

A semiderivative approach for shape optimization problems constrained by variational inequalities

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Abstract

Shape optimization problems constrained by variational inequalities (VI) are non-smooth and non-convex optimization problems. The non-smoothness arises due to the variational inequality constraint, which makes it challenging to derive optimality conditions. Besides the non-smoothness there are complementary aspects due to the VIs as well as distributed, non-linear, non-convex and infinite-dimensional aspects due to the shapes which complicate to set up an optimality system and, thus, to develop efficient solution algorithms. In this paper, we consider the Hadamard semiderivative in order to formulate optimality conditions. In this context, we set up a Hadamard shape semiderivative approach and demonstrate its advantages over an proposed approach based on regularizations.

Key words. Hadamard semiderivative, variational inequality, shape optimization, material derivative, shape derivative, optimality conditions

AMS subject classifications. 49Q10, 49J40, 35Q93, 65K15

1 Introduction

Optimal control problems with constraints in the form of variational inequalities (VI) are challenging, since classical constraint qualifications for deriving Lagrange multipliers generally fail. Therefore, not only the development of stable numerical solution schemes but also the development of suitable first order optimality conditions is an issue. By usage of tools of modern analysis, such as monotone operators in Banach spaces, significant results on properties of the solution operator of variational inequalities have been achieved since the 1960s (cf. [6, 7, 33]). Comprehensive studies of variational inequalities and more references can be found in [17, 28, 29, 46]. The generic non-smoothness and non-convexity in the feasible set described by variational inequalities causes difficulties already in finite dimensional versions of the problem. In fact, finite dimensional bilevel optimization (i.e., optimization with optimization problems in the constraints) is its own field of research since the 1970s (cf., e.g., [5]) and has been generalized to mathematical programming with equilibrium constraints (MPECs) for the optimization of stationary systems of constrained problems in [18]. For a survey on bilevel programming and MPECs see,

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e.g., [37]. In [47], the authors concentrate on the typical complementarity structure of variational inequalities and derive a hierarchy of stationarity concepts (depending on constraint qualification conditions) for the more general problem class of mathematical programs with complementarity constraints (MPCCs). During the last decade, these concepts have partly been transferred to respective concepts in function space in [21, 22, 23]. The optimal control of variational inequalities that are posed in function space has been studied since the 1970s and necessary stationary conditions have been derived by use of penalty and smoothing techniques and strengthened by the usage of instruments from convex analysis and differentiability, see, e.g., [2, 40, 44]. The conditions that a solution can be shown to verify have a complex structure and the problem to find candidates for solutions leads to a system of non-linear and non-smooth equations. This demands for the development of numerical algorithms and a proper mathematical analysis on their convergence behavior, see, e.g., the discussion in [30, 45].

In this paper, we consider shape optimization problems constrained by variational inequalities. These problems are non-smooth and non-convex optimization problems. The non-smoothness arises due to the variational inequality constraint, which makes it challenging to derive optimality conditions. Moreover, besides the non-smoothness there are complementary aspects due to the VIs as well as distributed, non-linear, non-convex and infinite dimensional aspects due to the shapes which complicate to set up an optimality system. In particular, one cannot expect for an arbitrary shape functional depending on solutions to VIs the existence of the shape derivative or to obtain the shape derivative as a linear mapping. In addition, the adjoint state can generally not be introduced and, thus, an optimality system cannot be set up. In this paper, we consider Hadamard semiderivatives instead of classical derivatives in order to formulate optimality conditions. As noted in [9], the Delfour-Zolesio approach of using Hadamard semiderivatives for evaluating shape sensitivities does not seem fully exploited so far. Thus, this paper aims at using it in order to obtain expressions for shape derivatives in the context of VI, which are computationally easier accessible.

So far, there are only very few approaches in the literature to the problem class of VI constrained shape optimization problems. In [31], shape optimization of 2D elasto-plastic bodies is studied, where the shape is simplified to a graph such that one dimension can be written as a function of the other. In [49, Chap. 4], shape derivatives of elliptic variational inequality problems are presented in the form of solutions to again variational inequalities. In [41], shape optimization for 2D graph-like domains are investigated. Also [34, 35] present existence results for shape optimization problems which can be reformulated as optimal control problems, whereas [14, 16] show existence of solutions in a more general set-up. In [42, 43], level-set methods are proposed and applied to graph-like two-dimensional problems. Moreover, [24] presents a regularization approach to the computation of shape and topological derivatives in the context of elliptic variational inequalities and, thus, circumventing the numerical problems in [49, Chap. 4]. In [19], the analysis of state material derivatives is significantly refined over [49, Chap. 4]. All these mentioned problems have in common that one cannot expect for an arbitrary shape functional depending on solutions to VIs to obtain the shape derivative as a linear mapping (cf. [49, Example in Chap. 1]). In general, the shape derivative for the obstacle problems fails to be linear with respect to the normal component of the vector field defined on the boundary of the open domain under consideration. In order to circumvent the problems related to the non-linearity of the shape derivative and in particular the non-existence of the shape derivative of a VI constrained shape optimization problem, this paper uses a Hadamard (shape) semiderivative approach in shape spaces. This could also open the door for formulating higher order optimization methods in shape spaces. With the help of a Hadamard se-

miderivative approach, VI constrained shape optimization problems which are not shape differentiable in the classical sense can be handled and solved without any regularization techniques.

This paper is structured as follows. In section 2, we recall and enhance a Hadamard semiderivative framework for non-smooth shape optimization problems. In particular, we define a Hadamard material semiderivative and also a Hadamard shape semiderivative. The developed framework allows the formulation of optimality conditions to VI constrained shape optimization problems in section 3. Finally, we apply the Hadamard shape semiderivative framework to a shape optimization problem constrained by VIs of first kind in section 4. More precisely, based on the Hadamard semiderivative framework of section 2 we set up the optimality system of section 3 for the obstacle-type problem.

2 Hadamard semiderivative

A main focus in shape optimization is in the investigation of shape functionals. A shape functional on an arbitrary shape space¹ \mathcal{U} is given by a function $J: \mathcal{U} \rightarrow \mathbb{R}$, $\Omega \mapsto J(\Omega)$. In general, a shape optimization problem can be formulated by

$$\min_{\Omega \in \mathcal{U}} J(\Omega). \quad (2.1)$$

Often, shape optimization problems are constrained by equations, e.g., equations involving an unknown function of two or more variables and at least one partial derivative of this function. The objective may depend on not only the shape u but also the state variable y , where the state variable is the solution of the underlying constraint. We concentrate on constraints in the form of variational inequalities in this paper. These problems are in particular highly challenging because one cannot expect for an arbitrary shape functional depending on solutions to VIs the existence of the adjoint and of the shape derivative or to obtain the shape derivative as a linear mapping.

In this section, we consider Hadamard semiderivatives instead of classical derivatives in order to be able to formulate optimality conditions in section 3.

We start by recalling the concept of a Hadamard semiderivative and its necessary rules in subsection 2.1, which ends in formulating necessary conditions of optimality for Hadamard semidifferentiable objective functions (cf. theorem 2.5). In subsection 2.2, we concentrate on shape optimization and extend the Hadamard semiderivative concepts to shape calculus.

2.1 Hadamard semiderivative

In this subsection, we first define Hadamard semiderivative and formulate some rules like the chain and product rule. Then we consider a simple example of importance for later discussions on variational inequalities.

We follow [12, 13] for the definition of the Hadamard semi-differential. Therefore, an admissible semitrajectory at x in a topological vector space X is a function $h: [0, \tau) \rightarrow X$, for some $\tau > 0$, such that

$$h(0) = x \quad \text{and} \quad h'(0^+) \stackrel{\text{def}}{=} \lim_{t \searrow 0} \frac{h(t) - h(0)}{t} \text{ exists in } X,$$

¹Various shapes spaces have been extensively studied in recent decades. In [27], a shape space is just modeled as a linear (vector) space, which in the simplest case is made up of vectors of landmark positions. However, there is a large number of different shape concepts, e.g., plane curves [39], surfaces in higher dimensions [3, 38], boundary contours of objects [32, 53], multiphase objects [52], characteristic functions of measurable sets [54], morphologies of images [15], and planar triangular meshes [20]. The choice of the shape space depends on the demands in a given situation. There exists no common shape space suitable for all applications.

where $h'(0^+)$ is the semitangent to the trajectory h at $h(0) = x$.

Definition 2.1. Let X and Y be topological vector spaces and $f: X \rightarrow Y$.

1. f is Hadamard semidifferentiable at $x \in X$ in the direction $v \in X$ if there exists $d_H f(x)[v] \in Y$ such that for all admissible semitrajectories h in X at x with $h'(0^+) = v$, we have

$$(f \circ h)'(0^+) \stackrel{\text{def}}{=} \lim_{t \searrow 0} \frac{(f \circ h)(t) - (f \circ h)(0)}{t} = d_H f(x)[v].$$

2. f is Hadamard semidifferentiable at $x \in X$ if there exists a function $v \mapsto d_H f(x)[v]: X \rightarrow Y$ such that for each admissible semitrajectory h in X at x , $(f \circ h)'(0^+)$ exists and $(f \circ h)'(0^+) = d_H f(x)[h'(0^+)]$.
3. f is Hadamard differentiable at $x \in X$ if f is Hadamard semidifferentiable at x and the function $v \mapsto Df(x)v \stackrel{\text{def}}{=} d_H f(x)[v]: X \rightarrow Y$ is linear.

For the Hadamard semiderivative, we have all the properties of the classical finite dimensional differential calculus including the chain rule (cf. [12]).

Lemma 2.2. Let X and Y be topological vector spaces and $f: X \rightarrow Y$ a function.

1. If f is Hadamard semidifferentiable at x , then $v \mapsto d_H f(x)[v]: X \rightarrow Y$ is positively homogeneous and sequentially continuous.
2. If f_1 and f_2 are Hadamard semidifferentiable at $x \in X$ in the direction $v \in X$, then for all α and β in \mathbb{R} ,

$$d_H(\alpha f_1 + \beta f_2)(x)[v] = \alpha d_H f_1(x)[v] + \beta d_H f_2(x)[v].$$

(iii) (Chain rule) Let X, Y, Z be topological vector spaces, $g: X \rightarrow Y$ and $f: Y \rightarrow Z$ be functions such as g is Hadamard semidifferentiable at x in the direction $v \in X$ and f is Hadamard semidifferentiable at $g(x)$ in the direction $d_H g(x; v)$. Then $f \circ g$ is Hadamard semidifferentiable at x in the direction $v \in X$ and

$$d_H(f \circ g)(x)[v] = d_H f(g(x)) [d_H g(x)[v]].$$

Remark 2.3. As for the finite dimensional differential calculus, the chain rule for the Hadamard semiderivative provides a product rule for the Hadamard semiderivative.

For later use, we give an example.

Example 2.4. Let $F(x) := \max\{0, x\}$ with $x \in \mathbb{R}$. The Hadamard semiderivative $d_H F(x)[v]$ of F at x in direction v is given by

$$d_H F(x)[v] = \begin{cases} v, & x > 0, \\ \max\{0, v\}, & x = 0, \\ 0, & x < 0. \end{cases} \quad (2.2)$$

This can be easily validated by following the definition of the Hadamard semiderivative and using the continuity of $\max\{0, x\}$:

$$\begin{aligned} d_H F(x)[v] &= \lim_{t \searrow 0} \frac{\max\{0, h(t)\} - \max\{0, h(0)\}}{t} \\ &= \begin{cases} 0, & x < 0 \\ \lim_{t \searrow 0} \frac{h(t) - h(0)}{t} = h'(0^+) = v, & x > 0 \\ \lim_{t \searrow 0} \frac{\max\{0, h(t)\} - 0}{t} = \max\left\{0, \lim_{t \searrow 0} \frac{h(t) - h(0)}{t}\right\} = \max\{0, v\}, & x = 0 \end{cases} \end{aligned}$$

Next, we consider an optimization problem in the following form:

$$\min_{x \in X} J(x), \quad (2.3)$$

where X is a Banach space and $J: X \rightarrow \mathbb{R}$ is assumed to be Hadamard semidifferentiable. Following standard reasoning, now we can formulate necessary conditions of optimality for the optimization problem (2.3).

Theorem 2.5. *We assume that the function $J: X \rightarrow \mathbb{R}$, where X is a Banach space, is Hadamard semidifferentiable and that $\hat{x} \in X$ is a local minimum of J . Then, there holds*

$$d_H J(\hat{x})[v] \geq 0 \quad \forall v \in X.$$

Proof. Due to the fact that \hat{x} is the minimum, there holds $J(z) \geq J(\hat{x})$, for all $z \in X$. We choose in particular $z := \hat{x} + tv$ for an arbitrary $v \in X$ and $t > 0$. From this, we conclude

$$\frac{1}{t} (J(\hat{x} + tv) - J(\hat{x})) \geq 0,$$

and thus we obtain the assertion by using the definition of the the Hadamard semiderivative. \square

2.2 Hadamard shape derivative calculus

In this subsection, we concentrate on shape optimization and extend the Hadamard semiderivative concepts from subsection 2.1 to shape calculus. For a detailed introduction into classical shape calculus, the reader is referred to the monographs [11, 49].

We define shapes Ω as open (Lebesgue-)measurable subdomains of an open hold-all domain $D \subset \mathbb{R}^n$ in the following. In addition, we consider a family $\{F_t\}_{t \in [0, T]}$ of mappings $F_t: \overline{D} \rightarrow \mathbb{R}^n$ such that $F_0 = \text{id}$, where \overline{D} denotes the closure of D and $T > 0$. This family transforms shapes Ω into new perturbed shapes

$$F_t(\Omega) = \{F_t(x) : x \in \Omega\}.$$

Such a transformation can be described by the *velocity method* or by the *perturbation of identity*; cf. [49, pages 45 and 49]. In the following, the perturbation of identity is considered. It is defined by $F_t = F_t(V) := \text{id} + tV$, where $V: \overline{D} \rightarrow \mathbb{R}^n$ denotes a sufficiently smooth vector field. In this setting, we recall the Hadamard shape semiderivative of a shape function as described in [11, Section 3.2] in our notation.

Definition 2.6 (Hadamard shape semiderivative). *Let $J: \Omega \mapsto \mathbb{R}$ be a shape functional. We consider all admissible families F_t of mappings with $F_0 = \text{id}$ and $F'_0 = V$ as semitrajectories in the space of mappings $\overline{D} \rightarrow \overline{D}$, such that $J \circ F_t(\Omega)$ evaluates the shape objective at the perturbed shape $F_t(\Omega)$ and the Hadamard derivative $d_H(J)[V]$ is a mapping acting on shapes. Then, we define the Hadamard shape semiderivative as the Hadamard semiderivative of J with the notation $D_H J(\Omega)[V] := d_H(J)[V](\Omega) = \lim_{\substack{F_0=V \\ t \rightarrow 0^+}} \frac{1}{t} (J \circ F_t(\Omega) - J \circ F_0(\Omega)).$*

With this, we define the Hadamard shape and material semiderivative analogously to the classical material derivative.

Definition 2.7 (Hadamard shape and material semiderivative). *Let $\{g_t: \Omega \rightarrow \mathbb{R} : t \leq T\}$ denote a family of mappings and $g(= g_0): \Omega \rightarrow \mathbb{R}$, which is Hadamard*

semidifferentiable in t at 0^+ . We define the Hadamard shape semiderivative $D_{Hs}g(\Omega)[V]$ at Ω in direction V as a directional derivative, i.e.,

$$D_{Hs}g(\Omega)[V] := \lim_{t \rightarrow 0^+} \frac{1}{t} (g_t(\Omega) - g_0(\Omega))$$

and the Hadamard material semiderivative by

$$D_{Hm}g(\Omega)[V] := D_{Hs}g(\Omega)[V] + d_Hg[V] = \lim_{\substack{F_0=V \\ t \rightarrow 0^+}} \frac{1}{t} (g_t \circ F_t(\Omega) - g_0 \circ F_0(\Omega)) .$$

Next, we formulate Hadamard material semiderivative rules, which are generalizations of the results in [4] regarding the material derivative.

Lemma 2.8. *Let $g, q: \Omega \rightarrow \mathbb{R}$ denote two functions that are Hadamard material semidifferentiable.*

(i) *For the Hadamard material semiderivative the product rule holds, i.e.,*

$$D_{Hm}(gq) = D_{Hm}gq + gD_{Hm}q.$$

(ii) *Let V_j denote the j th component of V . In case that g be Hadamard shape semidifferentiable the following equality holds:*

$$D_{Hm}(\partial_i^H g) = \partial_i^H D_{Hm}(g) - \sum_{j=1}^n \partial_j^H g \partial_i^H V_j \quad \text{for } i = 1, \dots, n,$$

which is equivalent to

$$D_{Hm}D_Hg = D_HD_{Hm}g - D_HV^\top D_Hg.$$

(iii) *If g and q are Hadamard shape semidifferentiable the following equality holds:*

$$\begin{aligned} & D_{Hm}(D_Hq^\top D_Hg) \\ &= D_Hg^\top D_HD_{Hm}q - D_Hg^\top (D_HV + D_HV^\top) D_Hq + D_Hq^\top D_HD_{Hm}g \end{aligned}$$

Proof. (i) This holds because the product rule holds for both parts of the sum defining the Hadamard material semiderivative in Definition 2.7 .

(ii) Definition 2.7 gives

$$D_{Hm}g = \lim_{t \searrow 0} \frac{g_t \circ F_t - g}{t}.$$

Therefore, we have

$$\partial_i^H D_{Hm}g = \partial_i^H \lim_{t \searrow 0} \frac{g_t \circ F_t - g}{t}$$

for $i = 1, \dots, n$. We can use the Moore-Osgood theorem to obtain

$$\partial_i^H D_{Hm}g = \lim_{t \searrow 0} \frac{\partial_i^H (g_t \circ F_t) - \partial_i^H g}{t}.$$

Let $\delta_{i,j}$ denote the Kronecker delta. The (multi-valued) chain rule leads to

$$\begin{aligned}
\partial_i^H D_{Hm} g &= \lim_{t \searrow 0} \frac{\partial_i^H (g_t \circ F_t) - \partial_i^H g}{t} \\
&= \lim_{t \searrow 0} \frac{\sum_{j=1}^n ((\partial_j^H g_t \circ F_t) \partial_i^H F_t) - \partial_i^H g}{t} \\
&= \lim_{t \searrow 0} \frac{\sum_{j=1}^n ((\partial_j^H g_t \circ F_t) (\delta_{i,j} + t \partial_i^H V_j)) - \partial_i^H g}{t} \\
&= \lim_{t \searrow 0} \frac{\sum_{j=1}^n ((\partial_j^H g_t \circ F_t) \delta_{i,j} + (\partial_j^H g_t \circ F_t) t \partial_i^H V_j) - \partial_i^H g}{t} \\
&= \lim_{t \searrow 0} \frac{(\partial_i^H g_t \circ F_t) + \sum_{j=1}^n ((\partial_j^H g_t \circ F_t) t \partial_i^H V_j) - \partial_i^H g}{t}
\end{aligned}$$

and, thus, to

$$D_{Hm}(\partial_i^H g) = \partial_i^H D_{Hg} - \sum_{j=1}^n (\partial_j^H g \partial_i^H V_j)$$

for $i = 1, \dots, n$.

- (iii) The combination of the product rule in (i) together with equality in (ii) proofs the claim. \square

As already mentioned above, shape optimization problems are often constrained by partial differential equations. Thus, we provide the following lemma which we apply in section 4 to get the Hadamard shape semiderivative expression of the considered shape optimization problem.

Lemma 2.9. *Let assumptions and notation be as in lemma 2.8. Given coefficient functions $a_{i,j}, d_j, b \in L^\infty(\Omega)$ of a strongly elliptic bilinear form² that fulfill the weak maximum principle, the following equality holds:*

$$\begin{aligned}
&D_{Hm} \left(\sum_{i,j=1}^n a_{i,j} \partial_i^H g \partial_j^H q + \sum_{i=1}^n d_i (\partial_i^H g q + g \partial_i^H q) + b g q \right) \\
&= \sum_{i,j=1}^n a_{i,j} \left(\left(\partial_i^H D_{Hm} g - \sum_{l=1}^n \partial_l^H g \partial_i^H V_l \right) \partial_j^H q \right. \\
&\quad \left. + \partial_i^H g \left(\partial_j^H D_{Hm} q - \sum_{l=1}^n (\partial_l^H q \partial_j^H V_l) \right) \right) \\
&\quad + \sum_{i=1}^n d_i \left(\left(\partial_i^H D_{Hm} g - \sum_{l=1}^n \partial_l^H g \partial_i^H V_l \right) q + \partial_i^H g D_{Hm} q + D_{Hm} g \partial_i^H q \right. \\
&\quad \left. + g \left(\partial_i^H D_{Hm} q - \sum_{l=1}^n \partial_l^H q \partial_i^H V_l \right) \right) \\
&\quad + b (D_{Hm} g q + g D_{Hm} q)
\end{aligned}$$

Proof. The combination of the product rule in lemma 2.8 (i) together with equality in lemma 2.8 (ii) proofs the claim. \square

²Such a bilinear form is defined in (4.5).

Next, we formulate a Hadamard shape semiderivative formula. For this purpose, we need to consider perturbed objective functions due to definition 2.6.

Lemma 2.10. *Let the family F_t of transformations be differentiable in the usual sense. We define the domain integral $J(\Omega) = \int_{\Omega} g \, dx$ for a function $g: \Omega \rightarrow \mathbb{R}$. Then, we have*

$$D_H J(\Omega)[V] = \int_{\Omega} D_{Hm} g + \operatorname{div} V g \, dx.$$

Proof. A straight forward calculation like in the proof of [51, Theorem 4.11] using common analysis, the product rule as well as definition 2.7 gives the result. \square

3 Hadamard optimality system

In this section, we focus on necessary optimality conditions for non-smooth shape optimization problems. In theorem 2.5, we observe that the Hadamard (shape) semiderivative can be used to characterize necessary optimality conditions. We consider constrained shape optimization problems of the following form:

$$\min_{\Omega \in \mathcal{U}} J(\Omega, y) \tag{3.1}$$

$$\text{s.t. } b(c(\Omega, y), p)_{\Omega} = 0 \quad \forall p \in \mathcal{H}(\Omega) \tag{3.2}$$

Here, $\mathcal{H}(\Omega)$ is a Hilbert space defined on the shape Ω containing the state variable $y \in \mathcal{H}(\Omega)$ and $b(\cdot, \cdot)_{\Omega}$ is a bilinear and in $\mathcal{H}(\Omega)$ a coercive form. Moreover, \mathcal{U} is the set of admissible shapes, i.e., an appropriate shape space. In this section, we follow the linear deformation space framework as investigated in [48], i.e., we consider a space Y as an appropriate vector space of deformations, such that the set \mathcal{U} of admissible shapes Ω is constructed as $\mathcal{S}^{\text{adm}} = \{W(\Omega^0): W \in Y\}$, where Ω^0 is a reference starting domain, which is assumed to be a subset of the open hold-all domain D . We assume that the mapping c is Hadamard semidifferentiable, and that the constraint (3.2) defines a unique solution $y(\Omega, f)$ on any shape Ω under consideration.

Because $y(\Omega)$ is assumed to satisfy the constraint, we may write for arbitrary $p(\Omega) \in \mathcal{H}(\Omega)$

$$J(\Omega, y(\Omega)) = J(\Omega, y(\Omega)) + b(c(\Omega, y(\Omega)), p(\Omega))_{\Omega}.$$

In order to derive necessary conditions of optimality, we differentiate the right-hand side with respect to Ω and simplify the expressions by introducing the notation

$$\mathcal{L}(\Omega, y, p) := J(\Omega, y) + b(c(\Omega, y), p)_{\Omega},$$

where we keep in mind the implicit dependence of y, p on Ω . Thus, the chain rule yields

$$D_H \mathcal{L}(\Omega, y, p)[V] = \partial_1^H \mathcal{L}(\Omega, y, p)[V] + \partial_2^H \mathcal{L}(\Omega, y, p) D_{Hm} y + \partial_3^H \mathcal{L}(\Omega, y, p) D_{Hm} p$$

for all $V \in Y$, where ∂_i^H denote the Hadamard partial semiderivative with respect to the i -th argument ($i \in \{1, 2, 3\}$).

Since y satisfies the state equation (3.2) in variational form, which is linear in p , we observe

$$\partial_3^H \mathcal{L}(\Omega, y, p) D_{Hm} p = 0. \tag{3.3}$$

Furthermore, we obtain

$$\partial_2^H \mathcal{L}(\Omega, y, p) D_{Hm} y = \partial_2^H J(\Omega, y) D_{Hm} y + b(\partial_2^H c(\Omega, y) D_{Hm} y, p)_{\Omega}$$

and, thus, we may obtain p from the Hadamard adjoint equation in variational form:

$$\partial_2^H J(\Omega, y) \tilde{y} + b(\partial_2^H c(\Omega, y) \tilde{y}, p)_\Omega = 0 \quad \forall \tilde{y} \in \mathcal{H}(\Omega) \quad (3.4)$$

The solvability of the Hadamard adjoint equation is in question in this rather general set-up. Therefore, we take it for granted now and show solvability, when confronted with a particular model problem as in the next section. Now, if y satisfies the state equation (3.2) and p satisfies the Hadamard adjoint equation (3.4), then the Hadamard shape semiderivative is given by

$$D_H \mathcal{L}(\Omega, y, p)[V] = \partial_1^H \mathcal{L}(\Omega, y, p)[V].$$

Nevertheless, it is a manually easier way to compute the Hadamard shape semiderivative of the full Lagrangian by employing shape and Hadamard calculus and later on eliminate expressions relating to the state and Hadamard adjoint equation, as exemplified in the next section. From Theorem 2.5, we conclude now the necessary condition of optimality for an optimal shape Ω as

$$\lim_{t \searrow 0} D_H \mathcal{L}((\text{id} + tV)(\Omega), y, p)[V] \geq 0 \quad \forall V \in Y, \quad (3.5)$$

where y satisfies the state equation (3.2) and p satisfies the Hadamard adjoint equation (3.4).

In many cases, as is demonstrated in the next section, the Hadamard shape semiderivative is continuous in $t \searrow 0$, although the constraints of the shape optimization problem are only semismooth. Then, the necessary condition is just the usual homogeneity of the shape derivative. In this case, the (Hadamard) shape (semi)derivative can be used in order to define a descent direction for algorithmical purposes. Nevertheless, finding a descent direction from the Hadamard semiderivative is a challenge in general.

In the next section, we study weak formulations of elliptic problems. These are typically formulated in the Sobolev space $H^1(\Omega)$ of weakly differentiable L^2 -functions. For the standard elliptic heat-equation-type problem, the solution is mostly in $H^2(\Omega) \subset H^1(\Omega)$ and, thus, their material derivative again in $H^1(\Omega)$ due to Definition

2.7. However, in the context of variational inequalities, the solution is only piecewise $H^2(\Omega)$, which means that material derivatives cannot be used as test functions like in (3.3). A similar problem arises in discontinuous Galerkin approximations, from where we borrow the notion of a “broken” Sobolev space here, which is analyzed in detail in [8]. This concept is based on a disjoint partitioning Ω_h of open subsets $\mathcal{K} \subset \Omega$ with Lipschitz boundaries such that $\overline{\cup_{\mathcal{K} \in \Omega_h} \mathcal{K}} = \Omega$. Then one defines

$$H^1(\Omega_h) := \{\Omega \in L^2(\Omega) : \Omega|_{\mathcal{K}} \in H^1(\mathcal{K}), \mathcal{K} \in \Omega_h\}$$

In [8], this space is used as test space and shown that a resulting weak formulation of the standard elliptic problem exists which inherits stability and, thus, existence of a unique solution. Thus, we mean this more general weak formulation in the following, whenever a test function is used, which is only piecewise H^1 .

4 Application of the Hadamard semiderivative approach

We consider a tracking-type shape optimization problem constrained by a variational inequality of the first kind, a so-called obstacle-type problem. Applications are manifold and arise, whenever a shape is to be constructed in a way not to violate constraints for the state solutions of partial differential equation depending on

a geometry to be optimized. Just think of a heat equation depending on a shape, where the temperature is not allowed to surpass a certain threshold. This example is basically the model problem already considered in [36] and that we are formulating in the following. In contrast to [36], which formulates an optimization approach based on the convergence of state, adjoint and shape derivative of the regularized problem to limit objects, we do not consider regularized versions of the VI. We apply the Hadamard semiderivative approach discussed above to the model problem and are able to formulate the optimality system. We will see that this system is in line with the limit objects of [36].

Problem class. Let $\mathcal{X} \subset \mathbb{R}^n$ be an open bounded domain equipped with a sufficiently smooth boundary $\partial\mathcal{X}$. This domain is assumed to be partitioned in an open subdomain $\mathcal{X}_{\text{out}} \subset \mathcal{X}$ and an open interior domain $\mathcal{X}_{\text{int}} \subset \mathcal{X}$ with boundary $\Gamma := \partial\mathcal{X}_{\text{int}}$ such that $\mathcal{X}_{\text{out}} \sqcup \Gamma \sqcup \mathcal{X}_{\text{int}} = \mathcal{X}$, where \sqcup denotes the disjoint union. The closure of \mathcal{X} is denoted by $\bar{\mathcal{X}}$. We consider \mathcal{X} depending on Γ , i.e., $\mathcal{X} = \mathcal{X}(\Gamma)$. In the following, the boundary Γ of the interior domain is called the *interface*. In the setting above, the shape Ω is represented by the interior domain \mathcal{X}_{int} . In contrast to the outer boundary $\partial\mathcal{X}$, which is assumed to be fixed, the inner boundary is variable. If $\Gamma (= \partial\Omega)$ changes, then the subdomains $\Omega, \mathcal{X}_{\text{out}} \subset \mathcal{X}$ change in a natural manner.

Let $\nu > 0$ be an arbitrary constant. For the objective function $J(y, \Omega) := \mathcal{J}(y, \Omega) + \mathcal{J}_{\text{reg}}(\Gamma)$ with

$$\mathcal{J}(y, \Omega) := \frac{1}{2} \int_{\mathcal{X}} (y - \bar{y})^2 dx, \quad (4.1)$$

$$\mathcal{J}_{\text{reg}}(\Gamma) := \nu \int_{\Gamma} 1 ds \quad (4.2)$$

we consider

$$\min_{\Omega \in \mathcal{U}} J(y, \Omega) \quad (4.3)$$

constrained by the obstacle type variational inequality

$$a(y, v - y) \geq \langle f, v - y \rangle \quad \forall v \in K := \{\theta \in H_0^1(\mathcal{X}) : \theta(x) \leq \varphi(x) \text{ in } \mathcal{X}\}, \quad (4.4)$$

where $y \in K$ is the solution of the VI, $f \in L^2(\mathcal{X})$ is explicitly dependent on the shape, $\langle \cdot, \cdot \rangle$ denotes the duality pairing and $a(\cdot, \cdot)$ is a general strongly elliptic, i.e. coercive, symmetric bilinear form

$$a: H_0^1(\mathcal{X}) \times H_0^1(\mathcal{X}) \rightarrow \mathbb{R} \\ (y, v) \mapsto \int_{\mathcal{X}} \sum_{i,j} a_{i,j} \partial_i y \partial_j v + \sum_i d_i (\partial_i y v + y \partial_i v) + b y v dx \quad (4.5)$$

defined by coefficient functions $a_{i,j}, d_j, b \in L^\infty(\mathcal{X})$, fulfilling the weak maximum principle.

With the tracking-type objective \mathcal{J} the model is fitted to data measurements $\bar{y} \in H^1(\mathcal{X})$. The second term \mathcal{J}_{reg} in the objective function J is a perimeter regularization. In (4.4), φ denotes an obstacle which needs to be an element of $L_{\text{loc}}^1(\mathcal{X})$ such that the set of admissible functions K is non-empty (cf. [49]). If additionally $\partial\mathcal{X}$ is Lipschitz and $\varphi \in H^1(\mathcal{X})$ with $\varphi|_{\partial\mathcal{X}} \geq 0$, then there is a unique solution to (4.4) satisfying $y \in H_0^1(\mathcal{X})$, given that the assumptions from above hold (cf. [25, 10, 50]). Further, (4.4) can be equivalently expressed as

$$a(y, v) + (\lambda, v)_{L^2(\mathcal{X})} = (f, v)_{L^2(\mathcal{X})} \quad \forall v \in H_0^1(\mathcal{X}) \quad (4.6)$$

$$\begin{aligned}
\lambda &\geq 0 && \text{in } \mathcal{X} \\
y &\leq \varphi && \text{in } \mathcal{X} \\
\lambda(y - \varphi) &= 0 && \text{in } \mathcal{X}
\end{aligned} \tag{4.7}$$

with $(\cdot, \cdot)_{L^2(\mathcal{X})}$ denoting the L^2 -scalar product and $\lambda \in L^2(\mathcal{X})$. It is well-known, e.g., from [10], that under these assumptions there exists a unique solution y to the obstacle type variational inequality (4.4) and an associated Lagrange multiplier λ . We assume this situation, which is also found in [26], giving us $\lambda \in L^2(\mathcal{X})$. It can be easily verified that this in turn gives the possibility to summarize the conditions (4.7) equivalently into a single condition of the form

$$\lambda = \max(0, \lambda + c(y - \varphi)) \quad \text{for any } c > 0. \tag{4.8}$$

In the following, we denote the active set corresponding to (4.6) and (4.7) by

$$A := \{x \in \mathcal{X} : y - \varphi \geq 0\}.$$

Hadamard adjoint equation. Since the perimeter regularization (4.2) is only used due to technical reasons to overcome ill-posedness of inverse problems (cf., e.g., [1]) and does not influence the adjoint system, we omit it for our investigations in the following. Thus, we consider the (reduced) Lagrangian function to the minimization of (4.1) constrained by

$$a(y, v) + (\max(0, \lambda + c(y - \varphi)), v)_{L^2(\mathcal{X})} = (f, v)_{L^2(\mathcal{X})} \quad \forall v \in H_0^1(\mathcal{X}), \tag{4.9}$$

which is given by

$$\begin{aligned}
\mathcal{L}(\Omega, y, v) &= \frac{1}{2} \int_{\mathcal{X}} (y - \bar{y})^2 dx - a(y, v) - \int_{\mathcal{X}} f v dx \\
&\quad + \int_{\mathcal{X}} \max\{0, \lambda + c(y - \varphi)\} v dx,
\end{aligned} \tag{4.10}$$

to formulate the Hadamard adjoint equation to the model problem (4.3)–(4.4) by computing $\partial_2^H \mathcal{L}(\Omega, y, v)$.

In order to compute $\partial_2^H \mathcal{L}(\Omega, y, v)$, we consider a variation of y . Let $t > 0$ and $\tilde{y} \in H_0^1(\mathcal{X})$. Then, we get

$$\begin{aligned}
\partial_2^H \mathcal{L}(\Omega, y, v) &= \frac{\partial^H}{\partial t} \Big|_{t=0^+} \mathcal{L}(\Omega, y + t\tilde{y}, v) \\
&= \int_{\mathcal{X}} (y - \bar{y}) \tilde{y} dx - a(\tilde{y}, v) + \int_{\mathcal{X}} \frac{\partial^H}{\partial t} \Big|_{t=0^+} (\max\{0, \lambda + c(y + t\tilde{y} - \varphi)\} v) dx.
\end{aligned}$$

Using the chain rule in lemma 2.2 we obtain

$$\begin{aligned}
&\frac{\partial^H}{\partial t} \Big|_{t=0^+} (\max\{0, \lambda + c(t\tilde{y} - \varphi)\} v) \\
&= D_H(\max\{0, \cdot\})(\lambda + c(y - \varphi)) \frac{\partial^H}{\partial t} \Big|_{t=0^+} (\lambda + c(t\tilde{y} - \varphi)) v \\
&= D_H(\max\{0, \cdot\})(\lambda + c(y - \varphi)) c\tilde{y} v.
\end{aligned}$$

Combining the Hadamard semiderivative of the maximum function given in (2.2) with the equality

$$\max\{0, \lambda - c(y - \varphi)\} = \begin{cases} \lambda + c(y - \varphi) & \text{in } A, \\ 0 & \text{in } \mathcal{X} \setminus A \end{cases} \tag{4.11}$$

gives

$$\partial_2^H \mathcal{L}(\Omega, y, v) = \int_{\mathcal{X}} (y - \bar{y}) \tilde{y} \, dx - a(\tilde{y}, v) + \int_X \mathbb{1}_A c v \tilde{y} \, dx,$$

where $\mathbb{1}_A$ denotes the indicator function on the active set A . Thus, the Hadamard adjoint equation is given in its weak form by

$$\int_{\mathcal{X}} (y - \bar{y}) \tilde{y} \, dx - a(\tilde{y}, v) = - \int_X \mathbb{1}_A c v \tilde{y} \, dx \quad \forall \tilde{y} \in H_0^1(\mathcal{X}). \quad (4.12)$$

Hadamard shape semiderivative. In order to set up the optimality system to the model problem (4.3)–(4.4), we need the Hadamard shape semiderivative of the (full) Lagrangian $\mathcal{L}_{\text{full}}(y, \Omega, v) = \mathcal{L}(y, \Omega, v) + \mathcal{J}_{\text{reg}}(\Gamma)$, where \mathcal{L} denotes the (reduced) Lagrangian (4.10). The Hadamard shape semiderivative of $\mathcal{L}_{\text{full}}$ is given by the sum of the Hadamard shape semiderivative of the (reduced) Lagrangian (4.10) and the shape derivative of \mathcal{J}_{reg} . Standard calculation techniques yield the shape derivative of \mathcal{J}_{reg} , which is given by $D\mathcal{J}_{\text{reg}}(\Gamma)[\cdot] = \nu \int_{\Gamma} \kappa \langle \cdot, n \rangle \, ds$ with $\kappa := \text{div}_{\Gamma}(n)$ denoting the mean curvature of Γ .

The next lemma gives the Hadamard shape semiderivative of the Lagrangian.

Lemma 4.1. *Let $\varphi \in H^2(\mathcal{X})$, $f \in L^2(\mathcal{X})$, $\bar{y} \in H^1(\mathcal{X})$, $v \in H_0^1(\mathcal{X})$ and $\lambda \in L^2(\mathcal{X})$. Then,*

$$\begin{aligned} D_H \mathcal{L}(\Omega, y, v)[V] &= \int_{\mathcal{X}} \text{div}(V) \left[\frac{1}{2} (y - \bar{y})^2 + \nabla y^\top \nabla v - f v \right] \, dx \\ &\quad - \int_{\mathcal{X}} (y - \bar{y}) \nabla \bar{y}^\top V \, dx + \int_{\mathcal{X}} \nabla f^\top V v \, dx \\ &\quad - \int_{\mathcal{X}} \sum_{i,j} a_{i,j} \left(-\partial_j v \sum_l \partial_l y \partial_i V_l - \partial_i y \sum_l \partial_l v \partial_j V_l \right) \, dx \\ &\quad - \int_{\mathcal{X}} \sum_i d_i \left(-v \sum_l \partial_l y \partial_i V_j - y \sum_l \partial_l v \partial_i V_j \right) \, dx \\ &\quad + \int_A (\varphi - \bar{y}) \nabla \varphi^\top V \, dx. \end{aligned} \quad (4.13)$$

Proof. For an easier understanding and notation purpose we define

$$\chi(y, v) := \sum_{i,j} a_{i,j} \partial_i y \partial_j v + \sum_i d_i (\partial_i y v + y \partial_i v) + b y v$$

such that

$$a(y, v) = \int_{\mathcal{X}} \chi(y, v) \, dx.$$

Let

$$\begin{aligned} G(\Omega, y, v)[V] &:= \int_{\mathcal{X}} D_{Hm} \left(\frac{1}{2} (y - \bar{y})^2 - \chi(y, v) + f v + \max\{0, \lambda + c(y - \varphi)\} v \right) \\ &\quad + \text{div}(V) \left[\frac{1}{2} (y - \bar{y})^2 + \chi(y, v) - f v \right] \, dx. \end{aligned} \quad (4.14)$$

We consider a variation $\Omega_t = F_t(\Omega)$ of Ω in the following. Since \mathcal{X} depends on Ω , we also use the notation $\mathcal{X}_t := F_t(\mathcal{X})$. We get

$$\begin{aligned} & \lim_{t \searrow 0} \frac{\mathcal{L}(\Omega, y, v) - \mathcal{L}(\Omega_t, y, v)}{t} \\ &= \lim_{t \searrow 0} \frac{\frac{1}{2} \int_{\mathcal{X}} (y - \bar{y})^2 dx - \frac{1}{2} \int_{\mathcal{X}_t} (y_t - \bar{y}_t)^2 dx}{t} - \frac{\int_{\mathcal{X}} \chi(y, v) dx - \int_{\mathcal{X}_t} \chi(y_t, v_t) dx}{t} \\ & \quad - \frac{\int_{\mathcal{X}} f v dx - \int_{\mathcal{X}_t} f_t v_t dx}{t} \\ & \quad + \frac{\int_{\mathcal{X}} \max(0, \lambda + c(y - \varphi)) v dx - \int_{\mathcal{X}_t} \max(0, \lambda_t + c_t(y_t - \varphi)) v_t dx}{t}. \end{aligned}$$

Using the definition of G together with the definition of the Hadamard material semiderivative (cf. definition 2.7) as well as lemma 2.10 we see

$$\lim_{t \searrow 0} \frac{\mathcal{L}(\mathcal{X}) - \mathcal{L}(\mathcal{X}_t)}{t} = G(\Omega, y, v)[V].$$

Therefore, $D_H \mathcal{L}$ is given by G . Combining lemma 2.8 and definition 2.7 with the state equation (4.9) and adjoint equation (2.2) leads to the expression on the right-hand side of (4.13) for $G(\Omega, y, v)[V]$. We refer to the appendix 6 for the calculation and details. \square

Remark 4.2. *It is worth mentioning that the Hadamard adjoint equation (4.12) and the Hadamard shape semiderivative given in lemma 4.1 are the limit object in [36, Theorem 3.3] and [36, Theorem 3.5], respectively. Consequently, if we consider the special case $a(y, v) := \int_{\mathcal{X}} \nabla y^\top \nabla v dx$ as in [36, section 4], the Lagrangian is given by $\mathcal{L}(y, \Omega, v) = \int_{\mathcal{X}} \frac{1}{2} (y - \bar{y})^2 - \nabla y^\top \nabla v - f v + \max\{0, \lambda + c(y - \varphi)\} v dx$. Then, lemma 4.1 yields the Hadamard shape semiderivative*

$$\begin{aligned} & D_H \mathcal{L}(\Omega, y, v)[V] \\ &= \int_{\mathcal{X}} - (y - \bar{y}) \nabla \bar{y}^\top V - \nabla y^\top (\nabla V^\top + \nabla V) \nabla p \\ & \quad + \operatorname{div}(V) \left[\frac{1}{2} (y - \bar{y})^2 + \nabla y^\top \nabla v - f v \right] dx + \int_A (\varphi - \bar{y}) \nabla \varphi^\top V dx, \end{aligned}$$

which confirms the limit object given in [36, equality (43)].

Hadamard optimality system. Here, we summarize the optimality conditions. For a solution shape Ω to problem (4.3)–(4.4), there holds the Hadamard adjoint variational equation (4.12). Since the Hadamard shape semiderivative, of the Lagrangian, $D_H \mathcal{L}(\Omega, y, v)[V]$ given in lemma 4.1 is continuous in V , we obtain from (3.5) the following necessary condition for the optimal shape Ω :

$$0 = D_H \mathcal{L}(\Omega, y, v)[V] \quad \forall V \in H^1(\Omega, \mathbb{R}^n)$$

The Hadamard adjoint equation, this necessary condition and the state equation (4.4) define together a set of equations, which is used for the computation of the solution in [36], where a perturbation approach is used for construction of $D_H \mathcal{L}(\Omega, y, v)[V]$. We observe also that $D_H \mathcal{L}(\Omega, y, v)[V]$ is an integral on $\mathcal{X}(\Omega)$, where the integrand is Hadamard semidifferentiable with respect to Ω and which lacks standard differentiability only at the the boundary of the active set A , which is a set of Lebesgue measure zero. Thus, $D_H \mathcal{L}(\Omega, y, v)[V]$ is a shape derivative and can therefore be used, in order to define a descent direction by employing an

appropriate scalar product. In [36], the same expression has been derived in a perturbation approach, which necessitates a safeguard technique. The fact observed here that the resulting step is a descent direction justifies also theoretically, why the safeguard technique has never been activated in the numerical computations in [36].

5 Conclusions

In this paper, the concept of Hadamard semiderivative is used to generalize some objects and methods for shape calculus. This includes the definition of Hadamard shape semiderivative and of a Hadamard material semiderivative. In addition to the chain rule given in [13], we provide a product rule—that is obtained using the chain rule. Further, rules for the material derivative calculus given in [4] are generalized to the Hadamard material semiderivative setting. One of the major advantages of the Hadamard shape semiderivative approach developed in this paper is that one no longer needs to regularize variational inequality constrained optimization problems and a limit process as in [36] can be avoided. Beyond that, this paper explains the limiting expression for the shape derivative given in [36] now as an expression derived from a Hadamard adjoint and, thus, safeguarding techniques as in [36] are no longer necessary. These observations open the door for further potential usage of Hadamard semiderivatives for more complicated variational inequalities than studied in section 4 and of Hadamard shape semiderivatives of even higher order.

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6 Appendix: Derivation Hadamard shape semiderivative expression

We consider the problem class stated in section 4. Let $\varphi \in H^2(\mathcal{X})$, $f \in L^2(\mathcal{X})$, $\bar{y} \in H^1(\mathcal{X})$, $v \in H_0^1(\mathcal{X})$ and $\lambda \in L^2(\mathcal{X})$. In this appendix, we show that G defined in (4.14) is given by the right-hand side of (4.13).

Let

$$\chi(y, v) := \sum_{i,j} a_{i,j} \partial_i y \partial_j v + \sum_i d_i (\partial_i y v + y \partial_i v) + b y v$$

such that

$$a(y, v) = \int_{\mathcal{X}} \chi(y, v) \, dx.$$

Then, lemma 2.9 leads to

$$\begin{aligned}
& G(\Omega, y, v)[V] \\
&= \int_{\mathcal{X}} \operatorname{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \chi(y, v) - fv \right] \\
&\quad + D_{Hm} \left(\frac{1}{2}(y - \bar{y})^2 \right) - D_{Hm}(\chi(y, v)) + D_{Hm}(fv) \\
&\quad + D_{Hm}(\max\{0, \lambda + c(y - \varphi)\}v) \, dx \\
&= \int_{\mathcal{X}} \operatorname{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \chi(y, v) - fv \right] \\
&\quad + (y - \bar{y})D_{Hm}y - (y - \bar{y})D_{Hm}\bar{y} + vD_{Hm}f + fD_{Hm}v \\
&\quad - D_{Hm} \left(\sum_{i,j} a_{i,j} \partial_i y \partial_j v + \sum_i d_i (\partial_i y v + y \partial_i v) + byv \right) \\
&\quad + D_{Hm}(\max\{0, \lambda + c(y - \varphi)\})v + \max\{0, \lambda + c(y - \varphi)\}D_{Hm}v \, dx \\
&= \int_{\mathcal{X}} \operatorname{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \chi(y, v) - fv \right] \\
&\quad + (y - \bar{y})D_{Hm}y - (y - \bar{y})D_{Hm}\bar{y} + vD_{Hm}f + fD_{Hm}v \\
&\quad - \chi(D_{Hm}y, v) + \chi(y, D_{Hm}v) \\
&\quad - \sum_{i,j} a_{i,j} \left(-\partial_j v \sum_l \partial_l y \partial_i V_l - \partial_i y \sum_l \partial_l v \partial_j V_l \right) \\
&\quad - \sum_i^n d_i (\partial_i y D_{Hm}v + D_{Hm}y \partial_i v) \\
&\quad + D_{Hm}(\max\{0, \lambda + c(y - \varphi)\})v + \max\{0, \lambda + c(y - \varphi)\}D_{Hm}v \, dx
\end{aligned}$$

Combining the Hadamard semiderivative of the maximum function given in (2.2) with the equality (4.11) and the fact that ∂A is a measure zero set, gives

$$\int_{\mathcal{X}} D_{Hm}(\max\{0, \lambda + c(y - \varphi)\})v \, dx = \int_{\mathcal{X}} \mathbb{1}_A(D_{Hm}\lambda + c(D_{Hm}y - D_{Hm}\varphi))v \, dx.$$

In addition, Definition 2.7 gives

$$D_{Hm}\bar{y} = \nabla \bar{y}^\top V \quad \text{and} \quad D_{Hm}f = \nabla f^\top V$$

if we assume \bar{y} and f independent of the shape. Thus, thanks to the state equa-

tion (4.9) and the Hadamard adjoint (4.12) we get

$$\begin{aligned}
G(\Omega, y, v)[V] = & \int_{\mathcal{X}} \operatorname{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \nabla y^\top \nabla v - f v \right] \\
& - (y - \bar{y}) \nabla \bar{y}^\top V + v \nabla f^\top V \\
& - \sum_{i,j} a_{i,j} \left(-\partial_j v \sum_l \partial_l y \partial_i V_l - \partial_i y \sum_l \partial_l v \partial_j V_l \right) \\
& - \sum_i^n d_i \left(-v \sum_l \partial_l y \partial_i V_j - y \sum_l \partial_l v \partial_i V_j \right) dx \\
& + \int_A (y - \bar{y}) D_{Hm} y dx.
\end{aligned}$$

In the active set A , we have $y = \varphi$. Moreover, $D_m \varphi = \nabla \varphi^\top V$ thanks to Definition 2.7. Thus, the integral over the active set is given by

$$\int_A (y - \bar{y}) D_{Hm} y dx = \int_A (\varphi - \bar{y}) \nabla \varphi^\top V dx.$$

References

- [1] H. AMEUR, M. BURGER, AND B. HACKL, *Level Set Methods for Geometric Inverse Problems in Linear Elasticity*, Inverse Problems, 20 (2004), pp. 673–696.
- [2] V. BARBU, *Optimal control of variational inequalities*, Research Notes in Mathematics, 100 (1984).
- [3] M. BAUER, P. HARMS, AND P. MICHOR, *Sobolev metrics on shape space of surfaces*, Journal of Geometric Mechanics, 3 (2011), pp. 389–438.
- [4] M. BERGGREN, *A unified discrete-continuous sensitivity analysis method for shape optimization*, in Applied and Numerical Partial Differential Equations, W. Fitzgibbon et al., eds., vol. 15 of Computational Methods in Applied Sciences, Springer, 2010, pp. 25–39.
- [5] J. BRACKEN AND J. MCGILL, *Mathematical programs with optimization problems in the constraints*, Operations Research, 21 (1973), pp. 37–44.
- [6] H. BRÉZIS, *Monotonicity methods in Hilbert spaces and some applications to nonlinear partial differential equations*, Contributions to Nonlinear Functional Analysis, (1971), pp. 101–156.
- [7] H. BRÉZIS AND G. STAMPACCHIA, *Sur la régularité de la solution d'inéquations elliptiques*, Bulletin de la Société Mathématique de France, 96 (1968), pp. 153–180.
- [8] C. CARSTENSEN, L. DEMKOWICZ, AND J. GOPALAKRISHNAN, *Breaking spaces and forms for the dpg method and applications including maxwell equations*, Computers & Mathematics with Applications, 72 (2016), pp. 494–522.
- [9] F. CAUBET, M. DAMBRINE, AND R. MAHADEVAN, *Shape sensitivity of eigenvalue functionals for scalar problems: Computing the semi-derivative of a minimum*, Applied Mathematics & Optimization, 86 (2022), <https://doi.org/10.1007/s00245-022-09827-6>.

- [10] G. S. D. KINDERLEHRER, *An Introduction to Variational Inequalities and Their Applications*, vol. 31, SIAM, 1980.
- [11] M. DELFOUR AND J.-P. ZOLÉSIO, *Shapes and Geometries: Metrics, Analysis, Differential Calculus, and Optimization*, vol. 22 of Adv. Des. Control, SIAM, 2nd ed., 2011.
- [12] M. C. DELFOUR, *Hadamard semidifferential of functions on an unstructured subset of a TVS*, Pure and Applied Functional Analysis, 5 (2020), pp. 1039–1072, www.yokohamapublishers.jp/online-p/Pafa/vol5/pafav5n5p1039.pdf.
- [13] M. C. DELFOUR, *Hadamard semidifferential, oriented distance function, and some applications*, Communications on Pure and Applied Analysis, 21 (2022), p. 1917, <https://doi.org/10.3934/cpaa.2021076>.
- [14] Z. DENKOWSKI AND S. MIGORSKI, *Optimal shape design for hemivariational inequalities*, Universitatis Iagellonicae Acta Mathematica, 36 (1998), pp. 81–88.
- [15] M. DROSKE AND M. RUMPF, *Multi scale joint segmentation and registration of image morphology*, IEEE Transactions on Pattern Analysis and Machine Intelligence, 29 (2007), pp. 2181–2194.
- [16] L. GASIŃSKI, *Mapping method in optimal shape design problems governed by hemivariational inequalities*, in Shape optimization and optimal design, J. Cagnol, M. Polis, and J.-P. Zolésio, eds., no. 216 in Lecture Notes in Pure and Applied Mathematics, Marcel Dekker, 2001, pp. 277–288.
- [17] R. GLOWINSKI, *Numerical methods for nonlinear variational problems*, Springer, 1984.
- [18] P. HARKER AND J.-S. PANG, *Existence of optimal solutions to mathematical programs with equilibrium constraints*, Operations Research Letters, 7 (1988), pp. 61–64.
- [19] C. HEINEMANN AND K. STURM, *Shape optimization for a class of semilinear variational inequalities with applications to damage models*, SIAM Journal on Mathematical Analysis, 48 (2016), pp. 3579–3617.
- [20] R. HERZOG AND E. LOAYZA-ROMERO, *A manifold of planar triangular meshes with complete Riemannian metric*.
- [21] R. HERZOG, C. MEYER, AND G. WACHSMUTH, *C-stationarity for optimal control of static plasticity with linear kinematic hardening*, SIAM Journal on Control and Optimization, 50 (2012), pp. 3052–3082.
- [22] R. HERZOG, C. MEYER, AND G. WACHSMUTH, *B- and strong stationarity for optimal control of static plasticity with hardening*, SIAM Journal on Control and Optimization, 23 (2013), pp. 312–352.
- [23] M. HINTERMÜLLER AND I. KOPACKA, *Mathematical programs with complementarity constraints in function space: C- and strong stationarity and a path-following algorithm*, SIAM Journal on Optimization, 20 (2009), pp. 868–902.
- [24] M. HINTERMÜLLER AND A. LAURAIN, *Optimal shape design subject to elliptic variational inequalities*, SIAM Journal on Control and Optimization, 49 (2011), pp. 1015–1047.

- [25] K. ITO AND K. KUNISCH, *Optimal Control of Elliptic Variational Inequalities*, Applied Mathematics and Optimization, 41 (2000), pp. 343–364.
- [26] K. ITO AND K. KUNISCH, *Semi-Smooth Newton Methods for Variational Inequalities of the First Kind*, ESIAM: Mathematical Modelling and Numerical Analysis, 37 (2003), pp. 41–62.
- [27] D. KENDALL, *Shape manifolds, procrustean metrics, and complex projective spaces*, Bulletin of the London Mathematical Society, 16 (1984), pp. 81–121.
- [28] N. KIKUCHI AND J. ODEN, *Contact problems in elasticity: A study of variational inequalities and finite element methods*, SIAM, 1988.
- [29] D. KINDERLEHRER AND G. STAMPACCHIA, *An introduction to variational inequalities and their applications*, Academic Press, 1980.
- [30] D. KLATTE AND B. KUMMER, *Nonsmooth Equations in Optimization: Regularity, Calculus, Methods, and Applications*, Kluwer Academic, 2002.
- [31] M. KOCVARA AND J. OUTRATA, *Shape optimization of elasto-plastic bodies governed by variational inequalities*, in Boundary Control and Variation, J.-P. Zolésio, ed., no. 163 in Lecture Notes in Pure and Applied Mathematics, Marcel Dekker, 1994, pp. 261–271.
- [32] H. LING AND D. JACOBS, *Shape classification using the inner-distance*, IEEE Transactions on Pattern Analysis and Machine Intelligence, 29 (2007), pp. 286–299.
- [33] J. LIONS AND G. STAMPACCHIA, *Variational inequalities*, Communications on Pure and Applied Mathematics, 20 (1967), pp. 493–519.
- [34] W. LIU AND J. RUBIO, *Optimal shape design for systems governed by variational inequalities, part 1: Existence theory for the elliptic case*, Journal of Optimization Theory and Applications, 69 (1991), pp. 351–371.
- [35] W. LIU AND J. RUBIO, *Optimal shape design for systems governed by variational inequalities, part 2: Existence theory for the evolution case*, Journal of Optimization Theory and Applications, 69 (1991), pp. 373–396.
- [36] D. LUFT, V. SCHULZ, AND K. WELKER, *Efficient techniques for shape optimization with variational inequalities using adjoints*, SIAM Journal on Optimization, 30 (2020), pp. 1922–1953, <https://doi.org/10.1137/19M1257226>.
- [37] Z. LUO, J. PANG, AND D. RALPH, *Mathematical Programs with Equilibrium Constraints*, Cambridge University Press, 1996.
- [38] P. MICHOR AND D. MUMFORD, *Vanishing geodesic distance on spaces of submanifolds and diffeomorphisms*, Documenta Mathematica, 10 (2005), pp. 217–245.
- [39] P. MICHOR AND D. MUMFORD, *An overview of the Riemannian metrics on spaces of curves using the Hamiltonian approach*, Applied and Computational Harmonic Analysis, 23 (2007), pp. 74–113.
- [40] F. MIGNOT AND J. PUEL, *Optimal control in some variational inequalities*, SIAM Journal on Control and Optimization, 22 (1984), pp. 466–476.

- [41] A. MYŚLIŃSKI, *Domain optimization for unilateral problems by an embedding domain method*, in Shape optimization and optimal design, J. Cagnol, M. Polis, and J.-P. Zolésio, eds., no. 216 in Lecture Notes in Pure and Applied Mathematics, Marcel Dekker, 2001, pp. 355–370.
- [42] A. MYŚLIŃSKI, *Level set approach for shape optimization of contact problems*, in European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS, P. Neittaanmäki, T. Rossi, K. Majava, O. Pironneau, and I. Lasiecka, eds., 2004.
- [43] A. MYŚLIŃSKI, *Level set method for shape and topology optimization of contact problems*, in IFIP Conference on System Modeling and Optimization, Springer, 2007, pp. 397–410.
- [44] P. NEITTAANMÄKI, J. SPREKELS, AND D. TIBA, *Optimization of Elliptic Systems: Theory and Applications*, Springer Monographs in Mathematics, 2006.
- [45] J. OUTRATA, M. KOČVARA, AND J. ZOWE, *Nonsmooth Approach to Optimization Problems with Equilibrium Constraints: Theory, Applications, and Numerical Results*, no. 152 in Nonconvex optimization and its applications, Kluwer Academic Publisher, 1998.
- [46] P. PANAGIOTOPOULOS, *Inequality problems in mechanics and applications*, Birkhäuser, 1985.
- [47] H. SCHEEL AND S. SCHOLTES, *Mathematical programs with complementarity constraints: Stationarity, optimality, and sensitivity*, Mathematics of Operations Research, 25 (2000), pp. 1–22.
- [48] S. SCHMIDT AND V. SCHULZ, *A linear view on shape optimization*, tech. report, 2022.
- [49] J. SOKOLOWSKI AND J. ZOLÉSIO, *Introduction to Shape Optimization*, vol. 16 of Computational Mathematics, Springer, 1992.
- [50] G. TROIANIELLO, *Elliptic Differential Equations and Obstacle Problems*, Springer Science & Business Media, 2013.
- [51] K. WELKER, *Efficient PDE Constrained Shape Optimization in Shape Spaces*, PhD thesis, Universität Trier, 2016.
- [52] B. WIRTH, L. BAR, M. RUMPF, AND G. SAPIRO, *A continuum mechanical approach to geodesics in shape space*, International Journal of Computer Vision, 93 (2011), pp. 293–318.
- [53] B. WIRTH AND M. RUMPF, *A nonlinear elastic shape averaging approach*, SIAM Journal on Imaging Sciences, 2 (2009), pp. 800–833.
- [54] J.-P. ZOLÉSIO, *Control of moving domains, shape stabilization and variational tube formulations*, International Series of Numerical Mathematics, 155 (2007), pp. 329–382.