

$$\partial_y J_\tau(\bar{x})S'(B_\tau\bar{u} + f_\tau, \delta\xi) + p\delta\xi \geq 0 \quad \text{for all } \delta\xi \in P_\tau^*$$

implying that  $(\delta y, \delta\xi) = (0, 0)$  is a global minimizer to the problem

$$\begin{aligned} \min \quad & \partial_y J_\tau(\bar{x})\delta y + p\delta\xi \\ & (\delta y, \delta\xi) \in Y_\tau \times P_\tau^* \\ & \delta y \in \mathcal{K}_{K_\tau} \\ & \delta\xi - A_\tau\delta y \in \mathcal{K}_{K_\tau}^\circ \\ & \langle \delta\xi - A_\tau\delta y, \delta y \rangle = 0 \end{aligned}$$

where  $\mathcal{K}_{K_\tau} = T_{K_\tau}(\bar{y}) \cap (B_\tau\bar{u} + f_\tau - D\bar{y})^\perp$ .

The mapping  $(\delta y, \delta\xi) \mapsto (\delta y, \delta\xi - A_\tau\delta y)$  is linear and surjective and we obtain the first order optimality conditions from [37, Prop. 4.8]:

$$\begin{aligned} \partial_y J_\tau(\bar{x}) + \mu + A_\tau^*p &= 0, & -p &\in T_{K_\tau}(\bar{y}) \cap (B_\tau\bar{u} + f_\tau - A_\tau\bar{y})^\perp \\ \partial_u J_\tau(\bar{x}) - B_\tau^*p &= 0, & \mu &\in (T_{K_\tau}(\bar{y}) \cap (B_\tau\bar{u} + f_\tau - A_\tau\bar{y})^\perp)^\circ \end{aligned}$$

□

Together with the state inequality (4.32c)-(4.32d) the adjoint problem (4.33) and the stationarity condition (4.34) form the first order optimality system. When we refer to (4.33) as the adjoint problem, this is meant to include the constraint on the multiplier  $\mu$ .

## 4.5 Discussion of the Optimality Conditions

In this subsection, we want to take a closer look at the optimality conditions to the problem (4.32) that were established in the previous section, specifically at the adjoint equation. We show, how to interpret the adjoint problem as a sequential step-by-step scheme and shortly discuss existence of solutions to the adjoint problem and their role in the optimality conditions.

We define  $\bar{\lambda} = B_\tau\bar{u} + f_\tau - A_\tau\bar{y}$  as the residual for the elastic problem at the optimizer. Recall, that  $\bar{\lambda}$  can be interpreted as a set of contact forces in the forward problem. Now, the adjoint problem in (4.33)-(4.34) consists of the conditions

$$-p \in \mathcal{K}_{K_\tau}, \quad \mu \in \mathcal{K}_{K_\tau}^\circ \quad (4.35)$$

for the adjoint state  $p$  and the multiplier  $\mu$ , with

$$\mathcal{K}_{K_\tau} = T_{K_\tau}(\bar{y}) \cap \{\bar{\lambda}\}^\perp$$

as well as the equation

$$\partial_y J_\tau(\bar{x}) + A_\tau^*p + \mu = 0. \quad (4.36)$$

**Variational Form.** Testing (4.36) with  $y \in Y_\tau$  yields

$$\langle A_\tau y, p \rangle_{P_\tau} + \langle \mu + \partial_y J_\tau(\bar{x}), y \rangle_{Y_\tau} = 0 \quad \forall y \in Y_\tau,$$

which can be rewritten as

$$\begin{aligned} & \sum_{k=1}^{N-1} (y_{k+1} - y_k - \tau \bar{v}_k, p_{k+1})_{\mathbf{L}^2} + \frac{\tau^2}{4} (a(y_{k+1}, p_{k+1}) + a(y_k, p_{k+1})) + \frac{\tau}{2} (b(y_{k+1}, p_{k+1}) - b(y_k, p_{k+1})) \\ & + \sum_{k=1}^N \left\{ \langle \partial_{y_k} J_\tau(\bar{x}), y_k \rangle_{\mathbf{H}_D^1} + \langle \mu_k, y_k \rangle_{\mathbf{H}_D^1} \right\} + (y_1, p_1)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(y_1, p_1) + \frac{\tau}{2} b(y_1, p_1) = 0 \quad \forall y \in Y_\tau, \end{aligned}$$

cf. the definition of  $A_\tau$  in the beginning of this section.

There is a close resemblance to the form in (4.19), where  $p$  was the test function. The decoupling into a time-stepping scheme was apparent in that case. Here,  $y$  is the test function, but the decoupling is inherent to the form of  $A_\tau$ , so when  $p$  is discretized, (4.36) decouples as well and reveals the same step-by-step structure when the components  $y_k$ ,  $k = 1 \dots N$  are varied independently. The adjoint problem (4.36) can then equivalently be interpreted as the following stepping scheme:

$$(p_N, \psi)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(p_N, \psi) + \frac{\tau}{2} b(p_N, \psi) + \langle \mu_N, \psi \rangle_{\mathbf{H}_D^1} = - \langle \partial_{y_N} J_\tau(\bar{y}, \bar{u}), \psi \rangle_{\mathbf{H}_D^1} \quad (4.37)$$

$$\begin{aligned} (p_k, \varphi)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(p_k, \varphi) + \frac{\tau}{2} b(p_k, \varphi) + \langle \mu_k, \varphi \rangle_{\mathbf{H}_D^1} &= (p_{k+1}, \varphi)_{\mathbf{L}^2} - \frac{\tau^2}{4} a(p_{k+1}, \varphi) + \frac{\tau}{2} b(p_{k+1}, \varphi) \\ &\quad - \tau (q_{k+1}, \varphi)_{\mathbf{L}^2} - \langle \partial_{y_k} J_\tau(\bar{y}, \bar{u}), \varphi \rangle_{\mathbf{H}_D^1}, \end{aligned} \quad (4.38)$$

for all  $\varphi, \psi \in \mathbf{H}_D^1$ ,  $k = 1 \dots N - 1$ , with the terms

$$q_N = -\frac{2}{\tau} p_N \quad (4.39)$$

$$q_k = \frac{2}{\tau} \left( \sum_{j=k}^{N-1} (-1)^{j+k} (p_{j+1} - p_j) + (-1)^{N-k+1} p_N \right). \quad (4.40)$$

This can be seen, when the components

The adjoint velocities are stated explicitly w.r.t.  $p_k$ ,  $k = 1 \dots N$ , just as the velocities in the forward problem have been earlier in this section, cf. Proposition 4.1. We also recognize the coercive, bounded, bilinear form  $d: \mathbf{H}_D^1 \times \mathbf{H}_D^1 \mapsto \mathbb{R}$  with  $d(\cdot, \cdot) = (\cdot, \cdot)_{\mathbf{L}^2} + \frac{\tau}{2} b(\cdot, \cdot) + \frac{\tau^2}{4} a(\cdot, \cdot)$  that defined the operator in all of the time steps to the state problem, c.f. Lemma 4.2. The structure with respect to the multiplier  $\mu$  is similar as well, as it is treated fully implicitly in each backward step. The linearization of the cost functional contributes to the right hand side of the adjoint problem as usual in adjoint problems.

Note, that the decoupled equation did not yet include the inclusions (4.35).

**Adjoint Stepping Scheme.** When we replace the explicit representation of the adjoint velocities (4.39)-(4.40) by a step-based update and include the restrictions (4.35) on  $p$  and  $\mu$ , this leads to the following backward time-stepping scheme with terminal condition

$$-p_N \in T_{\mathcal{K}_{\bar{K}_\tau}(\bar{y}_N)} \cap \{\bar{\lambda}_N\}^\perp \quad (4.41a)$$

$$\mu_N \in (T_{\mathcal{K}_{\bar{K}_\tau}(\bar{y}_N)} \cap \{\bar{\lambda}_N\}^\perp)^\circ \quad (4.41b)$$

$$(p_N, \psi)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(p_N, \psi) + \frac{\tau}{2} b(p_N, \psi) + \langle \mu_N, \psi \rangle_{\mathbf{H}_D^1} = - \langle \partial_{y_N} J_\tau(\bar{y}, \bar{u}), \psi \rangle_{\mathbf{H}_D^1} \quad (4.41c)$$

$$q_N = -\frac{2}{\tau} p_N \quad (4.41d)$$

and time steps for  $k = 1 \dots N - 1$

$$-p_k \in T_{\mathcal{K}_{\bar{K}_\tau}(\bar{y}_k)} \cap \{\bar{\lambda}_k\}^\perp \quad (4.42a)$$

$$\mu_k \in (T_{\mathcal{K}_{\bar{K}_\tau}(\bar{y}_k)} \cap \{\bar{\lambda}_k\}^\perp)^\circ \quad (4.42b)$$

$$\begin{aligned} (p_k, \varphi)_{\mathbf{L}^2} + \frac{\tau^2}{4} a(p_k, \varphi) + \frac{\tau}{2} b(p_k, \varphi) + \langle \mu_k, \varphi \rangle_{\mathbf{H}^1} &= (p_{k+1}, \varphi)_{\mathbf{L}^2} - \frac{\tau^2}{4} a(p_{k+1}, \varphi) + \frac{\tau}{2} b(p_{k+1}, \varphi) \\ &\quad - \tau (q_{k+1}, \varphi)_{\mathbf{L}^2} - \langle \partial_{y_k} J_\tau(\bar{y}, \bar{u}), \varphi \rangle_{\mathbf{H}^1} \end{aligned} \quad (4.42c)$$

$$q_k = -q_{k+1} + \frac{2}{\tau} (p_{k+1} - p_k) \quad (4.42d)$$

In the numerical implementation, this scheme is what will be solved in practice. Here

$$\bar{\lambda}_k = l_{k+1}(\bar{y}_0, \dots, \bar{y}_k, w) - Dy_{\bar{k}+1} \in T_{\bar{K}_\tau}(y_{\bar{k}+1})^\circ$$

as defined in (4.22b). The system decouples with respect to the values  $p_k, q_k$  and involves computing  $p_k$  from (4.42c) under the constraints (4.42a)-(4.42b), which has the structure of a variational inequality, due to the influence of the multiplier  $\mu$ . The value to  $q_k$  is then computed from an explicit update in (4.42d) and the same holds for the terminal condition.

**Adjoint boundary conditions.** It remains to give a more concrete interpretation of the relations (4.42a) and (4.42b) for  $k = 1 \dots N$  (thus including the case of terminal conditions). To this end let  $y \in Y_\tau$  and

$$\mathcal{A}_k = \{\omega \in \Gamma_C : y_k(\omega) \cdot \nu_\Phi(\omega) = \psi(\omega)\} \subset \Gamma_C$$

be the region of contact, defined up to sets of capacity 0 and  $\mathcal{S}_k \subset \mathcal{A}_k$  be the fine support of  $\bar{\lambda}_k$  (cf. e.g. [38, Lemma A.4]), which we call region of strong contact. We call the set  $\mathcal{W}_k = \mathcal{A}_k \setminus \mathcal{S}_k$ , where  $\bar{\lambda}_k = 0$ , region of weak contact.

In these terms,  $p_k \in T_{\mathcal{K}_{\bar{K}_\tau}(y_k)}$  can be interpreted with the help of [29, Lem. 3.2] and Lemma 4.10 (4), which yields

$$T_{\mathcal{K}_{\bar{K}_\tau}(y_k)} = \{\delta y \in \mathbf{H}_D^1 \mid \delta y \cdot \nu_\Phi \leq 0 \text{ q.e. on } \mathcal{A}_k\},$$

and thus

$$p_k \cdot \nu_\Phi \geq 0 \quad \text{q.e. on } \mathcal{A}_k.$$

Since additionally,  $p_k \in \{\bar{\lambda}_k\}^\perp$ , we have  $\langle \bar{\lambda}_k, p_k \rangle_{\mathbf{H}_D^1} = 0$ , and thus, since  $\langle \bar{\lambda}_k, \delta y \rangle_{\mathbf{H}_D^1} \geq 0$  for all  $\delta y$  with the property  $\delta y \cdot \nu_\Phi \geq 0$  and  $p_k \cdot \nu_\Phi \geq 0$  on  $\mathcal{A}_k$  the result

$$p_k \cdot \nu_\Phi = 0 \quad \text{q.e. on } \mathcal{S}_k$$

follows from the definition of the fine support. We thus have sliding boundary conditions for  $p_k$  on  $\mathcal{S}_k$  and unilateral contact conditions for  $p_k$  on  $\mathcal{A}_k$ . On  $\Gamma_C \setminus \mathcal{A}_k$ , there are no restrictions on  $p_k$ , so that we have homogeneous Neumann boundary conditions on this part of the boundary.

By duality, we obtain that the fine support of  $\mu_k$  is a subset of  $\mathcal{A}_k$ , and that  $\langle \mu_k, \delta y \rangle_{\mathbf{H}_D^1} \geq 0$  for all  $\delta y \in T_{\mathcal{K}_{\bar{K}_\tau}(y_k)}$  that vanish on  $\mathcal{S}_k$ . A ‘‘pointwise’’ interpretation would thus be as follows:  $\mu_k \cdot \nu_\Phi \geq 0$  on  $\mathcal{W}_k$  and  $\mu_k \cdot \nu_\Phi = 0$  on  $\bar{\Omega} \setminus \mathcal{A}_k$ . On  $\mathcal{S}_k$ , no sign restrictions on  $\mu_k$  apply.

Comparing these adjoint conditions on  $p_k$  and  $\mu_k$  with the complementarity conditions for  $y_k$  and  $\bar{\lambda}_k$  that come from the contact problem, we observe that instead of the complementarity condition  $\langle \bar{\lambda}_k, y_k \rangle = 0$  we only have  $\langle \mu_k, p_k \rangle_{\mathbf{H}_D^1} \geq 0$ . In particular, on  $\mathcal{W}_k$ ,  $p_k$  may be non-zero on subsets of the fine support of  $\mu_k$ . If, however  $\mathcal{W}_k$  has zero capacity, complementarity  $\langle \mu_k, p_k \rangle_{\mathbf{H}_D^1} = 0$  holds. Exploiting these relations, we can recapitulate our considerations by the following result:

**Theorem 4.26.** *The terminal condition (4.41a)-(4.41d) and each time step (4.42a)-(4.42d) have a solution  $(p_k, \mu_k)$ . If  $\mathcal{W}_k$  has zero capacity, this solution is unique, and the corresponding solution operator is linear.*

*Proof.* From the analysis of contact problems, we know that there is a unique solution  $(p_k, \mu_k)$  that additionally satisfies complementarity  $\langle \mu_k, p_k \rangle_{\mathbf{H}_D^1} = 0$ , but there may be others, for which  $\langle \mu_k, p_k \rangle_{\mathbf{H}_D^1} > 0$ . If  $\mathcal{W}_k$  has zero capacity, such solutions cannot occur, which yields uniqueness. In that case, the time-stepping problem is just a problem of linear elasticity with sliding boundary conditions on  $\mathcal{S}_k$  and Dirichlet conditions on the initial boundary segment  $\Gamma_D$ , i.e., a linear problem.  $\square$

**Relation to Crank-Nicolson Scheme.** Condition (4.42d) can be restated explicitly for  $p_k$  and from (4.42c) we can compute an expression for  $p_{k+1} - p_k$  that can be plugged into (4.42d). Combining the two resulting conditions, we obtain

$$(q_k, \varphi)_{\mathbf{L}^2} = (q_{k+1}, \varphi)_{\mathbf{L}^2} + \frac{\tau}{2} (a(p_{k+1}, \varphi) + a(p_k, \varphi) - b(q_k, \varphi) - b(q_{k+1}, \varphi)) + \frac{2}{\tau} \langle \mu_k, \varphi \rangle_{\mathbf{H}^1} + \frac{2}{\tau} \langle \partial_{y_k} J_\tau(\bar{y}, \bar{u}), \varphi \rangle_{\mathbf{H}^1} \quad (4.43a)$$

$$p_k = p_{k+1} - \frac{\tau}{2} (q_{k+1} + q_k) \quad (4.43b)$$

$$p_k \in T_{\mathcal{K}_{\bar{K}_\tau}}(y_k) \cap (\tilde{l}_k(w) - Dy_k)^\perp, \quad \mu_k \in (T_{\mathcal{K}_{\bar{K}_\tau}}(y_k) \cap (\tilde{l}_k(w) - Dy_k)^\perp)^\circ. \quad (4.43c)$$

Structurally, this resembles a reversed Crank-Nicolson scheme which is implicit in the multiplier  $\mu$ , cf. 3.2. The different signs on the viscosity part  $b: \mathbf{H}^1 \times \mathbf{H}^1 \mapsto \mathbb{R}$  and in the update match with the time reversal.

## 5 Numerics

This section is dedicated to the presentation of numerical results for a simple optimization scheme, based on the adjoint problem in Section 4.5.

We consider a problem of the type (4.18) with a linearly viscoelastic body in the shape of a half sphere of radius 15 m with a Kelvin-Voigt type response that comes into contact with a rigid plane on the time interval  $I = [0, 0.075 \text{ s}]$ , which equals 150 time steps of length  $\tau = 5e^{-5} \text{ s}$ . The body is considered to be at rest at time  $t = 0$  and homogeneous Dirichlet conditions are prescribed on the top section of the boundary while the contact boundary is assumed to lie within the middle third of the spherical boundary section.

Young's modulus and Poisson's ratio of the body's material were chosen to be  $E = 10^8 \text{ Pa}$ ,  $\nu = 0.3$  and viscosity bulk and shear modulus were taken as  $10^4 \text{ Pa}$ .

We search for minimizers to an approximation of the tracking type objective functional (4.2) where the reference control is taken to act on the whole domain in all of  $I$ . A desired state  $y_d$  was computed as solution of the variational inequality (4.21) to the temporally and spatially constant force  $w = B_\tau u_{\text{ref}}$  with the reference control  $u_{\text{ref}} \in U_\tau$  being

$$u_{\text{ref}} = u_{\text{const}}^N,$$

where  $u_{\text{const}} \in \mathbf{L}^2$  and

$$u_{\text{const}}(\omega) = ue_n, \\ u \in \mathbb{R}^n$$

for the  $n^{\text{th}}$  normal vector  $e_n$ , resulting in a bouncing motion of the ball with contact being established and released several times, where the viscose part has a damping effect on the motion of the body.

We chose the Tychonoff parameter to be  $\alpha = 10^{-2}$ . The control  $u$  was of first order of magnitude and was scaled by  $10^6 \text{ N/m}^2$  when entering the right hand side as a force distribution in order to avoid handling controls with high order magnitudes, which would lead to very small Tychonoff parameters and poor optimizer behavior in the first iterations, especially w.r.t. the scaling of descent directions.

This amounts to the optimal control problem

$$\begin{aligned} \min J_\tau(y, u) &= \frac{1}{2}\tau \sum_{k=1}^N \frac{1}{2} (\|y_{k-1} - y_{d,k-1}\|_{\mathbf{L}^2}^2 + \|y_k - y_{d,k}\|_{\mathbf{L}^2}^2) + \frac{\alpha}{2}\tau \sum_{k=1}^N \|u_k\|_{\mathbf{L}^2}^2 \\ \text{s.t. } (y, u) &\in Y_\tau \times U_\tau \\ y &\in K_\tau = \{y \in Y_\tau \mid y_{(n)}(\omega) \geq -\omega_{(n)} \text{ a.e. on } \Gamma_C\} \\ B_\tau u + f_\tau - A_\tau y &\in T_{K_\tau}(y)^\circ \end{aligned}$$

The proposed algorithm to finding minimizers is based on an iterative procedure in the framework of [31], where a one dimensional search space, i.e. the descent direction, is computed from the stationarity condition stated in Theorem 4.25 and appropriate stepsize control factors are calculated based on a quadratic regularization technique.

Our implementation is based on the Distributed and Unified Numerics Environment (DUNE) [5, 4, 6] and the finite element toolbox Kaskade 7.2 [15].

For the numerical treatment, we extend the time discretization to a full discretization with a P1 nodal basis for a spatial triangulation of the domain  $\Omega \subset \mathbb{R}^2$ . The resulting time-independent variational inequalities (4.22) in each of the time steps have been solved by a monotone multigrid solver [25] with (projected) block Gauß-Seidel schemes being used as base solver and smoothers. No weak contact occurred in the forward problems of our setting and therefore no additional treatment was required.

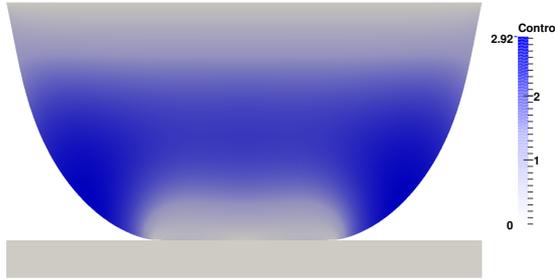


Fig. 5 Magnitude of control at  $t = 0.0013 \text{ s}$

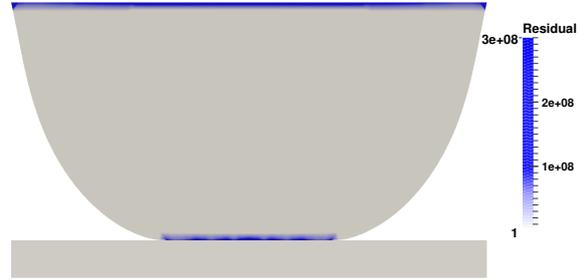


Fig. 6 Magnitude of residual at  $t = 0.0013 \text{ s}$

In this example, the stationarity condition (4.34) requires  $u = \frac{1}{\alpha}p$  and the adjoint state  $p$  has sliding boundary conditions and homogeneous Dirichlet conditions on the sections of active contact and the Dirichlet boundary section, respectively. Therefore, any minimizing control to the problem necessarily will have no input on the Dirichlet boundary patch and no input in y-direction on active contact patches. Fig. 5 shows that the resulting control is being reduced to values close to zero where contact is active and where the body is clamped by the Dirichlet conditions, as expected. The symmetry of the problem is responsible for the entire control being reduced to zero on the contact patch, instead of only its y-component. Over the course of the algorithm, the distance of the iterates to the reference control decreases at first and starts increasing again after the first 200 iterations, see Fig. 8. From 200 iterations on, the Tychonoff term in the costfunctional becomes increasingly relevant.

Fig. 6 shows the residual of the variational inequality at  $t = 0.0013 \text{ s}$ . The residual can be interpreted as the forces acting on the body upon restriction, i.e. Dirichlet or contact conditions. The development of the functional value during the iteration is shown in Fig. 7 as the difference of the current iterate's value and the functional value of the resulting control after 1000 iterations and behaves close to linearly.

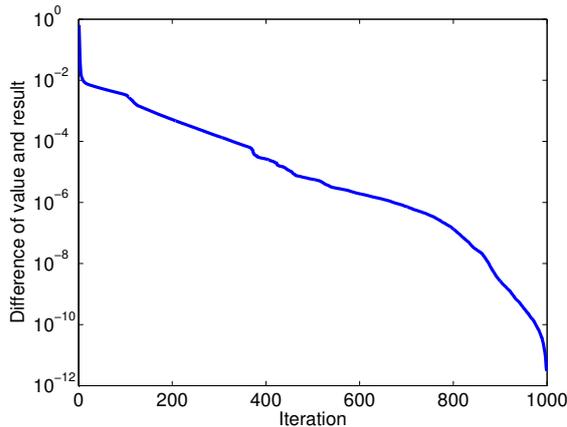


Fig. 7 Functional values

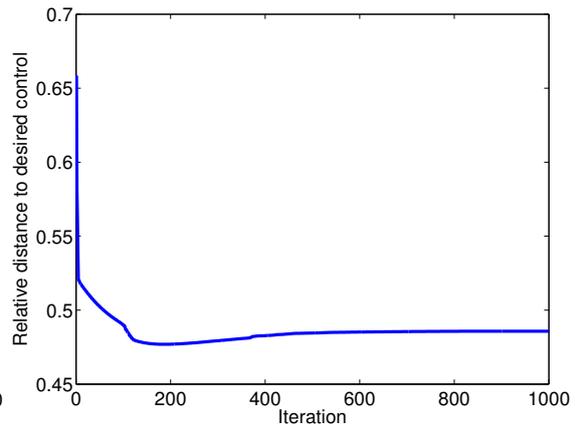


Fig. 8 Relative distance to reference control

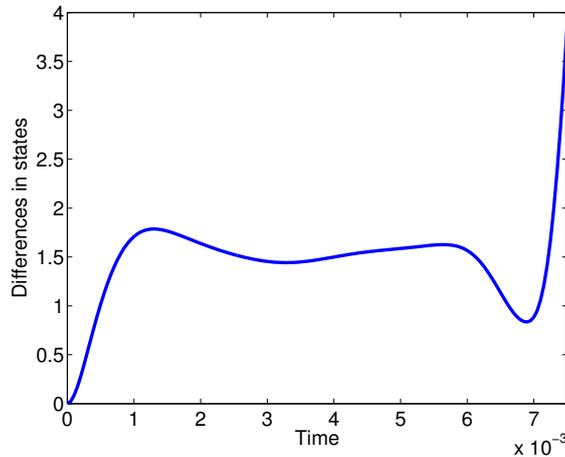


Fig. 9 Difference of result state and desired state over time

At times close to the endpoint  $T = 0.075$  s, there is a notable difference between the desired state and the result state, as shown in Fig. 9, which can be attributed to all adjoint states having close to zero terminal conditions, c.f. (4.37), because the continuous cost functional does not involve a final time observation.

## 6 Conclusion and Outlook

In this work, some steps towards the optimal control of dynamic contact problems, particularly in finding numerical solutions, have been taken. While the lack of theoretical understanding of the forward problem currently impedes a rigorous analysis of the optimal control problem in the time continuous case, we were able to establish a satisfactory theory for the time-discretized case.

Key to this analysis and to the numerical solution was the construction of a finite element method in time that represents a variant of the contact implicit Newmark scheme due to Kane et. al. For this discretization, we were able to extend the results of Mignot on strong stationarity from the scalar valued stationary case to the vector valued time-sequential case. Key ideas were the study of inheritance of polyhedricity under linear mappings and the use of Hadamard differentiability. A further extension to the time continuous case seems to be a very difficult, but also rewarding task. The straightforward idea of passing to the limit for  $\tau \rightarrow 0$  involves severe mathematical difficulties.

A major aim of our analysis was the derivation of a time discrete adjoint equation, that can be evaluated numerically by a backward time-stepping scheme. This is the foundation for our gradient

based algorithm, which enabled us to numerically solve an optimal control problem subject to time discretized dynamic contact. Up to now, this algorithm relies on the circumstance that the non-smoothness due to weak contact plays a minor role in the examples, considered so far. It is subject to current research to extend this algorithm to situations, where the effects of non-smoothness are more severe.

Up to now, the applied model is only valid for small deformations and thus only for small movements of the elastic body. For practical applications, an extension to larger movements, like rotations, which is often done by factoring out rigid body motions, will be necessary. While things become more involved numerically and notationally, we conjecture that our theoretical findings will carry over to that case. The treatment of dynamic contact in the context of finite strains, where the difficulties of nonlinear elasticity and dynamic contact merge, is a lot more demanding. The optimal control of such problems will certainly require a major research effort in the future.

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