

Gâteaux semiderivative approach applied to shape optimization of obstacle problems*

by

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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 setting up an optimality system and, thus, developing efficient solution algorithms. In this paper, we consider Gâteaux semiderivatives for the purpose of formulating optimality conditions. In the application, we concentrate on a shape optimization problem constrained by the obstacle problem.

Keywords: obstacle problem, directional derivative, variational inequality, shape optimization, shape derivative, material derivative, optimality conditions, Gâteaux semiderivatives

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

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optimality conditions is an issue. By the 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. Brézis, 1971; Brézis and Stampacchia, 1968; Lions and Stampacchia, 1967). Comprehensive studies of variational inequalities and more references can be found in Glowinski (1984), Kikuchi and Oden (1988), Kinderlehrer and Stampacchia (1980) or Panagiotopoulos (1985). 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., Bracken and McGill, 1973) and has been generalized to mathematical programming with equilibrium constraints (MPECs) for the optimization of stationary systems of the constrained problems in Harker and Paine (1988). For a survey on bilevel programming and MPECs see, e.g., Luo, Pang and Ralph (1996). In Scheel and Scholtes (2000), 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 Herzog, Meyer and Wachsmuth (2012, 2013) and Hintermüller and Kopacka (2009). The optimal control of variational inequalities that are posed in function space has been studied since the 1970s, and the necessary stationarity conditions have been derived by the use of penalty and smoothing techniques and strengthened by the usage of instruments from convex analysis and differentiability, see, e.g., Barbu (1984), Mignot and Puel (1984), or Neittaanmäki, Sprekels and Tiba (2006). The conditions that a solution can be shown to verify have a complex structure and the problem of finding candidates for solutions leads to a system of non-linear and non-smooth equations. This necessitates the development of numerical algorithms and a proper mathematical analysis on their convergence behavior, see, e.g., the discussion in Klatte and Kummer (2002), Outrata, Kočvara and Zowe (1998).

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 complementarity aspects due to the VIs, as well as distributed, non-linear, non-convex and infinite dimensional aspects, due to the shapes, which complicate setting up of 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. A common way to handle the non-smoothness is to regularize the given problem, e.g., by replacing the max-function by a smoothed approximation or by replacing certain functions with regularized version, and then considering the obtained regularized problem (see, for example, Christof et al., 2018; Schiela and Wachsmuth, 2013; Mordukhovich, 2006; Hintermüller and Kopacka, 2011). A mollification is also a tool that can be used to tweak non-smoothness, as it is done in Kovtunen and Kunisch (2023). They also discuss directional derivatives for shape optimization problems with VI. This paper aims at establishing a way to treat VI constrained shape optimization problems without the use of regularizations. We also aim at avoiding regularization techniques. Therefore, we use Gâteaux semiderivatives in order to obtain a useful kind of derivative, such that we can deal with the unregularized obstacle problem.

So far, there are only very few approaches in the literature to the problem class of VI constrained shape optimization problems. In Kocvara and Outrata (1994), 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 Sokolowski and Zolésio (1992, Chap. 4), shape derivatives of elliptic variational inequality problems are presented in the form of solutions to, again, variational inequalities. In Myśliński (2001), shape optimization for 2D graph-like domains is investigated. Also Liu and Rubio (1991 a,b) present existence results for shape optimization problems, which can be reformulated as optimal control problems, whereas Denkowski and Migórski (1998) and Gasiński (2001) show existence of solutions in a more general setup. In Myśliński (2004, 2007), level-set methods are proposed and applied to graph-like two-dimensional problems. Moreover, Hintermüller and Laurain (2011) present a regularization approach to the computation of shape and topological derivatives in the context of elliptic variational inequalities and, thus, circumvent the numerical problems arising in Sokolowski and Zolésio (1992, Chap. 4). In Heinemann and Sturm (2016), the analysis of state material derivatives is significantly refined over Sokolowski and Zolésio (1992, 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. Sokolowski and Zolésio, 1992, Example in Chap. 1). In general, the shape derivative for VI-constrained 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 concentrates on presenting a Gâteaux approach using Gâteaux semiderivatives.

This paper is structured as follows. In Section 2, a VI constrained shape optimization problem is introduced and reformulated. Then, we derive the

optimality system in the approach usually employed for Fréchet differentiable problems for VI constrained shape optimization in Section 3, in order to prepare the reader to Section 4, in which we apply our Gâteaux approach to tackle an obstacle problem. Within this context, we consider the Lagrangian associated with the obstacle problem and we use the concept of Gâteaux semiderivatives in order to calculate its derivative. This process enables us to generalize various objects and introduce a Gâteaux adjoint to the system under consideration. A conclusion is given in Section 5.

2. Problem formulation

The main focus in shape optimization is on 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

$$\min_{\Omega \in \mathcal{U}} J(\Omega). \quad (1)$$

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 Ω but also the state variable y , where the state variable is the solution of the underlying constraint.

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 Luft, Schulz and Welker (2020) and that we are also formulating in the following. In contrast to Luft, Schulz and Welker (2020), which formulates an optimization approach based on the convergence of state, adjoint and shape derivative of the

¹Various shapes spaces have been extensively studied in recent decades. In Kendall (1984), a shape space is just modelled 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 smooth curves, see Michor and Mumford (2007), piecewise-smooth curves, Pryymak, Suchan and Welker (2023), surfaces in higher dimensions, Bauer, Harms and Michor (2011), Michor and Mumford (2005), boundary contours of objects, Ling and Jacobs (2007) and Wirth and Rumpf (2009), multiphase objects, Wirth et al. (2011), characteristic functions of measurable sets, Zolésio (2007), morphologies of images, Droske and Rumpf (2007), and planar triangular meshes, Herzog and Loayza-Romero (2020). The choice of the shape space depends on the requirements for a given situation. There exists no common shape space suitable for all applications.

regularized problem to limit objects, we do not consider regularized versions of the VI. We consider a Gâteaux semiderivative approach in order to formulate an optimality system. We will see that this system is in line with the limit objects of Luft, Schulz and Welker (2020).

Model formulation

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 into an open subdomain $\mathcal{X}_{\text{out}} \subset \mathcal{X}$ and an open interior domain $\Omega \subset \mathcal{X}$ with boundary $\Gamma := \partial\Omega$, such that $\mathcal{X}_{\text{out}} \sqcup \Gamma \sqcup \Omega = \mathcal{X}$, where \sqcup denotes the disjoint union. The closure of \mathcal{X} is denoted by $\bar{\mathcal{X}}$. In the following, the boundary Γ of the interior domain Ω is called the interface. In the setting as above, Ω denotes the shape. In contrast to the outer boundary $\partial\mathcal{X}$, which is assumed to be fixed, the inner boundary is variable. If Γ changes, then the subdomains Ω , $\mathcal{X}_{\text{out}} \subset \mathcal{X}$ change in a natural manner. Thus, one can consider \mathcal{X} depending on Γ , i.e., $\mathcal{X} = \mathcal{X}(\Gamma)$.

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

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

$$\mathcal{J}_{\text{reg}}(\Gamma) := \nu \int_{\Gamma} 1 \, ds \quad (3)$$

we consider

$$\min_{\Omega \in \mathcal{U}} J(y, \Omega) \quad (4)$$

constrained by the obstacle type variational inequality

$$a(y, v - y) \geq \langle f, v - y \rangle \quad \forall v \in K := \{\theta \in H_0^1(\mathcal{X}) : \theta(x) \leq \varphi(x) \text{ in } \mathcal{X}\}, \quad (5)$$

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

$$\begin{aligned} a: H_0^1(\mathcal{X}) \times H_0^1(\mathcal{X}) &\rightarrow \mathbb{R} \\ (y, v) &\mapsto \int_{\mathcal{X}} \sum_{i,j} a_{i,j} \partial_i y \partial_j v + \sum_i d_i (\partial_i y v + y \partial_i v) + b y v \, dx \end{aligned} \quad (6)$$

defined by coefficient functions $a_{i,j}, d_j, b \in L^\infty(\mathcal{X})$ fulfilling the weak maximum principle, where ∂_i denotes the partial derivative to the i -th component.

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 (5), φ denotes an obstacle, which needs to be an element of $L^1_{\text{loc}}(\mathcal{X})$, such that the set of admissible functions K is non-empty (cf. Sokolowski and Zolésio, 1992). 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 (5), satisfying $y \in H^1_0(\mathcal{X})$, given that the assumptions from above hold (cf. Ito and Kunisch, 2000; Kinderlehrer and Stampacchia, 1980; Troianiello, 2013). Further, (5) can be equivalently expressed as

$$a(y, v) + (\lambda, v)_{L^2(\mathcal{X})} = (f, v)_{L^2(\mathcal{X})} \quad \forall v \in H^1_0(\mathcal{X}) \quad (7)$$

$$\begin{aligned} \lambda &\geq 0 && \text{in } \mathcal{X} \\ y &\leq \varphi && \text{in } \mathcal{X} \\ \lambda(y - \varphi) &= 0 && \text{in } \mathcal{X} \end{aligned} \quad (8)$$

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 Kinderlehrer and Stampacchia (1980), that under these assumptions there exists a unique solution y to the obstacle type variational inequality (5) and an associated Lagrange multiplier λ . We assume this situation, which is also found in Ito and Kunisch (2003), giving us $\lambda \in L^2(\mathcal{X})$. It can be easily verified that this, in turn, gives the possibility to summarize the conditions (8) equivalently into a single condition of the form

$$\lambda = \max(0, \lambda + \mathcal{C}(y - \varphi)) \quad \text{for any } \mathcal{C} > 0. \quad (9)$$

In the following, we denote the active set, corresponding to (7) and (8), by

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

After formulating the optimization problem under consideration and introducing the active set, we continue with the formulation of an optimality system for VI constrained shape optimization in the next section. For this, we will focus on Gâteaux semiderivatives to derive the state and adjoint system and on the Eulerian derivative of the shape functional to set up the design equation. For further details on Gâteaux semiderivatives as well as on the Eulerian derivative we refer to Sokolowski and Zolésio (1992) and for a more general point of view to Delfour (2020). Given a functional $\mathcal{F}(\Omega, y, z)$, depending on a shape Ω and elements y, z of topological spaces, we will denote the (total) Gâteaux semiderivative of \mathcal{F} by $d^G \mathcal{F}$. The notation $\partial_y^G \mathcal{F}(\Omega, y, z)[\hat{y}]$ (and $\partial_z^G \mathcal{F}(\Omega, y, z)[\hat{z}]$) means the Gâteaux semiderivative of \mathcal{F} with respect to y (and z) in direction \hat{y} (and \hat{z}). The Eulerian derivative of \mathcal{F} at Ω in the direction of a sufficiently

smooth vector field V is denoted by $\partial_{\Omega}^E \mathcal{F}(\Omega, y, z)[V]$. In order to be consistent with this notation we denote the material derivative by d_m , for a definition see, e.g., Sokolowski and Zolésio (1992). Given a functional $\mathcal{G}(y_1, \dots, y_n)$, depending on elements y_1, \dots, y_n of topological spaces, we denote its Gâteaux semiderivative with respect to the i -th component y_i by $\partial_i^G \mathcal{G}$ or $\partial_{y_i}^G \mathcal{G}$.

3. Optimality system for VI constrained shape optimization

In this section, we briefly discuss the necessary optimality conditions for non-smooth shape optimization problems in our setting and terminology. Although shapes do not define a linear space, the shape derivative can be viewed as a directional derivative in the space of deformations of the shape under investigation. This aspect is investigated further in Schmidt and Schulz (2023), where a linear deformation space framework is established. 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 $\mathcal{S}^{\text{adm}} = \{T(\Omega^0) : T \in Y\}$, where Ω^0 is a reference starting domain, which is assumed to be a subset of the open hold-all domain D . Thus, we can write the shape derivative of a functional $\mathcal{J} : \Omega \mapsto \mathbb{R}$ as

$$d\mathcal{J}(\Omega)[V] = \partial_W^G \mathcal{J}((I + W)(\Omega))[V]$$

i.e., as a Gâteaux semiderivative with respect to W , where I denotes the identity deformation and W an arbitrary small deformation. We denote this derivative for convenience as $d^G \mathcal{J}(\Omega)[V]$. Thus, for functionals with more arguments, like above, we define

$$\begin{aligned} d^G \mathcal{F}(\Omega, y(\Omega), p(\Omega))[V] &= d_W^G((I + W)(\Omega), y((I + W)(\Omega)), p((I + W)(\Omega)))[V] \\ \partial_{\Omega}^G \mathcal{F}(\Omega, y(\Omega), p(\Omega))[V] &= d_W^G((I + W)(\Omega), y(\Omega), p(\Omega))[V]. \end{aligned}$$

Partial Gâteaux derivatives with respect to the other arguments are denoted as $\partial_y^G \mathcal{F}$ and $\partial_p^G \mathcal{F}$.

We consider constrained shape optimization problems of the following form:

$$\begin{aligned} \min_{\Omega \in \mathcal{U}} \quad & J(\Omega, y) & (10) \\ \text{s.t.} \quad & b(c(\Omega, y), p)_{\Omega} = 0 \quad \forall p \in \mathcal{H}(\Omega). & (11) \end{aligned}$$

Here, $\mathcal{H}(\Omega)$ is a Hilbert space, defined on the domain Ω , containing the state variable $y \in \mathcal{H}(\Omega)$, and $b(\cdot, \cdot)_{\Omega}$ is a bilinear form that is coercive in $\mathcal{H}(\Omega)$. Moreover, \mathcal{U} is the set of admissible shapes, i.e., an appropriate shape space. We assume that the mapping c is Gâteaux semidifferentiable, and that the constraint (11) 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 the necessary conditions of optimality, we differentiate the right-hand side with respect to Ω , i.e. compute the shape derivative, 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

$$d^G \mathcal{L}(\Omega, y, p)[V] = \partial_\Omega^E \mathcal{L}(\Omega, y, p)[V] + \partial_y^G \mathcal{L}(\Omega, y, p) d_m y + \partial_p^G \mathcal{L}(\Omega, y, p) d_m p$$

for all $V \in Y$.

Since y satisfies the state equation (11) in variational form, which is linear in p , we observe that

$$\partial_p^G \mathcal{L}(\Omega, y, p) d_m p = 0. \quad (12)$$

Furthermore, we obtain

$$\partial_y^G \mathcal{L}(\Omega, y, p) d_m y = \partial_y^G J(\Omega, y) d_m y + b(\partial_y^G c(\Omega, y) d_m y, p)_\Omega$$

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

$$\partial_y^G J(\Omega, y) \tilde{y} + b(\partial_y^G c(\Omega, y) \tilde{y}, p)_\Omega = 0 \quad \forall \tilde{y} \in \mathcal{H}(\Omega). \quad (13)$$

The solvability of the Gâteaux adjoint equation is in question in this rather general setup. Therefore, we take it for granted now and show solvability, when confronted with the particular model problem as in the next section. Now, if y satisfies the state equation (11) and p satisfies the Gâteaux adjoint equation (13), then the Gâteaux shape semiderivative is given by

$$d^G \mathcal{L}(\Omega, y, p)[V] = \partial_\Omega^E \mathcal{L}(\Omega, y, p)[V].$$

Nevertheless, it is a manually easier way to compute the Gâteaux shape semiderivative of the full Lagrangian by employing shape and Gâteaux calculus and later on to eliminate expressions relating to the state and Gâteaux adjoint equation, as exemplified in the next section.

First, we formulate the necessary conditions of optimality for the minimization problem.

THEOREM 1 *We assume that the function $J: X \rightarrow \mathbb{R}$, where X is a Banach space, is Gâteaux semidifferentiable and that $\hat{x} \in X$ is a local minimum of J . Then, there holds*

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

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 that

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

and thus we obtain the assertion by using the definition of the Gâteaux semiderivative. ■

From Theorem 1, we derive now the necessary condition of optimality for an optimal shape Ω as

$$\partial_{\Omega}^G \mathcal{L}(\Omega, y, p)[V] \geq 0 \quad \forall V \in Y, \quad (14)$$

where y satisfies the state equation (11) and p satisfies the Gâteaux adjoint equation (13). This means that we can observe from Theorem 1 that the Gâteaux (shape) semiderivative can be used to characterize the necessary optimality conditions. For further exploration on first order optimality conditions in the Gâteaux framework, we refer to the literature, e.g., Bracken and Mc Gill (1973).

In many cases, as is demonstrated in the next section, the Gâteaux shape semiderivative is continuous, 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 (Gâteaux) shape (semi)derivative can be used in order to define a descent direction for algorithmical purposes. Nevertheless, finding a descent direction from the Gâteaux 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, its material derivative is again in $H^1(\Omega)$. 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 (12). A similar problem arises in discontinuous Galerkin approximations, where we borrow the notion of a “broken” Sobolev space here, which is analyzed in detail in Carstensen, Demkowicz and Gopalakrishnan (2016). 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

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

In Carstensen, Demkowicz and Gopalakrishnan (2016), this space is used as the test space, and it is shown that resulting weak formulation of the standard elliptic problem is stable, thereby ensuring the 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 to shape optimization for obstacle problems

In this section, we apply the Gâteaux semiderivative approach to an obstacle problem. In particular, we introduce the Lagrangian of the problem, compute its Gâteaux semiderivative and focus on a Gâteaux adjoint associated with the system under consideration.

Gâteaux adjoint equation

Since the perimeter regularization (3) is only used due to technical reasons to overcome ill-posedness of inverse problems (cf., e.g., Ameer, Burger and Hackl, 2004) 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 (2), constrained by

$$a(y, v) + (\max(0, \lambda + \mathcal{C}(y - \varphi)), v)_{L^2(\mathcal{X})} = (f, v)_{L^2(\mathcal{X})} \quad \forall v \in H_0^1(\mathcal{X}), \quad (15)$$

which is given by

$$\begin{aligned} \mathcal{L}(\Omega, y, v) &= \frac{1}{2} \int_{\mathcal{X}} (y - \bar{y})^2 dx - a(y, v) - \int_{\mathcal{X}} f v dx \\ &\quad + \int_{\mathcal{X}} \max\{0, \lambda + \mathcal{C}(y - \varphi)\} v dx, \end{aligned} \quad (16)$$

to formulate the Gâteaux adjoint equation to the model problem (4)–(5) by computing $\partial_y^G \mathcal{L}(\Omega, y, v)$.

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

$$\begin{aligned} \partial_y^G \mathcal{L}(\Omega, y, v)[\tilde{y}] &= \partial_t^G \mathcal{L}(\Omega, y + t\tilde{y}, v) \\ &= \int_{\mathcal{X}} (y - \bar{y})\tilde{y} dx - a(\tilde{y}, v) + \int_{\mathcal{X}} \partial_t^G (\max\{0, \lambda + \mathcal{C}(y + t\tilde{y} - \varphi)\}v) dx. \end{aligned}$$

Using the chain rule, we obtain

$$\begin{aligned} & \partial_t^G (\max\{0, \lambda + \mathcal{C}(t\tilde{y} - \varphi)\}v) \\ &= \partial_y^G (\max\{0, \cdot\})(\lambda + \mathcal{C}(y - \varphi)) [\partial_t^G (\lambda + \mathcal{C}(t\tilde{y} - \varphi))v] \\ &= \partial_y^G (\max\{0, \cdot\})(\lambda + \mathcal{C}(y - \varphi)) [\mathcal{C}\tilde{y}v]. \end{aligned}$$

Then, the Gâteaux semiderivative yields

$$\begin{aligned} & \partial_t^G (\max\{0, \lambda + \mathcal{C}(y + t\tilde{y} - \varphi)\}v) \\ &= \begin{cases} \mathcal{C}\tilde{y}v, & \lambda + \mathcal{C}(y + t\tilde{y} - \varphi) > 0, \\ \max\{0, \mathcal{C}\tilde{y}v\}, & \lambda + \mathcal{C}(y + t\tilde{y} - \varphi) = 0, \\ 0, & \lambda + \mathcal{C}(y + t\tilde{y} - \varphi) < 0. \end{cases} \quad (17) \\ &= \begin{cases} \mathcal{C}\tilde{y}v, & \text{in } A, \\ \max\{0, \mathcal{C}\tilde{y}v\}, & \text{in } \{x \in \mathcal{X} : y = \varphi\}, \\ 0, & \text{in } \{x \in \mathcal{X} : y < \varphi\}. \end{cases} \end{aligned}$$

This results in

$$\begin{aligned} d_t^G \mathcal{L}(\Omega, y + t\tilde{y}, v) &= \int_{\mathcal{X}} (y - \bar{y})\tilde{y} \, dx - a(\tilde{y}, v) + \int_{\mathcal{X}} \mathbf{1}_A \mathcal{C}\tilde{y}v \, dx \\ &\quad + \int_{\{x \in \mathcal{X} : y = \varphi\}} \max\{0, \mathcal{C}\tilde{y}v\} \, dx, \end{aligned}$$

where $\mathbf{1}_A$ denotes the indicator function on the active set A . As a result, the Gâteaux adjoint equation is given in its weak form by

$$\begin{aligned} \int_{\mathcal{X}} (y - \bar{y})\tilde{y} \, dx - a(\tilde{y}, v) &= - \int_{\mathcal{X}} \mathbf{1}_A \mathcal{C}v\tilde{y} \, dx \\ &\quad - \int_{\{x \in \mathcal{X} : y = \varphi\}} \max\{0, \mathcal{C}\tilde{y}v\} \, dx \quad \forall \tilde{y} \in H_0^1(\mathcal{X}). \end{aligned}$$

REMARK 1 *The additional integral over $\max\{0, \mathcal{C}\tilde{y}v\}$ on $\{x \in \mathcal{X} : y = \varphi\}$ seems to constitute further challenges. However, numerical experiments have shown that this expression never holds any numerical significance; see Suchan, Schultz and Welker (2024). As a consequence, we are going to neglect it and assume that $\max\{0, \mathcal{C}\tilde{y}v\}$ is of measure zero, and thus*

$$\int_{\mathcal{X}} (y - \bar{y})\tilde{y} \, dx - a(\tilde{y}, v) = - \int_{\mathcal{X}} \mathbf{1}_A \mathcal{C}v\tilde{y} \, dx \quad \forall \tilde{y} \in H_0^1(\mathcal{X}) \quad (18)$$

holds. This results in the necessity of a safeguard technique, since we cannot be sure that the Gâteaux semiderivative provides a descent direction. Such a technique is presented in Luft, Schultz and Welker (2020).

Gâteaux semiderivative of the (full) Lagrangian

In order to set up the optimality system to the model problem (4)–(5), we need the Gâteaux 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 (16). The Gâteaux semiderivative of $\mathcal{L}_{\text{full}}$ is given by the sum of the Gâteaux semiderivative of the (reduced) Lagrangian (16) and the shape derivative of \mathcal{J}_{reg} . Standard calculation techniques yield the shape derivative of \mathcal{J}_{reg} , which is given by $d^E \mathcal{J}_{\text{reg}}(\Gamma)[\cdot] = \nu \int_{\Gamma} \kappa \langle \cdot, n \rangle ds$ with $\kappa := \text{div}_{\Gamma}(n)$ denoting the mean curvature of Γ .

The next lemma gives the Gâteaux semiderivative of the Lagrangian.

LEMMA 1 *Let $\varphi \in H^2(\mathcal{X})$, $f \in L^2(\mathcal{X})$, $\bar{y} \in H^1(\mathcal{X})$, $v \in H_0^1(\mathcal{X})$, $\lambda \in L^2(\mathcal{X})$ and $V \in H^1(\mathcal{X}, \mathbb{R}^n)$. Then,*

$$\begin{aligned}
d^G \mathcal{L}(\Omega, y, v)[V] &= \int_{\mathcal{X}} \text{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \nabla y^{\top} \nabla v - f v \right] dx \\
&\quad - \int_{\mathcal{X}} (y - \bar{y}) \nabla \bar{y}^{\top} V dx + \int_{\mathcal{X}} \nabla f^{\top} V v dx \\
&\quad - \int_{\mathcal{X}} \sum_{i,j} a_{i,j} \left(-\partial_j^G v \sum_l \partial_l^G y \partial_i^G V_l - \partial_i^G y \sum_l \partial_l^G v \partial_j^G V_l \right) dx \\
&\quad - \int_{\mathcal{X}} \sum_i d_i \left(-v \sum_l \partial_l^G y \partial_i^G V_j - y \sum_l \partial_l^G v \partial_i^G V_j \right) dx \\
&\quad + \int_A (\varphi - \bar{y}) \nabla \varphi^{\top} V dx.
\end{aligned} \tag{19}$$

To prove Lemma 1, we need a rule for differentiating the perturbed domain integrals. Thus, we consider a family $\{F_t\}_{t \in [0, T]}$ of mappings $F_t: \bar{\mathcal{X}} \rightarrow \mathbb{R}^n$ such that $F_0 = \text{id}$, where $\bar{\mathcal{X}}$ denotes the closure of \mathcal{X} 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. Brézis (1971, pages 45 and 49) and Sokolowski and Zolésio (1992). The transformation defined by perturbation of identity is given by

$$F_t(x) := F_t^V(x) := \text{id}(x) + tV(x) \tag{20}$$

for $x \in \Omega$, where $V: \bar{\mathcal{X}} \rightarrow \mathbb{R}^n$ denotes a sufficiently smooth vector field. For $x \in \Omega$, the transformation defined by the velocity method is given by

$$\begin{aligned}
F_t(x) &:= \xi(t, x), \text{ where} \\
\partial_t \xi(t, x) &= v(t, \xi(t, x)) \text{ and } \xi(0, x) = x \text{ holds.}
\end{aligned} \tag{21}$$

Here, $v: [0, \tau] \times \overline{\mathcal{X}} \rightarrow \mathbb{R}^n$ denotes a non-autonomous vector field, which is at least continuous in the first argument for some $\tau > 0$ and Lipschitz continuous in the second argument. In the following lemma, we concentrate on these two transformations.

LEMMA 2 *Let Ω be as above and $t \leq T$ with $T \geq 0$. Moreover, let Ω_t be a shape perturbed by the perturbation of identity or the velocity method. Consider the domain integral $J(\Omega) = \int_{\Omega} g \, dx$ for a function $g: \Omega \rightarrow \mathbb{R}$. Moreover, let $x_t = F_t(x)$ for $x \in \Omega$ and let $\{g_t: \Omega_t \rightarrow \mathbb{R} \mid t \leq T\}$ denote a family of mappings with $g = g_0$. Then, we have*

$$(\partial_t^G)_{|_{t=0^+}} \left(\int_{\Omega_t} g_t \, dx_t \right) = \int_{\Omega} d_m g + \operatorname{div} V g \, dx.$$

PROOF *Case 1: Domain Ω_t perturbed by the perturbation of identity.* For a proof for considering the perturbation of identity, see, for example, Welker (2016, Theorem 4.11).

Case 2: Domain Ω_t perturbed by the velocity method. In this case, we denote the Jacobian of F_t with DF_t . Moreover, the vector field $V = V(x)$ is understood as $v(0, x)$ in (21). Then, we get

$$\begin{aligned} (\partial_t^G)_{|_{t=0^+}} \left(\int_{\Omega_t} g_t \, dx_t \right) &= (\partial_t^G)_{|_{t=0^+}} \left(\int_{\Omega} (g_t \circ F_t) \cdot \det(DF_t) \, dx \right) \\ &= \int_{\Omega} (\partial_t^G)_{|_{t=0^+}} ((g_t \circ F_t) \cdot \det(DF_t)) \, dx \\ &= \int_{\Omega} \underbrace{(\partial_t^G (g_t \circ F_t))_{|_{t=0^+}}}_{=d_m g} \underbrace{\det(DF_0)}_{=\det \operatorname{id}=1} + \underbrace{(g_0 \circ F_0)}_{=g} \partial_t^G (\det(DF_t))_{|_{t=0^+}} \, dx. \end{aligned}$$

Moreover, we have

$$\partial_t^G (\det(DF_t))_{|_{t=0^+}} = \underbrace{\det(DF_0)}_{=1} \operatorname{tr} \left((DF_0)^{-1} \partial_t^G (DF_t)_{|_{t=0^+}} \right) = \operatorname{tr}(DV) = \operatorname{div} V,$$

$$\text{where } DV = \begin{bmatrix} \frac{\partial V_1}{\partial x_1} & \cdots & \frac{\partial V_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial V_n}{\partial x_1} & \cdots & \frac{\partial V_n}{\partial x_n} \end{bmatrix}. \text{ This completes the proof. } \blacksquare$$

We are now able to prove Lemma 1.

PROOF For an easier understanding and notation purpose we define

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

such that

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

Let

$$\begin{aligned} G(\Omega, y, v)[V] &:= \int_{\mathcal{X}} d_m \left(\frac{1}{2}(y - \bar{y})^2 - \chi(y, v) + fv + \max\{0, \lambda + \mathcal{C}(y - \varphi)\}v \right) \\ &\quad + \operatorname{div}(V) \left[\frac{1}{2}(y - \bar{y})^2 + \chi(y, v) - fv \right] \, dx. \end{aligned} \quad (22)$$

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

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

$$\begin{aligned}
& - \sum_i^n d_i(\partial_i^G y d_m v + d_m y \partial_i^G v) \\
& + d_m(\max\{0, \lambda + \mathcal{C}(y - \varphi)\})v + \max\{0, \lambda + \mathcal{C}(y - \varphi)\}d_m v \, dx,
\end{aligned}$$

as well as

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

Combining the Gâteaux semiderivative of the maximum function with the equality (17) and the assumption that ∂A is a measure zero set, gives

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

In addition, we know that

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

if we assume that \bar{y} and f are independent of the shape.

Next, we consider the state equation (15) and the Gâteaux adjoint (18). Since the state and adjoint equation are formulated in weak forms, we can use $d_m y$ and $d_m v$ as test functions by piecewise integration and splitting the integral over \mathcal{X} even if they are only from broken Sobolev spaces.

Thus, we get

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

$$\begin{aligned}
& - \sum_i^n d_i \left(-v \sum_l \partial_l^G y \partial_i^G V_j - y \sum_l \partial_l^G v \partial_i^G V_j \right) dx \\
& + \int_A (y - \bar{y}) d_m y \, dx.
\end{aligned}$$

In the active set A , we have $y = \varphi$.

Moreover, the equation $d_m \varphi = \nabla \varphi^\top V$ holds. Thus, the integral over the active set is given by

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

Combining this with Lemma 2 we see that

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

Therefore, $d^G \mathcal{L}$ is given by G . ■

REMARK 2 *It is worth mentioning that the Gâteaux adjoint equation (18) and the Shape derivative given in Lemma 1 are the limit object in Luft, Schultz and Welker (2020, Theorem 3.3) and Luft, Schultz and Welker (2020, 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 Luft, Schultz and Welker (2020, Section 4), the Lagrangian is given by*

$$\mathcal{L}(y, \Omega, v) = \int_{\mathcal{X}} \frac{1}{2} (y - \bar{y})^2 - \nabla y^\top \nabla v - f v + \max\{0, \lambda + \mathcal{C}(y - \varphi)\} v \, dx.$$

Then, Lemma 1 yields the Gâteaux semiderivative

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

which confirms the limit object given in Luft, Schultz and Welker (2020, equality (43)).

Gâteaux optimality system

Here, we summarize the optimality conditions. For a solution shape Ω to problem (4)–(5), there holds the Gâteaux adjoint variational equation (18). Since

the Gâteaux semiderivative $d^G \mathcal{L}(\Omega, y, v)[V]$, given in Lemma 1, is continuous in V , we obtain from (14) the following necessary condition for the optimal shape Ω :

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

The Gâteaux adjoint equation, this necessary condition and the state equation (5) define together a set of equations, which is used for the computation of the solution in Luft, Schultz and Welker (2020), where a perturbation approach is used for construction of $d^G \mathcal{L}(\Omega, y, v)[V]$. We observe also that $d^G \mathcal{L}(\Omega, y, v)[V]$ is an integral on \mathcal{X} , where the integrand is Gâteaux 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, $d^G \mathcal{L}(\Omega, y, v)[V]$ is a Gâteaux shape semiderivative and can therefore be used, in order to define a descent direction by employing an appropriate scalar product. In Luft, Schultz and Welker (2020), the same expression has been derived in a perturbation approach, which necessitates a safeguard technique. To be more precise, there are limit objects of the regularized problem, used in Luft, Schultz and Welker (2020), but it is not guaranteed that the limit object of the regularized shape derivative yields a gradient in the classical sense in such a way that it is a descent direction. Therefore, a safeguard technique that checks if the limit object provides a descent direction is necessary in the algorithm based on the approach in Luft, Schultz and Welker (2020).

5. Conclusion

In this paper, the concept of the Gâteaux semiderivative is used to generalize some objects and methods for shape calculus. One of the major advantages of the Gâteaux approach is that one no longer needs to regularize the variational inequality constraint in optimization problems. Moreover, a limit process as in Luft, Schultz and Welker (2020) can be avoided. Considering Gâteaux semiderivatives results in an approach for the obstacle problem. In addition, this paper explains the limiting expression for the shape derivative, given in Luft, Schultz and Welker (2020) now as an expression derived from a Gâteaux adjoint.

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