On shape optimization with non-linear partial differential equations

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Abstract

This thesis is concerned with shape optimization problems under non-linear PDE (partial differential equation) constraints.

We give a brief introduction to shape optimization and recall important concepts such as shape continuity, shape derivative and the shape differentiability. In order to review existing methods for proving the shape differentiability of PDE constrained shape functions a simple semi-linear model problem is used as constraint. With this example we illustrate the conceptual limits of each method.

In the main part of this thesis a new theorem on the differentiability of a minimax function is proved. This fundamental result simplifies the derivation of necessary optimality conditions for PDE constrained optimization problems. It represents a generalization of the celebrated Theorem of Correa-Seeger for the special class of Lagrangian functions and removes the saddle point assumption. Although our method can also be used to compute sensitivities in optimal control, we mainly focus on shape optimization problems. In this respect, we apply the result to four model problems: (i) a semi-linear problem, (ii) an electrical impedance tomography problem, (iii) a model for distortion compensation in elasticity, and finally (iv) a quasi-linear problem describing electro-magnetic fields.

Next, we concentrate on methods to minimise shape functions. For this we recall several procedures to put a manifold structure on the space of shapes. Usually, the boundary expression of the shape derivative is used for numerical algorithms. From the numerical point of view this expression has several disadvantages, which will be explained in more detail. In contrast, the volume expression constitutes a numerically more accurate representation of the shape derivative. Additionally, this expression allows us to look at gradient algorithms from two perspectives: the Eulerian and Lagrangian points of view. In the Eulerian approach all computations are performed on the current moving domain. On the other hand the Lagrangian approach allows to perform all calculations on a fixed domain. The Lagrangian view naturally leads to a gradient flow interpretation. The gradient flow depends on the chosen metrics of the underlying function space. We show how different metrics may lead to different optimal designs and different regularity of the resulting domains.

In the last part, we give numerical examples using the gradient flow interpretation of the Lagrangian approach. In order to solve the severely ill-posed electrical impedance tomography problem (ii), the discretised gradient flow will be combined with a level-set method. Finally, the problem from example (iv) is solved using B-Splines instead of level-sets.

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Contents

Chapter 1

Introduction

He who seeks for methods
without having a definite problem in mind
seeks in the most part in vain.
David Hilbert

Shape optimization

Shape optimization has gained an increasing attention from the theoretical and application points of view. Many problems from real world applications can be recasted as shape optimization problems. It has proved its indispensability in many applications such as drag reduction of aircrafts, cars and boats, electrical impedance tomography [32, 54] and image segmentation [56].

In general, a shape optimization problem consists of a *cost/shape function* $J(\Omega, u(\Omega))$ with arguments $\Omega \subset \mathbf{R}^d$ and $u(\Omega)$, where the *state* u satisfies the *constraint* $E(\Omega, u(\Omega)) = 0$. The objective then is to minimize the cost function $J : \Xi \to \mathbf{R}$ over some *admissible subset* Ξ of $2^{\mathbf{R}^d} := \{\Omega : \ \Omega \subset \mathbf{R}^d\}$, i.e.

$$\begin{aligned} &\text{minimize } J(\Omega, u(\Omega)) \text{ over } \ (\Omega, u) \in \Xi \times \mathcal{X}(\Omega) \\ &\text{subject to } u = u(\Omega) \text{ solves } E(\Omega, u(\Omega)) = 0, \end{aligned} \tag{1.1}$$

where $\mathcal{X}(\Omega)$ is usually a function space. The constraint $E(\Omega, u(\Omega)) = 0$ could be a partial differential equation (PDE) or systems of PDEs such as the Navier-Stokes equation [84] or Maxwell's equations [53, 102]. A specific Ξ could be the set of all open subsets of a set D.

A unique characteristic of shape optimization is that it makes bonds from different areas of mathematics, such as *differential geometry, Riemmanian geometry, real and complex analysis, partial differential equations*, *topology* and *set theory*. The main difficulty arises because of the absence of a vector space structure of the set of sets $2^{\mathbf{R}^d}$. Thus one cannot apply standard tools from real analysis such as the Fréchet or the Gateaux derivative to investigate (1.1). One may circumvent this obstacle by identifying sets with functions and giving the space of these functions a *Lie group* or *manifold structure* as detailed below; cf. [37, 72, 73, 95].

In order to study the behavior of shape functions with respect to domain variations *shape sensitivity analysis* was introduced. In [100] the hereafter described velocity method was adopted for this purpose. We refer to [90] for the computation of material derivatives for various PDEs. Let a shape function $J : \Xi \to \mathbf{R}$ on some admissible set $\Xi \subset \{\Omega : \ \Omega \subset D \subset \mathbf{R}^d\}$ and a set $\Omega \subset D$ contained in a bigger set D be given. Then the domain Ω is perturbed by a suitable family of diffeomorphisms $\Phi_t : \overline{D} \to \overline{D}$, $t \geq 0$, with $\Phi_0 = \mathrm{id}$. The result is a family of new domains $\Omega_t := \Phi_t(\Omega)$, $t \geq 0$. One may define the diffeomorphisms Φ_t as the flow of a vector field $\theta : \overline{D} \to \mathbf{R}^d$. We define then the *Eulerian semi-derivative* (if it exists) as limit

$$dJ(\Omega)[\theta] := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}.$$

If the map $\theta \mapsto dJ(\Omega)[\theta]$ is linear and continuous, then it is termed *shape derivative*. Shape sensitivity was first used by Hadamard in his study of elastic plates; cf. [49]. The famous "structure theorem" of shape optimization states that under certain assumptions the shape derivative is a distribution acting on the normal part $\theta \cdot n$ of the perturbation field θ on the boundary $\partial\Omega$. In 1907, J. Hadamard [49] used displacements along the normal to the boundary Γ of a C^∞-domain to compute the derivative of the first eigenvalue of the clamped plate. The structure theorem for shape functionals on open domains with a C^{k+1}-boundary is due to J.-P. Zolésio [101] in 1979. The generalization of the structure theorem to an arbitrary domain was done in the paper [40, Thm. 3.2 and Rem. 3.1, Cor. 1] in 1992. It says that the shape gradient is a finite order distribution with support the boundary of the set and normal to the boundary.

In most cases, when the boundary is regular enough the boundary expression may be written in integral form

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} \tilde{g}\, n \cdot \theta \, ds, \tag{1.2}$$

where $\tilde{g} : \Gamma \to \mathbf{R}$ is usually the restriction of a function defined in a neighborhood of $\partial\Omega$. The formula (1.2) is often called the Hadamard formula.

For *state constrained* shape optimization problems, where the state is a partial differential equation, the shape differentiability may be difficult to prove depending on the PDE. One procedure is to derive the shape differentiability as follows. One may express the cost function $g(z)$ (z being an element of a topological vector space) of PDE constrained shape optimization problems as a minimax of a Lagrangian function G taken over vector spaces X and Y, i.e.,

$$g(z) = \min_{x \in X} \max_{y \in Y} G(z, x, y).$$

The problem of the shape differentiability of the cost function is transported to the differentiability of the minimax. Theorems on the differentiability of a minimax function with or without saddle point condition have a long history. The pioneering work in this area was done by Demjanov (cf. [42]) as early as 1968. Correa and Seeger gave in [30] a direct theorem on the differentiability of $g(z)$, where $z \in Z$, Z a locally convex space, and $(x, y) \in X \times Y$, X and Y two Hausdorff topological spaces (see also methods of non-smooth analysis in their bibliography). Since spaces of shapes or domains are not locally convex spaces[1], [36] reformulated the hypotheses of the previous theorems to make them readily applicable to the computation of the shape derivative. Some of those theorems were sharpened by Delfour and Morgan [33, Thm. 3] and extended to ϵ-solutions in [34]. In [35] an interesting penalization method was introduced where the state is the solution of a variational inequality. We would like to emphasize that until now none of the mentioned methods are applicable to non-linear problems without further assumptions, such as that G has saddle points.

Other methods which may be used to derive the shape differentiability are the following:

[1] In fact certain spaces of shapes can be identified as infinite dimensional Riemannian manifolds. We come back to this topic in Chapter 6.

1. The "chain rule approach" or material derivative method is as follows. In this approach the *material derivative* is introduced to derive the shape differentiability. The material derivative can be interpreted as the derivative of the state with respect to the domain and only occurs in an intermediate step and is not present in the final formula of the shape derivative. The terminology of the material derivative originates from continuum mechanics where it describes the time rate of change of some physical quantity, such as the mass, for a material element subjected to a time dependent velocity field. From the optimal control point of view this is nothing but the derivative of the control–solution operator, where the control is the domain and the solution is some function solving a PDE.

2. Another (formal) method that is often used to derive the boundary expression, which has to be used with caution because it *may yield the wrong formula*[2] is due to [23]. This method, also known as *Céa's Lagrange method*, uses the same Lagrangian as the minimax formulation, but requires that the shape derivatives of the state and the adjoint equation exist and belong to the solution space of the PDE. There are examples (see [82]), where Céa's Lagrange method fails.

3. In the recent paper [60] a *rearrangement method* was proposed. This method allows to prove the shape differentiability under the assumption that the domain-solution operator is Hölder continuous with an exponent bigger than $1/2$ and admits a second order expansion with respect to the unknown. No convexity of the state or the cost is needed. However it requires a first order expansion of the PDE and cost function with respect to the unknown such that the remainder vanishes with order two. Finally, we mention that there is an interesting *penalization method* introduced in [35].

Current trends

A natural way to deal with domains is by identifying them with functions. There are several methods to identify domains with functions, two of these will be further explained for the planar case of $\mathbf{R}^2$.

In the first approach simply connected domains Ω in the plane, with boundary Γ, are identified with immersed or embedded[3] curves γ which map from the circle S^1 onto the boundary Γ as done in [72]. Since a reparametrization of the curve does not affect the image Γ one is led to consider equivalence classes of curves. Two curves are equivalent, written $\gamma \sim \tilde{\gamma}$, if there exists $\varphi \in \mathrm{Diff}(S^1)$ such that $\gamma = \tilde{\gamma} \circ \varphi$. The space $B_e := \mathrm{Emb}(S^1; \mathbf{R}^2)/\mathrm{Diff}(S^1)$ comprising equivalence classes of embedded curves is a special case of a *manifold of mappings*. It can be given a Riemannian structure by introducing appropriate metrics; [71, 73, 93, 98]. With the identification of domains $\Omega \subset \mathbf{R}^2$ with functions $\gamma \in B_e$, we may identify a shape function $J(\Omega)$ with $\tilde{J}(\gamma) := J(\mathrm{int}(c))$, where $\mathrm{int}(\gamma)$ is the interior of $\Gamma := \partial\Omega$, that is, Ω. The link between the shape derivative in the form (1.2) and the derivative of $\hat{J}$ on the shape space B_e was given by [86]. The main benefit of this view is that on Riemannian manifolds minimization methods such as *BFGS*[4], *steepest descent, Newton* and *quasi-Newton methods* as well as their convergence analysis are available; cf. [2, 85, 86].

[2] We come back to this method in Subsection 3.5.

[3] The quotient $B_i := \mathrm{Imm}(S^1; \mathbf{R}^2)/\mathrm{Diff}(S^1)$ is no manifold, but only an orbifold.

[4] Is an abbreviation for Broyden-Fletcher-Goldfarb-Shanno.

An alternative approach of [70] defines admissible domains $\Omega \subset \mathbf{R}^2$ by $\Omega = (f+\mathrm{id})(\omega_0)$, $f \in C_0^k(\mathbf{R}^2, \mathbf{R}^2), k \geq 1$ and some fixed open domain $\omega_0 \subset \mathbf{R}^d$. Formally, setting $\Theta := C_b^{0,1}(\mathbf{R}^d, \mathbf{R}^d)$[5], an appropriate space is given by

$$\mathcal{F}(\Theta) := \{\mathrm{id} + f : \, f \in \Theta, \, f + \mathrm{id} \text{ is bijective and } (f+\mathrm{id})^{-1} - \mathrm{id} \in \Theta\}.$$

Since one is usually interested in the image of the mappings, we consider the group $\mathcal{S}_{\omega_0} := \{F \in \mathcal{F}(\Theta) : F(\omega_0) = \omega_0\}$. Now we introduce the equivalence relation between two functions $F, \tilde{F} \in \mathcal{F}(\Theta)$, written $F \sim \tilde{F}$ by $F \circ h = \tilde{F}$ for some $h \in \mathcal{S}_{\omega_0}$. As for the space B_e the important role plays the quotient $H_e := \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$ on which a right invariant metric, called *Courant metric*, can be introduced to make the space H_e a complete metric group [37]. The equivalence relation is nothing but the right action of $\mathcal{S}_{\omega_0}$ on the group $\mathcal{F}(\Theta)$ and induces a natural projection $\pi : \mathcal{F}(\Theta) \to \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$, by $f \mapsto f \circ \mathcal{S}_{\omega_0}$. By construction, we may identify the quotient $\mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$ with the image set $\mathcal{Z}(\omega_0) := \{F(\omega_0) : F \in \mathcal{F}(\Theta)\}$ via the bijection $F \mapsto F(\omega_0)$.

In 1993, the problem of comparing medical scans arising in medical imaging led to the construction of deformations defined by $\varphi(x) := x - u(x)$, where u is a smooth displacement in the plane [69] which is smoothed by a Sobolev type energy minimization. Since this displacement allows not for arbitrary large deformations the velocity method was used by [14, 95] to construct deformations via the flow of a vector fields. More precisely the authors considered the group $\mathcal{G} := \{\Phi_1^\theta : \theta \text{ vector field}\}$ of all flows evaluated at $t = 1$. Also in this case a right invariant metric may be introduced making the space $\mathcal{G}$ a complete metric group.

Finally, we mention that spaces of shapes can also be generated by distance functions, signed distance functions and characteristic functions, but lead to less differentiable structures.

The previous considerations show that by identifying sets with functions, we can employ most of the features from smooth analysis on infinite dimensional manifolds. This will be a cornerstone for future numerical and theoretical investigations of constrained shape optimization problems.

The objective of this thesis

The main contributions of this thesis are:

- In this thesis, we present a novel approach to the differentiability of a minimax, without a saddle point assumption when the function G is a Lagrangian, that is, a utility function plus a linear penalization of the state equation. Until now the assumptions to apply the minimax theorems required that the Lagrangian is a concave-convex function or other hypotheses have to be satisfied that are not easy to be proved or even fail to be true. The novelty of the new approach is to replace the usual adjoint state equation by an averaged adjoint state equation. For problems where the function is a Lagrangian this result allows us now to compute sensitivities for a very broad class of shape optimization problems contained by linear, semi-linear and also quasi-linear partial differential equations.

- Most numerical simulations use the boundary expression (1.2) or to be more precise the pointwise descent direction $\theta := -g\,n$. It is well known that due to low regularity of

[5]The space $C_c^{0,1}(\mathbf{R}^d, \mathbf{R}^d)$ comprises all bounded Lipschitz continuous functions $f : \mathbf{R}^d \to \mathbf{R}^d$. This space is a Banach space when endowed with the usual norm.

g the algorithm may be unstable and can lead to oscillations of the moving boundary. The low regularity of g may occur if Ω is less regular or the cost function involves high order derivatives of the solution of the PDE or the solution of the PDE has low regularity. Besides introducing penalizations, one way to get around this is to consider the alternative representation of the shape derivative as a domain integral, i.e. $dJ(\Omega)[\theta] = \int_\Omega F(\theta)\,dx$, where F is an operator acting on θ. This expression is more general than the boundary expression and is even defined for quite irregular domains Ω, where no boundary expression is available. It has been overlooked for mainly two reasons:

- the difficulty to obtain descent directions,
- the computational effort seems to be bigger since a space dimension is added.

We will make the volume expression accessible for numerical simulations. Also we discuss why the volume expression is advantageous when combined with the level-set method.

- With the volume expression it is possible to interpret gradient algorithms as gradient flows taking values in certain groups of diffeomorphisms. This interpretation allows us to distinguish between two different ways to look at gradient algorithms: (i) from the Eulerian and (ii) from the Lagrangian. In the Eulerian approach all computations in an algorithm are performed on the current domain. On the other hand the Lagrangian approach allows to perform all calculations on a fixed domain. The gradient flow depends on the chosen metric of the underlying space. We present several possible metrics and different regularity of the resulting domains.

The structure of this thesis

Outline:

Chapter 2: This chapter gives a brief introduction to shape optimization is given and recalls some basic material from shape calculus. The essential notation used throughout this thesis is introduced. We introduce the notion of the shape derivative and the structure theorem of Zolésio. Many useful properties of the flow associated with vector field are derived.

Chapter 3: In this chapter various methods available to calculate the so-called shape derivative are reviewed. The methods range from the classical material derivative method [90] (also called chain rule approach), over the minimax approach of Correa-Seeger applied to shape optimization by Delfour and Zolésio ([36]), to the recent rearrangement method of [60]. Finally, we consider a theorem on the differentiability of a min function, that allows the calculation of sensitivities for energy functionals. In order to illustrate the methods a simple quasi-linear partial differential equation is used.

Chapter 4: A novel approach to the differentiability of a minimax, without a saddle point assumption when the function is a Lagrangian, that is, a utility function plus a linear penalization of the state equation, is presented. Its originality is to replace the usual adjoint state equation by an averaged adjoint state equation. When compared to the former theorems in [36, Sect. 4, Thm. 3, p. 842] and in [33, Thm. 3, p. 93], all the hypotheses are now verified for a Lagrangian function without going to the dual problem and it relaxes the classical continuity assumptions on the derivative of the Lagrangian involving both the state and adjoint state to continuity assumptions that only involve the averaged adjoint state.

Chapter 5: The results from Chapter 4 are applied to three transmission problems and the semi-linear problem from Chapter 3: (i) a sharp interface model of distortion compensation in elasticity (ii) an electrical impedance tomography problem, (iii) a quasi-linear transmission problem and (iv) a simple quasi-linear problem. For the examples (i) – (iii) the existence of optimal shapes via a standard perimeter and a Gagliardo penalization (also called fractional perimeter penalization) is discussed.

Chapter 6: This chapter deals with the theoretical treatment of shape optimization problems. The novel part is the usage of the volume expression of the shape derivative, which has been ignored so far. We compare different metrics generating gradient flows in the spaces of shapes.

Chapter 7: The methods introduced in Chapter 3 are applied to the examples introdcued before. It is shown that the volume expression is superior when compared to the boundary expression.

Chapter 2

Introduction to shape optimization

In this chapter, we introduce shape functions along with an appropriate notion of continuity and differentiability. We recall the celebrated structure theorem of Hadamard-Zolésio which provides us with the canonical structure of shape derivatives. Finally, we study flows generated by vector fields. For the convenience of the reader, we list below all used symbols and function spaces.

2.1 Notation

We mostly use notations and definitions of the Amman-Escher book series [7, 8, 9]. Some definitions can be found in [37]. Let $\boldsymbol{f} : \Omega \subset \mathbf{R}^d \to \mathbf{R}^d$ and $\phi : \Omega \subset \mathbf{R}^d \to \mathbf{R}$ be given functions defined on a set Ω with boundary Γ.

- Measures and sets:

$\mathbf{N}, \mathbf{Z}, \mathbf{R}$	natural numbers, integers, real numbers
$\overline{\mathbf{R}}, \overline{\mathbf{R}}^+$	extended (non-negative) real numbers $\mathbf{R} \cup \{\pm\infty\}$
	and $\{x \geq 0\} \cap \mathbf{R} \cup \{\infty\}$
$\mathbf{R}^d$	d - times product of $\mathbf{R}$
E, F	Banach spaces with norms $\\|\cdot\\|_E, \\|\cdot\\|_F$
$\mathrm{int}(\Omega),\ \partial\Omega,\ \overline{\Omega}$	interior, boundary and closure of a set $\Omega \subset \mathbf{R}^d$
2^Ω	set of all subsets of Ω, *i.e.*, $\{\tilde{\Omega} : \tilde{\Omega} \subset \Omega\}$
$T_D(x), C_D(x)$	Bouligand and Clarke tangent cone of D at $x \in \overline{D}$
$\mathrm{supp}(\phi)$	support of a function ϕ, i.e., $\overline{\{x \in \mathbf{R}^d :\ \phi \neq 0\}}$
Y^X	set of all functions from X into Y
$\lfloor s \rfloor$	the biggest integer less or equal to s
$df(x; v)$	directional derivative of $f : \Omega \subset E \to F$
	at $x \in \Omega$ in direction v
$d_{\mathrm{H}} f(x; v)$	Hadamard semi-derivative at $x \in \Omega$ in direction $v \in E$
$\partial f(x)$	Fréchet derivative at x; it is an element of $\mathcal{L}(E, F)$
$\partial_\gamma f(x)$	partial derivative $\frac{\partial^{\|\gamma\|} f}{\partial^{\gamma_1} x_1 \cdots \partial^{\gamma_d} x_d}$, where $\gamma = (\gamma_1, \ldots, \gamma_d)^\top \in \mathbf{N}^d$
	and $\|\gamma\| := \gamma_1 + \cdots + \gamma_d$
$\nabla\phi$	gradient defined by $\partial f(x)(v) = \nabla\phi \cdot v$ for all $v \in \mathbf{R}^d$
$\nabla_\Gamma \phi$	tangential gradient $\nabla\phi_{\,\|\Gamma} - \partial_n \phi_{\,\|\Gamma}\, n$

$\partial_\Gamma \boldsymbol{f}\|_\Gamma$	tangential gradient $\partial \boldsymbol{f}\|_\Gamma - (\partial_n \boldsymbol{f}) \otimes n$
$\varepsilon(\boldsymbol{f})$	symmetrised gradient $\frac{1}{2}(\partial \boldsymbol{f} + \partial \boldsymbol{f}^\top)$
J	rotation matrix $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$A^\top, A^{-1}$	transpose and inverse of a matrix

- Function spaces:

$\mathcal{L}(\mathbf{E}, \mathbf{F})$	space of linear and continuous mappings from E into F
$\mathcal{L}\mathrm{is}(\mathbf{E}, \mathbf{F})$	space of mappings $A \in \mathcal{L}(\mathbf{E}, \mathbf{F})$ with inverse $A^{-1} \in \mathcal{L}(\mathbf{F}, \mathbf{E})$
$C^k(\Omega)$	space of k-times continuously differentiable mappings from Ω into $\mathbf{R}$
$C_c^k(\Omega)$	space of function $f \in C^k(\Omega)$ such that $\mathrm{supp} f \subset \Omega$
$C^{0,\alpha}(\Omega)$	Hölder space with exponent $0 < \alpha < 1$ (also denoted $C^\alpha(\Omega)$)
$C^{k,\alpha}(\Omega)$	subspace of function $f \in C^k(\Omega)$ such that the k-th order derivatives belong to $C^\alpha(\Omega)$, $0 < \alpha < 1$, $k \geq 0$
$C(\overline{\Omega})$	space of continuous functions that are bounded on $\overline{\Omega}$
$L_p(\Omega)$	standard space of measurable function that are p-integrable $(1 \leq p < \infty)$
$L_\infty(\Omega)$	space of essentially bounded functions on Ω
$W_p^k(\Omega)$	standard Sobolev space of k-times weakly differentiable functions with weak derivative in $L_p(\Omega)$ $(1 \leq p \leq \infty, 0 \leq k < \infty)$
$W_p^s(\Omega)$	standard fractional Sobolev space with $s \geq 0$ a real number (see the appendix for a definition)
$\mathrm{Hom}(\mathbf{E})$	space of continuous functions $f : \mathbf{E} \to \mathbf{E}$ with continuous inverse f^{-1}
$\mathrm{Diff}^k(\mathbf{E}, \mathbf{F})$	space of k-times Fréchet differentiable functions $f : \mathbf{E} \to \mathbf{F}$ with inverse $f^{-1} \in C^k(\mathbf{F}, \mathbf{E})$
$X(D)$	characteristics function χ_Ω, with Lebesgue measurable $\Omega \subset D$
$BV(D)$	function space of bounded variations
$\mathfrak{B}(D)$	subspace of $X(D)$ such that $\chi \in BV(D)$
$\mathrm{Lip}_0(D, \mathbf{R}^d)$	Lipschitz continuous functions $\theta : \overline{D} \to \mathbf{R}^d$ such that $\pm\theta(x) \in C_D(x)$ for all $x \in \overline{D}$
$C^{0,1}(\overline{D}, E)$	space of Banach space valued functions $f : \overline{D} \to E$ that are Lipschitz continuous
$C_b^k(\mathbf{R}^d, \mathbf{R}^d)$	space of k-times differentiable functions, whose derivatives are bounded
$C_{b,0}^k(\mathbf{R}^d, \mathbf{R}^d)$	space of k-times differentiable functions, whose derivatives vanish at infinity
$C_b^{0,1}(\mathbf{R}^d, \mathbf{R}^d)$	space of bounded and Lipschitz continuous functions

The vector valued versions of $C^k(\Omega), C_c^k(\Omega), C^{k,\alpha}(\Omega), C^{0,\alpha}(\Omega), \ldots,$ etc. are denoted by $C^k(\Omega, \mathbf{R}^d), C_c^k(\Omega, \mathbf{R}^d), C^{k,\alpha}(\Omega, \mathbf{R}^d), C^{0,\alpha}(\Omega, \mathbf{R}^d), \ldots,$.

$$
\begin{array}{lll}
\|f\|_{L_p(\Omega)} & := & \left(\int_\Omega |f|^p dx\right)^{1/p} \\
\|f\|_{L_\infty(\Omega)} & := & \operatorname{ess\,sup}_{x\in\Omega} |f(x)| \\
|f|_{C^{0,\alpha}(\Omega)} & := & \sup_{\substack{x\neq y\\ x,y\in\Omega}} \frac{|f(x)-f(y)|}{|x-y|^\alpha} \\
\|f\|_{C(\overline{\Omega})} & := & \sup_{x\in\Omega} |f(x)| \\
\|f\|_{C^{k,\alpha}(\Omega)} & := & \sum_{|\gamma|\le k} \|\partial_\gamma f\|_{C(\Omega)} + \sum_{|\gamma|=k} |\partial_\gamma f|_{C^{0,\alpha}(\Omega)} \quad (\gamma = (\gamma_1,\ldots,\gamma_d)^\top \in \mathbf{N}^d) \\
|f|_{W_p^s(\Omega)} & := & \int_\Omega\int_\Omega \frac{|f(x)-f(y)|^p}{|x-y|^{sp+d}} dxdy \quad p\ge 1, 0<s<1 \\
\|f\|_{W_p^k(\Omega)} & := & \left(\sum_{|\gamma|\le k} \|\partial_\gamma f\|^p_{L_p(\Omega)}\right)^{1/p} \quad 1<p<\infty \\
\|f\|_{W_\infty^k(\Omega)} & := & \sum_{|\gamma|\le k} \|\partial_\gamma f\|_{L_\infty(\Omega)} \\
\|f\|_{W_p^s(\Omega)} & := & \|f\|_{W_p^{\lfloor s\rfloor}(\Omega)} + \sup_{|\gamma|=\lfloor s\rfloor} |\partial_\gamma f|_{W_\eta^p(\Omega)} \\
\|f\|_{L_p(\Omega)} & := & \left(\int_\Omega |f|^p dx\right)^{1/p} \\
\|f\|_{L_\infty(\Omega)} & := & \operatorname{ess\,sup}_{x\in\Omega} |f(x)| \\
|f|_{C^{0,\alpha}(\Omega)} & := & \sup_{\substack{x\neq y\\ x,y\in\Omega}} \frac{|f(x)-f(y)|}{|x-y|^\alpha} \\
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\|f\|_{W_p^k(\Omega)} & := & \left(\sum_{|\gamma|\le k} \|\partial_\gamma f\|^p\right)^{1/p} \quad 1<p<\infty \\
\|f\|_{W_\infty^k(\Omega)} & := & \sum_{|\gamma|\le k} \|\partial_\gamma f\|_{L_\infty(\Omega)} \\
\|f\|_{W_p^s(\Omega)} & := & \|f\|_{W_p^{\lfloor s\rfloor}(\Omega)} + \sup_{|\gamma|=\lfloor s\rfloor} |\partial_\gamma f|_{W_\eta^p(\Omega)}
\end{array}
$$

Next we list some useful operations from tensor algebra. The coordinate free definitions from [12, pp. 399-404] are used.

- Tensor algebra:

$$
\begin{aligned}
(\mathbf{u}\otimes \boldsymbol{v})\boldsymbol{w} &:= (\boldsymbol{v}\cdot\boldsymbol{w})\mathbf{u} \qquad (\mathbf{u},\boldsymbol{v}\in\mathbf{R}^d,\ \forall \boldsymbol{w}\in\mathbf{R}^d) \\
(\mathbf{a}\otimes\mathbf{b}) : (\mathbf{c}\otimes\mathbf{d}) &:= (\mathbf{a}\cdot\mathbf{c})\ (\mathbf{b}\cdot\mathbf{d}) \qquad (\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\in\mathbf{R}^d) \\
|\mathbf{A}| &:= \sqrt{(\mathbf{A}:\mathbf{A})} \qquad (\mathbf{A}\in\mathbf{R}^{d,d}) \\
\operatorname{tr}(\mathbf{A}) &:= \mathbf{A} : I
\end{aligned}
$$

- Tensor algebra calculus rules:

Let $\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\in\mathbf{R}^d$ and $\mathbf{A},\mathbf{B}\in\mathbf{R}^{d,d}$ then

$$
\begin{aligned}
(\mathbf{a}\otimes\mathbf{b})\cdot(\mathbf{c}\otimes\mathbf{d}) &= (\mathbf{b}\cdot\mathbf{c})\ \mathbf{a}\otimes\mathbf{d} \\
\mathbf{A} : (\mathbf{c}\otimes\mathbf{d}) &= \mathbf{c}\cdot\mathbf{A}\mathbf{d} \\
(\mathbf{a}\otimes\mathbf{b}) : (\mathbf{c}\otimes\mathbf{d}) &= (\mathbf{c}\otimes\mathbf{d}) : (\mathbf{a}\otimes\mathbf{b}) \\
\mathbf{A} : \mathbf{B} = \mathbf{B} : \mathbf{A} &= \mathbf{A}^\top : \mathbf{B}^\top \\
\operatorname{tr}(\mathbf{A}\mathbf{A}^\top) = \mathbf{A} : \mathbf{A} &= |\mathbf{A}|^2
\end{aligned}
$$

2.2 General shape optimization problems

The main focus of shape optimization is to examine shape functions. Their domain of definition is no subset of a topological vector space and thus a direct application of standard tools known from topological vector spaces is not possible. These functions require therefore the development of special notions of continuity and differentiability, which will be recalled subsequently.

Definition 2.1. *Let $D \subset \mathbf{R}^d$ be a set and $\Xi \subset 2^D := \{\Omega : \Omega \subset D\}$*[1] *be a set of subsets. Then a function*

$$J : \Xi \to \mathbf{R} : \quad \Omega \to J(\Omega)$$

is called shape function*.*

A typical shape optimization problem is of the form

$$\min J(\Omega) \qquad \text{over } \Omega \in \Xi, \tag{2.1}$$

where $\Xi \subset 2^{\mathbf{R}^d}$ is called *admissible* set. As already indicated in (1.1), the shape function J might implicitly depend on a partial differential equation (PDE) or other constraints. For examples we refer the reader to Chapter 5. When J depends on the solution of a PDE, we call the shape optimization problem *PDE constrained* or *state constrained*.

Example 2.2. *A possible choice of an admissible set Ξ could be the set of all open subsets $\Omega \subset D$ of an open and bounded subset $D \subset \mathbf{R}^d$. Examples of unconstrained shape functions are*

$$J_1(\Omega) = \int_\Omega f\,dx \qquad \text{and} \qquad J_2(\Omega) = \int_{\partial\Omega} \kappa\,ds.$$

Here, for J_1 we may assume $f \in L_1(\mathbf{R}^d)$ and for J_2 the boundary $\partial\Omega$ has to be sufficiently smooth, say C^2, in order to make sense of the curvature κ of $\partial\Omega$. An example of a PDE constrained shape function is

$$J_3(\Omega) = \int_\Omega |u(\Omega) - u_r|\,dx, \qquad \text{where } \begin{aligned} -\Delta u(\Omega) &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

where $u_r \in L_1(D)$ is a given target function.

Throughout this thesis we choose to work with special sets $D \subset \mathbf{R}^d$.

Definition 2.3. *We call a subset $D \subset \mathbf{R}^d$ a* regular domain *if it is a simply connected and bounded domain with Lipschitz boundary $\Sigma := \partial D$. Moreover, we say that D is a k-*regular domain*, $k \geq 1$, if D is a regular domain and its boundary Σ is of class C^k in the sense of [37, p. 68, Definition 3.1].*

Regular sets according to our definition are not the most general sets we could consider, but they serve our purpose and are sufficient for the applications. If not stated otherwise, we assume the subset $D \subset \mathbf{R}^d$ is regular.

[1] This notation motivates from the fact, that we can associate to each $\Omega \subset D$ a characteristic function $\chi_\Omega : D \to \{0,1\} =: 2$. Then $\{\chi_\Omega : D \to \{0,1\} : \Omega \subset D\} \to \{\Omega : \Omega \subset D\} : \chi_\Omega \mapsto \Omega$ is a bijection. Moreover, for finite sets $D \subset \mathbf{R}^d$, we have $\#\{\Omega : \Omega \subset D\} = 2^{\#D}$. Here, $\#$ denotes the cardinality of a set.

There are three typical questions related to the problem (2.1): *Does an optimal solution exist?*, *What regularity does an optimal shape have?* and *Are there criteria to detect an optimum?* The first question is quite delicate. There are examples where the optimal solution is no longer a set, but a measure; cf. [19]. The reason for those obscure scenarios is the lack of compactness of the underlying space of admissible sets. One may avoid these cases by penalizing the cost function with the perimeter or the Gagliardo perimeter. Also it is possible to consider other special classes of domains in order to obtain existence of solutions; cf. [37, Chap. 8]. We discuss this topic in more detail in the present chapter, Chapter 6 and study some examples in Chapter 5. The question of regularity of optimal solutions is important for the applications since highly irregular sets that model optimal shape designs may be not manufacturable in a factory. However, this will not be further explained in the following chapters and we refer the reader to [51, Sect. 6]. The following chapters are mostly devoted to the third question.

2.3 Flows, homeomorphism and a version of Nagumo's theorem

In this section we recall important properties of *flows* (also called transformations), generated by vector fields. If a sufficiently smooth vector field has compact support in a bounded subset of $\mathbf{R}^d$, then Nagumo's classical theorem yields that the associated flows are diffeomorphisms, mapping this subset bijectively into itself. Function compositions of these flows with Sobolev functions enjoy special properties which will be reviewed in the subsequent sections.

2.3.1 The flow of a vector field

Let $D \subset \mathbf{R}^d$ be a regular domain according to Definition 2.3, $\tau > 0$ and $s \in [0, \tau]$. Then to each *vector field* $\theta : [0, \tau] \times \overline{D} \to \mathbf{R}^d$, we associate (if it exists) a *flow*.

Definition 2.4. *For fixed $\tau > 0$, $s \in [0, \tau)$ and given $x_0 \in \overline{D}$, we consider the solution $x : [0, \tau] \to \mathbf{R}^d$ of the initial value problem*

$$\dot{x}(t) = \theta(t, x(t)), \quad x(s) = x_0. \tag{2.2}$$

The flow *at $(t, x_0) \in [0, \tau] \times \overline{D}$ associated with the vector field θ is defined by $\Phi(t, s, x_0) := x(t)$. We write $\Phi_{t,s}(x) := \Phi(t, s, x)$ and define $\Phi_{t,s}^{-1}(z) := \Phi^{-1}(t, s, z)$ for each $t \in (0, \tau)$ for which $x \mapsto \Phi(t, s, x)$ is invertible. If $s = 0$ we use the abbreviation $\Phi_t := \Phi_{t,0}$.*

A flow $\Phi_{t,s}$ generated by a time-dependent vector field θ fulfills the following well-known equations for all $0 \le s' \le s \le t$

$$\begin{aligned} \Phi_{t,s} \circ \Phi_{s,s'} &= \Phi_{t,s'} \\ \Phi_{s,t} \circ \Phi_{t,s} &= \mathrm{id}. \end{aligned}$$

This identity is sometimes called *Chapman-Kolmogorov law*. Moreover, if θ is *autonomous* the previous equation reduces to: for all $s, t \ge 0$ with $s + t \in [0, \tau]$

$$\Phi_s \circ \Phi_t = \Phi_{s+t}.$$

Of course the vector fields θ has to have a certain regularity in space and time to guarantee the existence and uniqueness of a flow Φ_t. Moreover, in order to generate a homeomorphism

Φ_t from $\overline{D}$ to itself, the vector field must be tangential to the boundary ∂D. This is discussed in more detail in the subsection below.

The topology of an optimal set of problem (2.1) can be determined with the help of the topological derivative; cf. [89]. Once the topology of an optimal set is known then it is only necessary to investigate diffeomorphic transformations which preserve the topology. Therefore, we are particularly interested in vector fields θ generating flows with the properties: for all $t \in [0, \tau]$

$$\boxed{\Phi_t \in \mathrm{Hom}(\overline{D}), \quad \Phi_t(\mathrm{int}(D)) = \mathrm{int}(D), \quad \Phi_t(\partial D) = \partial D.} \tag{2.3}$$

To derive a general class of vector fields whose associated flows satisfy (2.3), we need the definition of the tangent cone at a point $x \in \overline{D}$. We write $x_n \to_D x$ if $x_n \in D$ for all $n \in \mathbf{N}$ and $x_n \to x$ as $n \to \infty$. The tangent cone is a generalisation of the tangent space for sets with non-smooth boundaries.

Definition 2.5. *The* tangent cone *of a set $D \subset \mathbf{R}^d$ at $x \in \overline{D}$ is defined as*

$$T_D(x) := \{h \in \mathbf{R}^d |\ (x_\nu - x)/\tau_\nu \to h \textit{ for some } x_\nu \to_D x,\ t_\nu \to 0\}.$$

Let $D \subset \mathbf{R}^d$ be an open and bounded set with C^1-boundary $\Sigma := \partial D$. Denote by $n := n(x)$ the unit normal vector at $x \in \Sigma$. Then $T_D(x)$ is the closed half space $H_n^+ = \{x \in \mathbf{R}^d |\ x \cdot n \geq 0\}$ and thus $h, -h \in H_n^+$ if and only if $h \cdot n = 0$ which means that h belongs to the tangent space of Σ at x, i.e. $h \in T_x\Sigma$. In other words $\pm h \in T_D(x)$ if and only if $h \in T_x\Sigma$ for $x \in \Sigma$.

Now let $x \in D$ be in the interior of D. Since we assumed D to be open, we have $\gamma(t) := x + ty \in D$ for $y \in \mathbf{R}^d$ and $t > 0$ small enough. Let $(t_n)_{n\in\mathbf{N}}$ be a sequence with $t_n \searrow 0$ as $n \to \infty$ and put $x_n := \gamma(t_n)$. Then we get $x_n \to_D x$ and $(x_n - x)/t_n \to y$. Since y was arbitrary, we conclude that if $x \in D$ then $T_D(x) = \mathbf{R}^d$. We summarise:

Lemma 2.6. *Let $D \subset \mathbf{R}^d$ be an open, bounded set with C^1-boundary $\Sigma := \partial D$. Denote the normal along Σ by n. Let a continuous function $\theta : \overline{D} \to \mathbf{R}^d$ be given. Then we have the following equivalence*

$$\forall x \in \Sigma :\ \pm\theta(x) \in T_D(x) \quad \Longleftrightarrow \quad \theta(x) \cdot n(x) = 0 \quad \Longleftrightarrow \quad \theta(x) \in T_x\Sigma.$$

Remark 2.7. *The commonly used equivalent definition of $T_D(x)$ is*

$$T_D(x) := \left\{ h \in \mathbf{R}^d :\ \liminf_{t \searrow 0} \frac{d_D(x + th)}{t} = 0 \right\},$$

where $d_D(x) := \inf_{y\in D} |x - y|$ is called distance function *associated with D. Notice also that $d_D = d_{\overline{D}}$ and hence $T_D(x) = T_{\overline{D}}(x)$.*

Remark 2.8. *Let $D \subset \mathbf{R}^d$ be a regular domain. It is essential to realise that if a bounded domain $\Omega \subset D$ has a C^k-boundary Γ, then the boundary $\Gamma_t := \Phi_t^\theta(\Gamma)$ of $\Omega_t := \Phi_t^\theta(\Omega)$ will be of class C^k too, provided θ is such that $\Phi_t(\cdot)$ belongs to $C^k(D)$. But, one has to be cautious with the notion of a Lipschitz domain, since there are several notions. We usually mean by "the boundary of Ω is Lipschitzian" that it can be locally represented by a graph of a Lipschitz function. So if Ω has a Lipschitz boundary in the above sense then it is in general not true that Γ_t is Lipschitzian if $\Phi_t(\cdot)$ is only bi-Lipschitzian, that is, $\Phi_t : \overline{D} \to \overline{D}$ and its inverse are both Lipschitzian.*

For a continuous function $\theta : \overline{D} \to \mathbf{R}^d$ the condition that $\pm\theta(x) \in T_D(x)$ for all $x \in \overline{D}$ is non-linear and equivalent to $\theta(x) \in \{-T_D(x)\} \cap T_D(x)$ for all $x \in \overline{D}$. By non-linear we understand that $\{-T_D(x)\} \cap T_D(x)$ is no linear subspace of $\mathbf{R}^d$ unless D is convex. It can be shown ([37, Thm. 5.2, p. 200]) that the condition can be reduced to the *Clarke cone* $C_D(x) \subset T_D(x)$, i.e. for all $x \in \overline{D}$: $\theta(x) \in \{-C_D(x)\} \cap C_D(x)$ if and only if for all $x \in \overline{D}$: $\theta(x) \in \{-T_D(x)\} \cap T_D(x)$. Moreover, $\{-C_D(x)\} \cap C_D(x)$ is a closed linear subspace of $\mathbf{R}^d$ and hence the constraint with the Clarke cone is now linear. Finally, the Clarke cone, which is always convex, is defined by

$$C_D(x) := \left\{ h \in \mathbf{R}^d : \liminf_{\substack{t \searrow 0 \\ y \to_D x}} \frac{d_D(x+th)}{t} = 0 \right\}.$$

2.3.2 A version of Nagumo's Theorem

Necessary and sufficient conditions to obtain viability solutions of (2.2), i.e., solutions that cannot leave the domain $\overline{D}$ and have no self intersections, were first given by [77]; cf. [13, Chap. 4].

Definition 2.9. *We call a set $D \subset \mathbf{R}^d$, (strictly) θ-*flow invariant *if $\Phi_t^\theta(\overline{D})(=) \subset \overline{D}$.*

The function Φ_t^θ is also called a (strict) *viability* solution of (2.2). It is known that the following conditions are sufficient to obtain strict viability solutions

$$\text{(V)} \qquad \theta \in C^{0,1}(\overline{D}, \mathbf{R}^d) \quad \text{and} \quad \forall x \in \overline{D} : \ \pm\theta(x) \in T_{\overline{D}}(x).$$

The first condition is the Lipschitz continuity of θ while the second ensures that the flow cannot leave the domain $\overline{D}$. To be more precise points in the interior are mapped to the interior and points of the boundary are mapped to the boundary. The following conditions are the analog to (V) for time-dependent vector fields

$$(\hat{V}\ ) \qquad \begin{aligned} \forall x \in \overline{D} :& \quad \theta(\cdot, x) \in C([0,\tau], \mathbf{R}^d) \\ \forall x, y \in \overline{D} :& \quad \|\theta(\cdot, x) - \theta(\cdot, y)\|_{C([0,\tau],\mathbf{R}^d)} \le c|x-y| \\ \forall x \in \overline{D} : \ \forall t \in [0,\tau] & \quad \pm\,\theta(t,x) \in T_{\overline{D}}(x). \end{aligned}$$

Notice that according to Lemma 2.6 for a smooth set D the last condition in (V) and $(\hat{V})$ means that $\theta(x) \cdot n(x) = 0$ on the boundary Σ of D. Moreover, any *autonomous* (time-independent) vector field θ which satisfies (V) also satisfies $(\hat{V})$.

The following result shows that the properties (V) or $(\hat{V})$ are indeed sufficient to conclude (2.3) for the associated flow.

Theorem 2.10. *Let $D \subset \mathbf{R}^d$ be a regular domain and $\tau > 0$. Then the following statements are true.*

(i) Let the flow Φ_t be generated by the vector field $\theta : \overline{D} \times [0,\tau] \to \mathbf{R}^d$ satisfying condition $(\hat{V})$. Then D is strictly θ-flow invariant. Moreover, it follows that for some constants $C, c > 0$

$$\begin{aligned} \forall x, y \in \overline{D} : \|\Phi(x) - \Phi(y)\|_{C^1([0,\tau],\mathbf{R}^d)} &\le C|x-y|, \\ \|\Phi^{-1}(x) - \Phi^{-1}(y)\|_{C([0,\tau],\mathbf{R}^d)} &\le c|x-y|, \end{aligned} \tag{2.4}$$

$$\begin{aligned} \forall x \in \overline{D} : t \mapsto \Phi_t(x) &\in C^1([0,\tau], \mathbf{R}^d), \\ t \mapsto \Phi_t^{-1}(x) &\in C([0,\tau], \mathbf{R}^d) \end{aligned}$$

and

$$\forall t \in [0,\tau] : \ x \mapsto \Phi_t(x) \in Hom(\overline{D}), \tag{2.5}$$

(ii) Assume that the family of functions $\phi_t : [0,\tau] \times \overline{D} \to \mathbf{R}^d$ satisfies (2.4)-(2.5) and $\phi_0 = id$. Then ϕ_t is the flow of the time-dependent vector field

$$\theta(t,x) := \partial_t \phi(t, \phi^{-1}(t,x)),$$

that is $\phi_t = \Phi_t^\theta$, which satisfies $(\hat{V})$.

Proof. A proof can be found in [37, Thm. 5.1, p. 194]. □

Subsequently, we use the notation ∂f to indicate the (Fréchet) derivative of f with respect to the space variable x (that should not be mixed up with the sub-differential). If we want to consider only the directional derivative of f at $x \in \Omega$ in direction v, we write

$$df(x;v) := \lim_{t \searrow 0} \frac{f(x+tv) - f(x)}{t} \qquad \text{(directional derivative)}$$

and for the Hadamard semi-derivative, we write

$$d_{\mathrm{H}} f(x;v) := \lim_{\substack{t \searrow 0 \\ \tilde{v} \to v}} \frac{f(x+t\tilde{v}) - f(x)}{t} \qquad \text{(Hadamard semi-derivative).}$$

Notice that the Hadamard semi-derivative is strictly weaker than the Fréchet derivative and stronger than the Gateaux derivative. The main difference between the Gateaux derivative and the Hadamard semi-derivative is that the latter guarantees that the chain rule is satisfied; see [38].[2]

Henceforth, it will be useful to introduce for $k \geq 0$ the following sets

$$C_c^k(D, \mathbf{R}^d) := \{\theta : \overline{D} \to \mathbf{R}^d |\ \theta \in C^k(\overline{D}, \mathbf{R}^d) \text{ and } \mathrm{supp}(\theta) \subset D\}.$$

In the case $k = 0$, we set $C_c(D, \mathbf{R}^d) := \{f \in C(D, \mathbf{R}^d)|\ \mathrm{supp} f \subset D\}$ and for $k = \infty$, we define $C_c^\infty(D, \mathbf{R}^d) := \bigcap_{k \in \mathbf{N}} C_c^k(D, \mathbf{R}^d)$. The space $C_c^\infty(D, \mathbf{R}^d)$ is a locally convex vector space, which is not metrisable. It is clear that every vector field $\theta \in C_c^k(D, \mathbf{R}^d)$, $k \geq 1$, satisfies (V). Define also the linear space

$$\mathrm{Lip}_0(D, \mathbf{R}^d) := \{\theta \in C^{0,1}(\overline{D}, \mathbf{R}^d) :\ \pm\theta(x) \in C_{\overline{D}}(x) \ \text{ for all } x \in \overline{D}\}.$$

The following result concerning the sensitivity of the flow with respect to x is well-known; cf. [1, Lem. 4, p. 64].

Lemma 2.11. *Let $\theta \in C_c^k(D, \mathbf{R}^d)$ be a vector field, where $1 \leq k \leq \infty$. Then $x \mapsto \Phi_t(x)$ belongs to $C^k(D, \mathbf{R}^d)$.*

[2] To be more precise, let $f : U \subset E \to F$ and $g : g(U) \to \mathbf{R}$ be two functions defined on open subsets $U \subset E$ and $g(U) \subset F$ of Banach spaces E, F. Suppose that the Gateaux derivative $dg(x;v)$ of g exists at $x \in g(U)$ in direction $v \in F$ and that $d_H f(g(x); dg(x;v))$ exists. Then

$$d(f \circ g)(x;v) = d_H f(g(x); dg(x;v)).$$

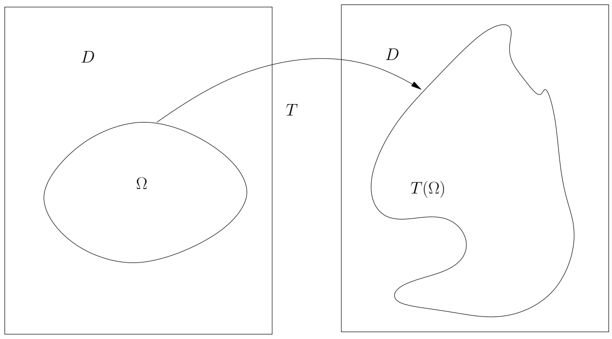

Figure 2.1: Admissible transformation $T : \overline{D} \to \overline{D}$

2.3.3 Compositions of Sobolev functions with flows

In the following let $\theta \in C_c^1(D, \mathbf{R}^d)$ be a given vector field and $\Phi_t = \Phi_t^\theta$ its associated flow. Notice that by the chain rule $\partial\Phi^{-1}(t, \Phi(t,x)) = (\partial\Phi(t,x))^{-1}$ (briefly $(\partial(\Phi_t^{-1})) \circ \Phi_t = (\partial\Phi_t)^{-1} =: \partial\Phi_t^{-1}$), which implies[3] $(\nabla f) \circ \Phi_t = \partial\Phi_t^{-\top}\nabla(f \circ \Phi_t)$. Throughout this thesis the following abbreviations are used

$$\boxed{\xi(t) := \det(\partial\Phi_t), \qquad A(t) := \xi(t)\partial\Phi_t^{-1}\partial\Phi_t^{-\top}, \quad B(t) := \partial\Phi_t^{-\top},} \tag{2.6}$$

where $\det : \mathbf{R}^{d,d} \to \mathbf{R}$ denotes the determinant. Step-by-step, we will derive properties of the functions ξ, B and A.

Proposition 2.12. *Let the mappings $A \in C([0,\tau]; C(\overline{D}, \mathbf{R}^{d,d}))$ and $\xi \in C([0,\tau]; C(\overline{D}))$ be given and assume that $A(0) = I$ and $\xi(0) = 1$. Then there are constants $\gamma_1, \gamma_2, \delta_1, \delta_2 > 0$ and $\tilde{\tau} > 0$ such that*

$$\forall \zeta \in \mathbf{R}^d,\ \forall t \in [0,\tilde{\tau}] : \qquad \gamma_1|\zeta|^2 \le \zeta \cdot A(t)\zeta \le \gamma_2|\zeta|^2, \qquad \text{(a)}$$
$$\delta_1 \le \xi(t) \le \delta_2. \qquad \text{(b)}$$

Proof. (a) For any $t \in [0,\tau]$, we may estimate

$$\begin{aligned} |\eta|^2 &= (I - A(t))\eta \cdot \eta + A(t)\eta \cdot \eta \\ &\le \|I - A(t)\|_{C(D,\mathbf{R}^{d,d})}\eta \cdot \eta + A(t)\eta \cdot \eta. \end{aligned}$$

By continuity of $t \mapsto A(t)$ there exists for all $\varepsilon > 0$, a $\tilde{\delta} > 0$ such that for all $t \in [0,\tilde{\delta}]$ we have $\|I - A(t)\|_{C(D,\mathbf{R}^{d,d})} \le \varepsilon$. Thus choosing $\varepsilon = \frac{1}{2}$, we obtain the desired inequality. Since $t \mapsto A(t)$ is bounded, we also have

$$A(t)\eta \cdot \eta \le \|A\|_{C(D\times[0,\tau],\mathbf{R}^{d,d})}|\eta|^2 \text{ for all } t \in [0,\tilde{\tau}], \text{ for all } \eta \in \mathbf{R}^d.$$

(b) It is clear that ξ is bounded in space and time. The inequalities in item (b) follow then from

$$1 = (1 - \xi(t)) + \xi(t) \le \|\xi(t) - 1\|_{C(D)} + \xi(t).$$

□

[3] For any scalar function $f \in H^1(\mathbf{R}^d)$, we have for all $v \in \mathbf{R}^d$ and all $x \in D$

$$\partial(f(\Phi_t(x))v = \partial f(\Phi_t(x))\partial\Phi_t(x)v = \nabla f(\Phi_t(x)) \cdot \partial\Phi_t(x)v = (\partial\Phi_t(x))^\top \nabla(f(\Phi_t(x))) \cdot v.$$

Proposition 2.13. *Let $B : [0,\tau] \to \mathbf{R}^{d,d}$ be a bounded mapping and $C > 0$ a constant such that $\|B^{-1}(t)\|_{L_\infty(D,\mathbf{R}^{d,d})} \le C$ for all $t \in [0,\tau]$. Then for any $p \ge 1$ there exist constants $C_1, C_2 > 0$ such that*

$$\begin{aligned} \forall t \in [0,\tau],\ \forall f \in W^1_p(D):\ \|\nabla f\|_{L_p(D,\mathbf{R}^d)} &\le C_1 \|B(t)\nabla f\|_{L_p(D,\mathbf{R}^d)} \\ \forall t \in [0,\tau],\ \forall f \in W^1_p(D,\mathbf{R}^d):\ \|\partial \varphi\|_{L_p(D,\mathbf{R}^{d,d})} &\le C_2 \|B(t)\partial\varphi\|_{L_p(D,\mathbf{R}^{d,d})}. \end{aligned} \tag{2.7}$$

Proof. Estimating

$$\|\nabla f\|_{L_p(D,\mathbf{R}^d)} = \|(B(t))^{-1}B(t)\nabla f\|_{L_p(D,\mathbf{R}^d)} \le C\,\|B(t)\nabla f\|_{L_p(D,\mathbf{R}^d)}$$

gives the first inequality. The proof of (2.7) is similar and omitted. □

Lemma 2.14. *Let $\theta \in C^1([0,\tau]; C^1_c(D,\mathbf{R}^d))$ be a vector field and Φ its flow. The functions $t \mapsto A(t)$, $t \mapsto \xi(t)$ and $t \mapsto B(t)$ given by (2.6) are differentiable*[4] *on $[0,\tau]$ and satisfy the following ordinary differential equations*

$$\begin{aligned} B'(t) &= -B(t)(\partial\theta^t)^\top B(t) \\ \xi'(t) &= tr(\partial\theta^t B^\top(t))\xi(t) \\ A'(t) &= tr(\partial\theta^t B^\top(t))A(t) - B^\top(t)\partial\theta^t A(t) - (B^\top(t)\partial\theta^t A(t))^\top, \end{aligned}$$

where $\theta^t(x) := \theta(t,\Phi_t(x))$ and $' := \frac{d}{dt}$.

Proof. (i) Let E, F be two Banach spaces. In [8, Satz 7.2, p. 222] it is proved that

$$\mathrm{inv} : \mathcal{L}\mathrm{is}(E,F) \to \mathcal{L}(F,E), \quad A \mapsto A^{-1}$$

is infinitely times continuously differentiable with derivative $\partial\mathrm{inv}(A)(B) = -A^{-1}BA^{-1}$. Now by the fundamental theorem of calculus, we have

$$\Phi_t(x) = x + \int_0^t \theta(s,\Phi_s(x))\,ds \ \Rightarrow\ \partial\Phi_t(x) = I + \int_0^t \partial\theta(s,\Phi_s(x)))\,ds,$$

where $I \in \mathbf{R}^{d,d}$ denotes the identity matrix. Therefore $t \mapsto \partial\Phi_t(x)$ is differentiable for each $x \in \overline{D}$ with derivative

$$\frac{d}{dt}(\partial\Phi_t(x)) = \partial\theta^t(x) = \partial\theta(t,\Phi_t(x))\partial\Phi_t(x).$$

Thus if we let $E = F = \mathbf{R}^{d,d}$ and take into account the previous equation, we get by the chain rule

$$\frac{d}{dt}(\mathrm{inv}(\partial\Phi_t(x))) = -(\partial\Phi_t(x))^{-1}\partial\theta^t(x)(\partial\Phi_t(x))^{-1}.$$

(ii) A proof may be found in [97, Prop. 10.6, p. 215].
(iii) Follows from the product rule together with (i) and (ii). □

[4] A function $f : [a,b] \to \mathbf{R}$ $(a,b \in \mathbf{R})$ is called differentiable if it is differentiable on (a,b) and the right sided, respectively left sided derivative of f exists in a, respectively in b, i.e. $(f')^-(a) := \lim_{h\searrow 0}(f(a+h) - f(a))/h$ and $(f')^+(b) := \lim_{h\nearrow 0}(f(b+h) - f(a))/h$ exist.

Remark 2.15. *Note that the first formula can also be derived by differentiating the identity $\partial\Phi_t\partial\Phi_t^{-1} = I$, where I is the identity matrix in $\mathbf{R}^d$. That the inverse $t \mapsto \partial\Phi_t^{-1}$ is differentiable can also be seen by the well known formula $\partial\Phi_t^{-1} = (\det(\partial\Phi_t))^{-1}(cofac(\partial\Phi_t))^\top$, where cofac denotes the cofactor matrix.*

Lemma 2.16. *Let $D \subset \mathbf{R}^d$ be a regular domain and $p > 1$ a real number. Denote by Φ_t the flow of $\theta \in C_c^1(D, \mathbf{R}^d)$.*

(i) For any $f \in L_p(D)$, we have

$$\lim_{t\searrow 0} \|f \circ \Phi_t - f\|_{L_p(D)} = 0 \quad \text{and} \quad \lim_{t\searrow 0} \|f \circ \Phi_t^{-1} - f\|_{L_p(D)} = 0.$$

(ii) For any $f \in W_p^1(D)$, we have

$$\lim_{t\searrow 0} \|f \circ \Phi_t - f\|_{W_p^1(D)} = 0. \tag{2.10}$$

(iii) For $k \in \{1,2\}$ and any $f \in W_p^k(D)$, we have

$$\lim_{t\searrow 0} \left\| \frac{f \circ \Phi_t - f}{t} - \nabla f \cdot \theta \right\|_{W_p^{k-1}(D)} = 0.$$

(iv) Fix $p \geq 1$ and let $t \to u_t : [0,\tau] \to W_p^1(D)$ be a continuous function in 0. Set $u := u_0$. Then $t \mapsto u_t \circ \Phi_t : [0,\tau] \to W_p^1(D)$ is continuous in 0 and

$$\lim_{t\searrow 0} \|u_t \circ \Phi_t - u\|_{W_p^1(D)} = 0.$$

Proof. (i) It is proved for instance in [37, p. 529].
(ii) In order to prove (2.16) it is sufficient to show

$$\lim_{t\searrow 0} \|\nabla(f \circ \Phi_t - f)\|_{L_p(D)} = \lim_{t\searrow 0} \|\partial\Phi_t^\top((\nabla f) \circ \Phi_t - \nabla f)\|_{L_p(D)} = 0.$$

By the triangle inequality, we have

$$\|\partial\Phi_t^\top((\nabla f) \circ \Phi_t - \nabla f)\|_{L_p(D)} \leq \|(\nabla f) \circ \Phi_t - \nabla f)\|_{L_p(D)} + \|(\partial\Phi_t^\top - I)\nabla f)\|_{L_p(D)}.$$

For the first term on the right hand side we can use (i) and the second term tends to zero since $\partial\Phi_t^\top \to I$ in $C(\overline{D}; \mathbf{R}^{d,d})$.
(iii) A proof can be found in [60, Lem. 3.6, p. 6].
(iv) By the triangle inequality, we get for all $t \in [0,\tau]$

$$\|u_t \circ \Phi_t - u\|_{W_p^1(D)} \leq \|u_t \circ \Phi_t - u \circ \Phi_t\|_{W_p^1(D)} + \|u \circ \Phi_t - u\|_{W_p^1(D)}.$$

The last term on the right hand side converges to zero as $t \searrow 0$ due to (ii). For the second inequality note that

$$\begin{aligned}\|u_t \circ \Phi_t - u \circ \Phi_t\|_{W_p^1(D)} &= \left(\int_D \xi^{-1}(t)(|u_t - u|^p + |B(t)\nabla(u_t - u)|^p)\right)^{1/p} \\ &\leq C\left(\int_D |u_t - u|^p + |\nabla(u_t - u)|^p\right)^{1/p}\end{aligned}$$

and the right hand side converges to zero as $t \searrow 0$. $\square$

Remark 2.17. *Item (i) remains true if θ only satisfies (V) and $D \subset \mathbf{R}^d$ is measurable.*

2.4 Shape continuity

In this section, we collect existence results of shape optimization problems for special types of shape functions. In Chapter 5 these will be applied to obtain existence of optimal shapes for several PDE constrained optimization problems defined on subsets of regular domains $D \subset \mathbf{R}^d$.

2.4.1 Topologies via L_p-metrics

The sets $\Xi \subset 2^{\mathbf{R}^d}$ respectively $\Xi \subset 2^D$ ($D \subset \mathbf{R}^d$ regular domain) are in general no subsets of a locally convex vector spaces. Therefore there is no 'canonical' choice of a topology as it is for functions $f : U \to \mathbf{R}$ defined on open subsets U of topological vector spaces $\boldsymbol{X}$. However, for special classes of shape functions there are natural choices of topologies. One such class consists of shape functions depending on the shape only via a characteristic function, i.e.

$$J(\Omega) = \hat{J}(\chi_\Omega),$$

for some function $\hat{J} : X_\mu(D) \to \mathbf{R}$, where

$$X_\mu(D) = \{\chi_\Omega : \ \Omega \text{ is } \mu - \text{measurable subset of } D\}$$

denotes the set of characteristic functions defined by μ-measurable subsets of D. Here, μ is Radon measure, that is, a measure on the σ-algebra of Borel sets of $\mathbf{R}^d$ that is locally finite and inner regular.[5] For simplicity, we can think of the Lebesgue measure m in which case we set $X(D) := X_m(D)$. We may equip $X_\mu(D)$ with the metric induced by the $L_p(D,\mu)$ norm, $p \in [1,\infty)$:

$$\delta_{p,\mu}(\chi_1,\chi_2) := \|\chi_1 - \chi_2\|_{L_p(D,\mu)}.$$

When μ is the Lebesgue measure m we put $\delta_p := \delta_{p,\mu}$. Convergence $\Omega_n \to_{L_{p,\mu}} \Omega$, where $\Omega_n, \Omega \in D$ means then $\lim_{n\to\infty} \delta_{p,\mu}(\chi_{\Omega_n},\chi_\Omega) = 0$.

Remark 2.18. *Note that we view μ-measurable subsets $\Omega \subset D$ as characteristic functions χ_Ω and the latter ones are seen as elements of $L_p(D,\mu)$. Therefore we loose information, because two characteristic functions are equal if they are equal μ-almost everywhere on D. That means two sets are equal if they are equal μ-almost everywhere. This is important to keep in mind when one is interested in cracks.*

Proposition 2.19. *Then $X_\mu(D) \cap L_1(D,\mu)$ is closed in $L_p(D,\mu)$ and the metric space $(X_\mu(D) \cap L_1(D,\mu), \delta_{p,\mu})$ is complete. The topologies generated by $\delta_{p,\mu}$ are equivalent for all $p \in [1,\infty)$.*

Thus we get a natural topology on $X_\mu(D) \cap L_1(D,\mu)$ induced by the norm $\|\cdot\|_{L_p(D,\mu)}$ and can speak of the continuity of $\chi \mapsto \hat{J}(\chi)$.

Unlike normal L_p-spaces for $p \in (1,\infty)$ the spaces $X_\mu(D) \cap L_1(D,\mu)$ are not weakly closed. This is problematic concerning the existence of optimal solutions of optimization problems, since we would like to extract a converging subsequence of minimizing sequence that converges in the same space. In order to obtain a certain compactness an additional stronger term can be added.

[5] Compare Definition A.4.

2.4.2 Topologies via BV-metric

Characteristic functions are not weakly differentiable since they are discontinuous along hypersurfaces of dimension one below the space dimension. That means a characteristic function defined by a subset of the plane has discontinuities along lines and in the three space it has discontinuities along surfaces. Nevertheless an appropriate notion of weak derivative allows us to talk of derivatives of characteristic functions.

We begin with the definition of this notion of weak derivative.

Definition 2.20. *Let $D \subset \mathbf{R}^d$ be open. We say that $u \in L_1(D)$ is of bounded variation if there exists a vector valued Radon measure μ such that*

$$\int_D u \operatorname{div}(\varphi)\, dx = -\int_D \varphi \cdot d\mu,$$

for all $\varphi \in C_c^1(D, \mathbf{R}^d)$. Then one writes $du = \mu$, that indicates the 'weak derivative' of u is a vector valued Radon measure. The space of all functions $u \in L_1(D)$ that have a derivative that is a vector valued Radon measure is denoted by $BV(D)$. It becomes a Banach space when equipped with the norm

$$\|f\|_{BV(D)} := \|f\|_{L_1(D)} + Var(f, D), \tag{2.11}$$

where

$$Var(f, D) := \sup\left\{\int_D \operatorname{div}(\boldsymbol{\varphi})\chi\, dx \mid \boldsymbol{\varphi} \in C_c^1(D, \mathbf{R}^d), \|\boldsymbol{\varphi}\|_{L_\infty(D)} \le 1\right\}$$

denotes the total variation of f with respect to D.

The set of all characteristic functions with finite total variation is denoted by

$$\mathfrak{B}(D) := \{\chi \in X(D) :\ \chi \in BV(D)\}. \tag{2.12}$$

We put $\hat{P}_D(\chi) := \mathrm{Var}(\chi, D)$ for $\chi \in X(D)$. Now we can say what a set of finite perimeter is.

Definition 2.21. *A subset $\Omega \subset \mathbf{R}^d$ is said to have finite perimeter relative to $D \subset \mathbf{R}^d$ if $P_D(\Omega) := \hat{P}_D(\chi_\Omega) < \infty$. If $D = \mathbf{R}^d$ then we define $\hat{P}(\chi) := Var(\chi, \mathbf{R}^d)$ and $P(\Omega) := \hat{P}(\chi_\Omega)$. In other words, a subset $\Omega \subset D$ has finite perimeter if the characteristic function $\chi = \chi_\Omega \in X(D)$ belongs to the space $BV(D)$.*

If $\Omega \subset D$, then $P_D(\Omega) = P(\Omega)$. One should keep in mind that a finite perimeter set $\Omega \subset \mathbf{R}^d$, that is $P_D(\Omega) < \infty$, can have non zero d-dimensional Lebesgue measure, i.e. $m(\partial\Omega) > 0$. This is even true for the relative boundary $\partial\Omega \cap D$; see [48, p. 7]. We have the following compactness result:

Theorem 2.22. *Let $D \subset \mathbf{R}^d$ be a Lipschitz domain. We endow $BV(D)$ with the norm (2.11). Then the space $BV(D)$ is compactly and continuously embedded into $L_q(D)$, $q \in [1, \frac{d}{d-1})$, written*

$$BV(D) \overset{c}{\hookrightarrow} L_q(D),$$

that is, the identity operator $id : BV(D) \to L_q(D)$ is continuous and compact for each $q \in [1, \frac{d}{d-1})$.

Proof. See [10, Corol. 3.49, p. 152]. □

Corollary 2.23. *Let $D \subset \mathbf{R}^d$ be a Lipschitz domain and $q \in [1, \frac{d}{d-1})$.*

(i) The set $\mathfrak{B}(D)$ is closed in $BV(D)$. For any bounded sequence $(\chi_n)_{n\in\mathbf{N}}, \chi_n \in \mathfrak{B}(D)$, there exists a subsequence $(\chi_{n_k})_{k\in\mathbf{N}}$ converging in $L_q(D)$ to some characteristic function $\chi \in X(D)$ such that

$$Var(D,\chi) \leq \liminf_{k\to\infty} Var(D,\chi_{n_k}) < \infty.$$

(ii) The space $\mathfrak{B}(D)$ equipped with the metric $\delta_{BV}(\chi_1,\chi_2) := \|\chi_1 - \chi_2\|_{BV(D)}$ $(\chi_1, \chi_2 \in BV(D))$ is a complete metric space.

Proof. (i) Fix $q \in [1, \frac{d}{d-1})$. Let $(\chi_n)_{n\in\mathbf{N}}$, $\chi_n \in \mathfrak{B}(D) = X(D) \cap BV(D)$ be any converging sequence with limit $\chi \in \overline{\mathfrak{B}(D)} \subset X(D)$ (closure and convergence with respect to δ_{BV}). Note that the sequence $(\chi_n)_{n\in\mathbf{N}}$ is bounded in $\mathfrak{B}(D)$. Therefore, according to Theorem 2.22, we may extract a subsequence $(\chi_{n_k})_{k\in\mathbf{N}}$ converging in $L_q(D)$ to $\chi \in X(D)$. We show that $\mathrm{Var}(\cdot, D) : BV(D) \to \mathbf{R}$ is lower semi-continuous with respect to the δ_1-topology. Let $(u_n)_{n\in\mathbf{N}}$ be a sequence in $BV(D)$ converging in $L_1(D)$ to $u \in BV(D)$. Set $j := \liminf_{n\to\infty} \mathrm{Var}(u_n, D)$, then by definition of the lim inf, we may extract a subsequence of $(u_n)_{n\in\mathbf{N}}$ such that $j = \lim_{k\to\infty} \mathrm{Var}(u_{n_k}, D)$. Then for any $\phi \in C^1_c(D, \mathbf{R}^d)$ with $\|\phi\|_{L_\infty(D)} \leq 1$, we have

$$\begin{aligned}
\liminf_{n\to\infty} \mathrm{Var}(u_n, D) = \lim_{k\to\infty} \mathrm{Var}(u_{n_k}, D) &\geq \lim_{k\to\infty} \int_D u_{n_k} \operatorname{div}(\phi)\, dx \\
&= \int_D \lim_{k\to\infty} u_{n_k} \operatorname{div}(\phi)\, dx \\
&= \int_D u \operatorname{div}(\phi)\, dx,
\end{aligned}$$

where we applied Lebesgue's dominated convergence theorem Theorem A.7. Since this inequality is true for all $\phi \in C^1_c(D, \mathbf{R}^d)$ with $\|\phi\|_{L_\infty(D)} \leq 1$, we obtain

$$\liminf_{n\to\infty} \mathrm{Var}(u_n, D) \geq \mathrm{Var}(u, D).$$

This shows that $\chi \in \mathfrak{B}(D)$.
(ii) Since a closed subset of a complete metric space is complete, the result directly follows from (i). □

Minimizing in $\mathfrak{B}(D)$-spaces is theoretically nice, but for applications may be not the optimal choice. One reason is that $\mathfrak{B}(D)$ yield a too big class of domains which includes highly irregular domains. The continuity of shape function with respect to this metric is defined as the following.

Definition 2.24. *Let $D \subset \mathbf{R}^d$ be Lebesgue measurable and bounded. We say that $\hat{J} : \mathfrak{B}(D) \to \mathbf{R}$ is continuous in $\chi \in \mathfrak{B}(D)$ with respect to the δ_{BV} metric if for any sequence $\chi_n \in \mathfrak{B}(D)$ converging with respect to this metric to χ, we have*

$$\lim_{n\to\infty} \hat{J}(\chi_n) = \hat{J}(\chi).$$

The following theorem states the existence of shape optimization problems defined on finite perimeter sets.

Theorem 2.25. *Let $\hat{J} : X(D) \to \mathbf{R}$ be a shape function that is continuous with respect to the δ_p-metric for some $p > 1$. Assume that $\inf_{\chi\in X(D)} \hat{J}(\chi) > -\infty$. Define for any $\alpha > 0$ the cost function $\hat{\mathcal{J}} : \mathfrak{B}(D) \to \mathbf{R}$ by $\hat{\mathcal{J}}(\chi) := \hat{J}(\chi) + \alpha\hat{P}_D(\chi)$. Then the minimisation problem*

$$\inf_{\chi\in X(D)} \hat{\mathcal{J}}(\chi)$$

has at least one solution $\chi \in \mathfrak{B}(D)$.

Proof. Set $j := \inf_{\chi\in X(D)} \hat{\mathcal{J}}(\chi)$. By definition we have $j \geq \inf_{\chi\in X(D)} \hat{J}(\chi) > -\infty$. Let $(\chi_n)_{n\in\mathbf{N}}$ be a minimizing sequence in $X(D)$, such that $\lim_{n\to\infty} \hat{\mathcal{J}}(\chi_n) = j$. Since $\inf_{\chi\in X(D)} \hat{J}(\chi) > -\infty$, there must be a constant $c > 0$ such that

$$\forall n \in \mathbf{N} : \ \hat{P}_D(\chi_n) \leq c.$$

Finally, taking into account Corollary 2.23, noting that $\hat{P}_D(\cdot) = \mathrm{Var}(D, \cdot) : BV(X) \to \mathbf{R}$ is lower semi-continuous and that $\hat{J}$ continuous with respect to the δ_p-metric, we get

$$\hat{\mathcal{J}}(\chi) \leq \lim_{n\to\infty} \hat{\mathcal{J}}(\chi_n) = j$$

□

2.4.3 Topologies via W_p^s-metrics

Although characteristic functions are not weakly differentiable in general, they can have a finite Gagliardo semi-norm. This leads to the notion of the Gagliardo[6] perimeter.

For every $p \in (1, \infty)$ and $0 < s < \infty$, the Gagliardo semi-norm is defined by

$$|u|^p_{W_p^s(D)} := \int_D \int_D \frac{|u(x) - u(y)|^p}{|x - y|^{d+sp}}\, dx\, dy.$$

The fractional Sobolev space $W_p^s(D)$ is defined as the completion of $C_c^\infty(D)$ with respect to the norm

$$u \mapsto \|u\|_{W_p^s(D)} := |u|_{W_p^s(D)} + \|u\|_{L_p(D)}.$$

It is a reflexive Banach space.

Note that the norms on $W_p^s(D)$ and $W_{p'}^{s'}(D)$ are equivalent if $sp = s'p'$. Moreover, notice that for a characteristic function χ_Ω, $\Omega \subset D$ the norm $|\chi_\Omega|_{W_p^s(D)}$ depends only on the value of the space dimension $d \geq 1$ and the product $sp \in (0, \infty)$, since

$$|\chi_\Omega|^p_{W_p^s(D)} = \int_D \int_D \frac{|\chi_\Omega(x) - \chi_\Omega(y)|}{|x - y|^{d+sp}}\, dx\, dy.$$

In other words $|\chi_\Omega|^p_{W_p^s(D)} = |\chi_\Omega|^{p'}_{W_{p'}^{s'}(D)}$ if $sp = s'p'$. This leads to the following definition.

Definition 2.26. *Let $\Omega \subset D$ be Lebesgue measurable and $s \in (0, \infty)$. We say that Ω has finite s-perimeter relatively to D if*

$$P_s(\Omega) := \int_D \int_D \frac{|\chi_\Omega(x) - \chi_\Omega(y)|}{|x - y|^{d+s}}\, dx\, dy < \infty$$

We call $P_D^s(\Omega)$ the s-perimeter of Ω relative to D and put $\hat{P}_D^s(\chi) := \int_D \int_D \frac{|\chi_\Omega(x) - \chi_\Omega(y)|}{|x-y|^{d+s}}\, dx\, dy$.

[6] E. Gagliardo introduced the fractional Sobolev norm to characterise traces. Usually, this norm is referred to as fractional Sobolev norm, but since it was Gagliardo who introduce it we use his name.

For every $\bar{s} \in (0, \infty)$, we define the space of characteristic functions having finite $\bar{s}$-perimeter by

$$\mathfrak{W}^{\bar{s}}(D) := \{\chi_\Omega : \mathbf{R} \to \mathbf{R} | \ \chi_\Omega \in X(D) \text{ and } \hat{P}_D^{\bar{s}}(\chi_\Omega) < \infty\}.$$

Note that for $0 \leq s < 1/p \leq 1$, we have $BV(D) \cap L_\infty(D) \subset W_p^s(D)$, see [37, Thm. 6.9., p. 253]. That means for $\bar{s} \in (0,1)$, we obtain $\mathfrak{B}(D) \subset \mathfrak{W}^{\bar{s}}(D)$ and $\mathfrak{W}^{\bar{s}}(D) = X(D) \cap W_p^s(D)$, when $\bar{s} := sp$.

Compared with the perimeter $P_D(\Omega)$ the s-perimeter $P_D^s(\Omega)$ provides a weaker regularisation. In particular, the regularisation term and its shape derivative are domain integrals, but they are non-local. Also note that an open and bounded set $\Omega \subset \mathbf{R}^d$ of class C^2 has finite perimeter and thus $\chi_\Omega \in BV(D) \cap L_\infty(D)$, which implies $\chi_\Omega \in \mathfrak{W}^{\bar{s}}(D)$ for all $\bar{s} \in (0,1)$.

Let $0 \leq s < 1/p \leq 1$ and $\bar{s} = sp$. Then we introduce the metrics $\delta_{s,p}$ on $\mathfrak{W}^{\bar{s}}(D)$ by

$$\delta_{s,p}(\chi_{\Omega_1}, \chi_{\Omega_2}) := |\chi_{\Omega_1} - \chi_{\Omega_2}|_{W_p^s(\Omega)} + \|\chi_{\Omega_1} - \chi_{\Omega_2}\|_{L_p(D)}.$$

These metrics are all generating the same topology on $\mathfrak{W}^{\bar{s}}(D)$.

Theorem 2.27 ([41]). *Let $D \subset \mathbf{R}^d$ be a Lipschitz domain and $s \in (0,1), p \in [1,\infty), q \in [1,p]$. Assume that $\mathcal{T}$ is a bounded subset of $W_p^s(D)$ such that*

$$\sup_{u \in \mathcal{T}} |u|_{W_p^s(D)} < \infty.$$

Then $\mathcal{T}$ is relatively compact in $L_q(D)$.[7]

Corollary 2.28. *Let $D \subset \mathbf{R}^d$ be a regular domain with boundary $\Sigma = \partial D$. Let $\bar{s} \in (0,\infty), s \in (0, \bar{s}]$ and $p := \bar{s}/s \geq 1$.*

(i) The set $\mathfrak{W}^{\bar{s}}(D)$ is closed in $W_p^s(D)$. For any bounded sequence $(\chi_n)_{n\in\mathbf{N}}, \chi_n \in \mathfrak{W}^{\bar{s}}(D)$, i.e. $P_D^{\bar{s}}(\chi_n) = |\chi_n|_{W_p^s(D)} \leq C$ for all $n \in \mathbf{N}$, where $C > 0$, there exist a subsequence $(\chi_{n_k})_{k\in\mathbf{N}}$ converging in $L_q(D)$ to some characteristic function $\chi \in X(D)$ such that

$$\hat{P}_D^{\bar{s}}(\chi) \leq \liminf_{k\to\infty} \hat{P}_D^{\bar{s}}(D, \chi_{n_k}) < \infty.$$

(ii) The space $(\mathfrak{W}^{\bar{s}}(D), \delta_{s,p})$ is a complete metric space.

Proof. (i) First note that any sequence converging in $\mathfrak{W}^s(D)$ also converges in $X(D)$ with respect to δ_1. Now let $(\chi_n)_{n\in\mathbf{N}}$, $\chi_n \in \mathfrak{W}^s(D)$ be any converging sequence with limit $\chi \in \overline{\mathfrak{W}^s(D)} \subset X(D)$ (closure and convergence with respect to δ_{BV}). We may extract based on Theorem 2.27 a subsequence $(\chi_{n_k})_{k\in\mathbf{N}}$ converging in $L_q(D)$ to $\chi \in X(D)$. To finish the prove it is sufficient to show that $P_D^{\bar{s}}(\,\cdot\,) = |\cdot|_{W_p^s(D)} : W_p^s(D) \to \mathbf{R}$ is lower semi-continuous with respect to the δ_1-metric. To prove this let $(u_n)_{n\in\mathbf{N}}$ be any sequence in $W_p^s(D)$ converging in $L_1(D)$ to $u \in W_p^s(D)$. Set $j := \liminf_{n\to\infty} |u_n|_{W_p^s(D)}^p$. Note that by definition of the lim inf, we may extract a subsequence denoted $(u_{n_k})_{k\in\mathbf{N}}$ such that $j = \lim_{k\to\infty} |u_n|_{W_p^s(D)}$ and a further subsequence still denoted $(u_n)_{n\in\mathbf{N}}$ such that $u_{n_k} \to u$ as $k \to \infty$ almost everywhere in D. Therefore setting

$$f_n(x,y) := \frac{|u_{n_k}(x) - u_{n_k}(y)|}{|x-y|^{d+sp}}, \quad f(x,y) := \frac{|u(x) - u(y)|}{|x-y|^{d+sp}},$$

[7] In a topological vector space X a subset A is called pre-compact or relatively compact if the closure $\overline{A}$ in X is compact.

we get $\lim_{n\to\infty} f_n = f$ a.e. in $D\times D$. Therefore applying Fatou's Lemma A.6 yields

$$\begin{aligned}\liminf_{n\to\infty} |u_n|^p_{W^s_p(D)} &= \liminf_{k\to\infty} \int_{D\times D} \frac{|u_{n_k}(x)-u_{n_k}(y)|}{|x-y|^{d+sp}}\, d(x,y)\\ &\geq \int_{D\times D} \frac{|u(x)-u(y)|}{|x-y|^{d+sp}}\, d(x,y)\\ &= |u|^p_{W^s_p(D)},\end{aligned}$$

where $d(x,y) = dx\, dy$ is the product measure. This concludes the prove.
(ii) Since a closed subset of a complete metric space is complete, we only need to show that $\mathfrak{W}^{\bar{s}}(D)$ is closed, but this follows directly from (i). $\square$

The following theorem is the key for shape optimization problems defined on finite Gagliardo perimeter sets.

THEOREM 2.29. *Let $\hat{J} : X(D) \to \mathbf{R}$ be a shape function that is continuous with respect to the δ_p-metric for some $p > 1$. Assume that $\inf_{\chi\in X(D)} \hat{J}(\chi) > -\infty$. Define for any $\alpha > 0$ and $s \in (0,1)$ the cost function $\hat{\mathcal{J}} : \mathfrak{W}^s(D) \to \mathbf{R}$*

$$\hat{\mathcal{J}}(\chi) := \hat{J}(\chi) + \alpha \hat{P}^s_D(\chi).$$

Then the minimisation problem

$$\inf_{\chi\in\mathfrak{W}^s(D)} \hat{\mathcal{J}}(\chi)$$

has at least one solution.

Proof. Put $j := \inf_{\chi\in\mathfrak{W}^s(D)} \hat{\mathcal{J}}(\chi)$. By definition $j \geq \inf_{\chi\in X(D)} J(\chi) > -\infty$. Let $(\chi_n)_{n\in\mathbf{N}}$ be a minimizing sequence in $X(D)$ such that $j = \lim_{n\to\infty} \hat{\mathcal{J}}(\chi_n)$. By Corollary 2.28 we may extract a subsequence $(\chi_{n_k})_{k\in\mathbf{N}}$ converging $L_p(D)$. Finally, taking into account Corollary 2.28 part (i) and that $\hat{\mathcal{J}}(\cdot)$ is continuous in $X(D)$ with respect to the δ_p metric, we obtain

$$\hat{\mathcal{J}}(\chi) \leq \lim_{k\to\infty} \hat{\mathcal{J}}(\chi_{n_k}) = \inf_{\chi\in\mathfrak{W}^s(D)} \hat{\mathcal{J}}(\chi).$$

$\square$

2.4.4 Shape continuity via flows

In the next section, we are going to introduce the shape derivative. A feature of a derivative should be that if a function is differentiable then it is continuous with respect to some topology. It is not clear if a shape function is continuous with respect to the previously introduced topologies even if the shape function is shape differentiable. Nevertheless, the following concept of continuity is well-suited.

DEFINITION 2.30. *Let $X \subset (\mathbf{R}^d)^{\mathbf{R}^d}$ be a given non-empty set.*

(i) We say that a subset $\Xi \subset 2^{\mathbf{R}^d}$ is X-stable at $\omega_0 \in \Xi$ if $F(\omega_0) \in \Xi$ for all $F \in X$. This definition is equivalent to $Z_{X,\omega_0} := \{F(\omega_0) |\, F \in X\} \subset \Xi$.

(ii) We say that Ξ is weakly flow stable if for every $\omega_0 \in \Xi$ there exists a $\tau > 0$ and an open, bounded set $D \supset \omega_0$ such that $\Phi^\theta_t(\omega_0) \in \Xi$ for all $t \in [0,\tau]$ and all $\theta \in C([0,1], Lip_0(D,\mathbf{R}^d))$.

Note that if Ξ is X-stable at all $\omega_0 \subset \Xi$ and $\mathrm{id} \in X$, then necessarily $\cup_{\omega_0 \in \Xi} Z_{X,\omega_0} = \Xi$. It is clear that if Ξ is X-stable at ω_0 then it is also Y-stable at ω_0 for any $Y \subset X$. Flow stable subsets of $2^{\mathbf{R}^d}$ are important for the shape continuity along flows.

Example 2.31. *Let $D \subset \mathbf{R}^d$ be open and bounded. The following sets are flow stable*

$$
\begin{aligned}
\Xi_1 &:= \{\Omega \subset D : \Omega \text{ is open } \} \\
\Xi_2 &:= \{\Omega \subset D : \Omega \text{ is closed } \} \\
\Xi_3 &:= \{\Omega \subset D : \Omega \text{ is open and Lipschitzian}\}.
\end{aligned}
$$

Definition 2.32. *Let $D \subset \mathbf{R}^d$ be a regular domain. Let $J : \Xi \to \mathbf{R}$ be a shape function defined on a weakly flow stable subset $\Xi \subset 2^D$ and Θ be a topological vector subspace of $Lip_0(D, \mathbf{R}^d)$. We say that a shape function J is* shape continuous[8] *at $\Omega \in \Xi$ on $C([0,1], \Theta)$ if*

$$\lim_{t \searrow 0} J(\Phi_t^\theta(\Omega)) = J(\Omega) \quad \text{for all } \theta \in C([0,1], \Theta).$$

We say that J is shape continuous on $C([0,1], \Theta)$ if it is shape continuous at all $\Omega \in \Xi$ on $C([0,1]; \Theta)$. If $\Theta = C_c^\infty(D, \mathbf{R}^d)$ then we denote the set of all real valued shape continuous shape functions $J : \Xi \subset 2^D \to \mathbf{R}$ by $C_D^0(\Xi, \mathbf{R}) = C_D^0(\Xi)$.

Later in Chapter 6, we introduce metrics on spaces of diffeomorphisms in $\mathbf{R}^d$. Definition 2.32 will give a criterion when a shape function is continuous with respect to this metric.

The existence of minimisers of minimisation problems over flows is redirected to Subsection 6.2.1. It involves more definitions and some basic tools from differential geometry, which will be introduced in Chapter 6.

2.5 Sensitivity analysis

The *Eulerian semi-derivative* of a shape functions $\Omega \mapsto J(\Omega)$ is similar to the Lie derivative on manifolds. It can be interpreted as a derivative of J with respect to the domain Ω. The *shape derivative* is then defined as the Eulerian semi-derivative with the additional property that it is continuous and linear with respect to the direction. The vanishing of the shape derivative can be interpreted as a necessary optimality condition, which does not necessarily guarantees that a local minimum is attained.

2.5.1 Eulerian semi-derivative and shape derivative

The *Eulerian semi-derivative* may be defined in two ways. We first describe what is known in the literature as *perturbation of identify*. For a fixed set $\Omega \subset D$ define the family of *perturbed* domains $\Omega_t := (\mathrm{id} + t\,\theta)(\Omega)$, where $\theta \in C^{0,1}(\overline{D}, \mathbf{R}^d)$ with $\theta = 0$ on ∂D and id denotes the identity mapping on $\mathbf{R}^d$. For $\tau > 0$ sufficiently small the mapping $x \mapsto \Phi_t(x) := x + t\theta(x)$ is invertible[9] for each $t \in [0, \tau]$. Then one defines the Eulerian semi-derivative as

$$d^{\mathrm{Id}} J(\Omega)[\theta] := \lim_{t \searrow 0} \frac{J((\mathrm{id} + t\,\theta)(\Omega)) - J(\Omega)}{t}. \tag{2.13}$$

[8] In [17, Def. 1, p. 50] this is called directional continuous.

[9] Let $D \subset \mathbf{R}^d$ be a regular domain. Pick an element $\theta \in C^{0,1}(D)$ and assume that $\partial\theta(x) < 1$ at $x \in D$. Now since for any matrix $A \in \mathbf{R}^{d,d}$ the perturbation $A + I$ is invertible if the series $\sum_{n=1}^{\infty} A^n$ converges absolutely, in particular if $\|A\| < 1$, we get that $(I + \partial\theta(x))^{-1}$ exists. Thus by the inverse function theorem we get that $(\mathrm{id} + \theta)^{-1}$ exists in $(\mathrm{id} + \theta)(\mathbf{B}_r(x))$ for some $r > 0$. Therefore assuming $\|\partial\theta\|_{C(D,\mathbf{R}^{d,d})} < 1$, we conclude $(\mathrm{id} + \theta)^{-1}$ exists everywhere in D.

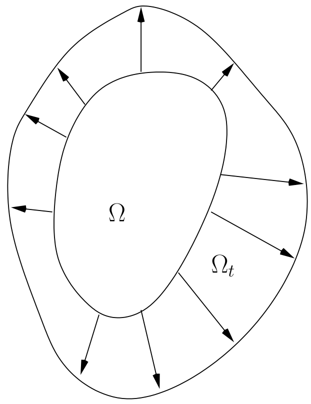

Figure 2.2: Perturbed Ω_t and unperturbed domain Ω

The second way to define the Eulerian semi-derivative is referred to as *velocity method* or *speed method*. Instead of considering $\mathrm{id} + t\,\theta$, we replace this function by the flow $\Phi_t^{\overline{\theta}}$ generated by a vector field $\overline{\theta}$ belonging to $\mathrm{Lip}_0(D, \mathbf{R}^d)$ and define the Eulerian semi-derivative at Ω in direction $\overline{\theta}$ as

$$d^{\mathrm{fl}} J(\Omega)[\overline{\theta}] := \lim_{t \searrow 0} \frac{J(\Phi_t^{\overline{\theta}}(\Omega)) - J(\Omega)}{t}.$$

Note that the function $\Phi_t^{\overline{\theta}} := \overline{(\mathrm{id} + t\,\theta)}$ is the flow of the time-dependent vector field $\overline{\theta}(t) := \theta \circ (\mathrm{id} + t\,\theta)^{-1}$ with $\mathrm{supp}(\overline{\theta}(t)) \subset \overline{D}$ for each $t \in [0, \tau]$. Thus if (2.13) exists then

$$d^{\mathrm{Id}} J(\Omega)[\theta] = d^{\mathrm{fl}} J(\Omega)[\overline{\theta}].$$

Let $\Theta \subset \mathrm{Lip}_0(D, \mathbf{R}^d)$ be a Banach subspace. Then if $C([0, \tau]; \Theta) \to \mathbf{R} : \tilde{\theta} \mapsto d^{\mathrm{fl}} J(\Omega)[\tilde{\theta}]$ is linear and continuous, we conclude by [37, Thm. 3.1, p. 474] that

$$d^{\mathrm{fl}} J(\Omega)[\overline{\theta}] = d^{\mathrm{fl}} J(\Omega)[\overline{\theta}(0)] = d^{\mathrm{fl}} J(\Omega)[\theta]$$

and thus both derivatives coincide. The following definition is given for autonomous vector fields, but can be immediately extended to the time-dependent case.

Definition 2.33. *Let $D \subset \mathbf{R}^d$ be a regular domain. Let $J : \Xi \to \mathbf{R}$ be a shape function defined on a flow stable set $\Xi \subset 2^D$ and Θ be a topological vector subspace of $C_c^\infty(D, \mathbf{R}^d)$. The* Eulerian semi-derivative *or* Lie semi-derivative *of J at Ω in direction $\theta \in \Theta$ is defined by*

$$dJ(\Omega)[\theta] := \lim_{t \searrow 0} \left(\frac{\Phi_t^* J - J}{t} \right) (\Omega), \tag{2.14}$$

where $\Phi_t^*(f) := f \circ \Phi_t$ denotes the pull-back. The semi-derivative is also denoted by $\mathcal{L}_\theta(J)|_\Omega := dJ(\Omega)[\theta]$.

(i) We call J shape differentiable *at Ω with respect to Θ if it has a Eulerian semi-derivative at Ω for all $\theta \in \Theta$ and the mapping*

$$\theta \mapsto dJ(\Omega)[\theta] =: G(\theta) : \Theta \to \mathbf{R}$$

is linear and continuous, in which case $G(\theta)$ is called the shape derivative *at Ω.*

(ii) We call J continuously shape differentiable *at Ω in Θ if it is shape differentiable at Ω in Θ and $\lim_{t \searrow 0} dJ(\Phi_t^\zeta(\Omega))[\theta] = dJ(\Omega)[\theta]$ for all $\zeta, \theta \in C([0, \tau], \Theta)$.*

(iii) The smallest integer $k \geq 0$ for which G is continuous with respect to the $C_c^k(D, \mathbf{R}^d)$-topology is called the order of G.

Let $\Theta = C_c^\infty(D, \mathbf{R}^d)$. Given a regular domain $D \subset \mathbf{R}^d$ and a stable subset $\Xi \subset 2^D$, we denote by

$$C_D^1(\Xi) := \{J : \Xi \subset 2^D \to \mathbf{R},\ J \text{ is continuously shape differentiable in each } \Omega \in \Xi\}$$

the set of continuously differentiable shape functions.

Remark 2.34.

(i) Note that the distribution G in (i) is frequently called shape gradient. *This terminology is not used in this thesis, since a gradient is defined in Hilbert spaces and always depends on the chosen metric in the space where the derivative is taken. In Chapter 6, we show how to obtain the gradient of G with respect to different metrics.*

(ii) Note that the semi-derivative given by (2.14) is equivalent to

$$dJ(\Omega)[\theta] = \lim_{t \searrow 0} \frac{J(\Phi_t(\Omega)) - J(\Omega)}{t}.$$

By (very) formally applying the 'chain rule', we get $\frac{d}{dt} J(\Phi_t(\Omega))|_{t=0} = \partial_\Omega J(\Omega) \cdot \theta$. As usually done in differential geometry, we may view θ as an operator, also called derivation, *acting on J by setting $(\theta J)(\Omega) := dJ(\Omega)[\theta] :\ C_D^1(\Xi) \to C_D^0(\Xi)$. This operator satisfies ($p := \Omega$)*

(i) $\forall a, b \in \mathbf{R}, \forall f, g \in C_D^1(\Xi) :\ \theta(af + bg)|_p = a\theta f|_p + b\theta g|_p$

(ii) $\forall f, g \in C_D^1(\Xi) :\ \theta(fg)|_p = ev_p(f)\theta g|_p + \theta f|_p ev_p(g)$,

where $ev_p J := J(p) = J(\Omega)$ denotes the evaluation map $ev : C_D^1(\Xi) \to \mathbf{R}$.

Therefore J is shape differentiable at Ω if and only if for each direction $\theta \in C_c^\infty(D, \mathbf{R}^d)$, there exists an operator $X = X_\theta : C_D^1(\Xi) \to C_D^0(\Xi)$ that is linear with respect to θ and satisfies (i)-(ii) with $(XJ)(\Omega) = dJ(\Omega)[\theta]$.

We continue with the definition of the second order Eulerian derivative.

Definition 2.35. *Let $J : \Xi \subset 2^{\mathbf{R}^d} \to \mathbf{R}$ be a shape function and Θ be a topological vector subspace of $C_c^\infty(D, \mathbf{R}^d)$. Assume that the Eulerian semi-derivative $dJ(\Phi_t^\zeta(\Omega))[\theta]$ exists for $\zeta \in \Theta$, for all $\theta \in \Theta$ and $0 \leq t \leq \tau$. Set $dJ(\Omega)[\theta] := (\theta dJ)(\Omega)$. Then the* second order Eulerian semi-derivative *or* second order Lie semi-derivative *is defined as*

$$dJ^2(\Omega)[\theta][\zeta] = \lim_{t \searrow 0} \left(\frac{\Phi_t^*(\theta dJ) - (\theta dJ)}{t} \right)(\Omega). \tag{2.15}$$

The second order semi-derivative is also denoted by $\mathcal{L}_{\theta,\zeta}(J)|_\Omega := dJ(\Omega)[\theta][\zeta]$.

(i) We say J is twice shape differentiable if for all $\hat{\theta}, \hat{\zeta} \in \Theta$ the mappings

$$\theta \mapsto dJ(\Omega)[\theta][\hat{\zeta}], \qquad \zeta \mapsto dJ(\Omega)[\hat{\theta}][\zeta]$$

are linear and continuous from Θ into $\mathbf{R}$.

Remark 2.36.

(i) Note that the second order semi-derivative (2.15) *is equivalent to*

$$\begin{aligned} dJ^2(\Omega)[\theta][\zeta] &= \lim_{t\searrow 0} \frac{dJ(\Phi_t^\zeta(\Omega))[\theta] - dJ(\Omega)[\theta]}{t} \\ &= \frac{d^2}{dt\,ds} J(\Phi_t^\theta(\Phi_s^\zeta(\Omega)))|_{t=s=0} \end{aligned}$$

(ii) Higher order derivatives can be defined in a similar fashion. Let n vector fields $\theta_1, \ldots, \theta_n \in C_c^\infty(D, \mathbf{R}^d)$ *be given. Then the nth order Eulerian or Lie semi-derivative is defined by*

$$dJ^n(\Omega)[\theta_1][\theta_2]\cdots[\theta_{n-1}][\theta_n] := \frac{d^n}{dt_1 \cdots dt_n} J((\Phi_{t_1}^{\theta_1} \circ \cdots \circ \Phi_{t_n}^{\theta_n})(\Omega))|_{t_1=\cdots=t_n=0}.$$

The nth order semi-derivative is also denoted by $\mathcal{L}_{\theta_1,\ldots,\theta_n}(J)|_\Omega := dJ(\Omega)[\theta_1]\cdots[\theta_n]$*. For a regular domain* $D \subset \mathbf{R}^d$ *and a flow stable subset* $\Xi \subset 2^D$*, we denote by*

$$C_D^k(\Xi) := \{J : \Xi \to \mathbf{R},\quad k\text{-times continuously shape differentiable in each } \Omega \subset \Xi\}$$

the set of k-times shape differentiable function.

We close this section with the following example of a very simple shape function and its derivatives.

Example 2.37. *Let an open, bounded set* $\Omega \subset \mathbf{R}^d$ *and a function* $f \in C^1(\mathbf{R}^d)$ *be given. The first order shape derivative (or simply shape derivative) of the shape function*

$$J(\Omega) := \int_\Omega f\,dx$$

reads

$$dJ(\Omega)[\theta] = \int_\Omega \mathrm{div}\,(\theta) f + \nabla f \cdot \theta\,dx.$$

When $f \in C^2(\mathbf{R}^d)$*, we can compute the second order shape derivative*

$$\begin{aligned} d^2J(\Omega)[\theta][\zeta] =& dJ(\Omega)[\partial\theta\zeta] + \int_\Omega -f\partial\theta : \partial\zeta^\top + f\ \mathrm{div}\,(\theta)\,\mathrm{div}\,(\zeta)\,dx \\ &+ \int_\Omega \nabla^2 f\zeta\cdot\theta + \nabla f\cdot\zeta\,\mathrm{div}\,(\theta) + \nabla f\cdot\theta\,\mathrm{div}\,(\zeta)\,dx \end{aligned}$$

One immediately sees that in a stationary *or* critical *point* $\Omega^* \subset \mathbf{R}^d$ *of* J*, that is,*

$$dJ(\Omega^*)[\theta] = 0 \quad \text{for all } \theta \in C_c^2(D, \mathbf{R}^d)$$

the asymmetrical term $dJ(\Omega^*)[\partial\theta\zeta]$ *vanishes and thus the second order shape derivative is symmetric in a critical point. Now we show that the second order shape derivative is positive definite in a critical point. Pick* $\Omega^* = (a, b) \subset \mathbf{R}$ *and* f *as depicted in Figure 2.3. Then* Ω^* *is a global optimum and, we get (note that* $\frac{1}{2}\frac{d}{dx}\theta^2 = \theta\theta'$*)*

$$\begin{aligned} d^2J(\Omega^*)[\theta][\theta] &= \int_{\Omega^*} f''\theta^2 + 2f'\theta\theta'\,dx \\ &= |_a^b f'\theta^2 - \int_{\Omega^*} f''\theta^2\,dx + \int_{\Omega^*} f''\theta^2\,dx \\ &= f'(b)\theta(b)^2 - f'(a)\theta(a)^2 \\ &\geq \min\{f'(b), -f'(a)\}(\theta(b)^2 + \theta(a)^2) \end{aligned}$$

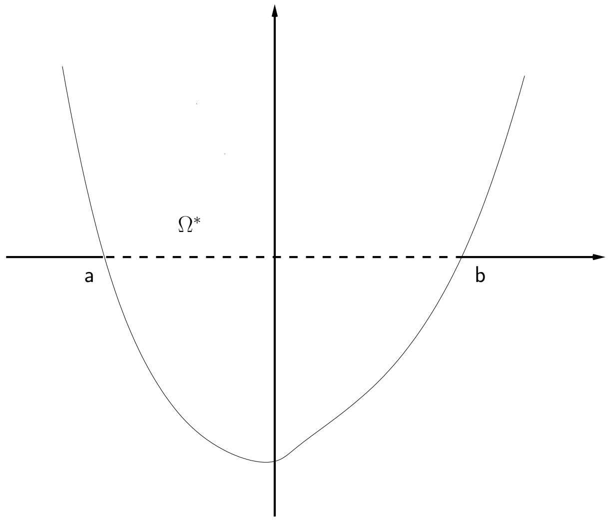

Figure 2.3: Function f and optimal set Ω^* (dashed)

since $f'(a) < 0$ and $f'(b) > 0$.

In the next chapter, we will see an example for the first order shape derivative, where the function f depends itself on the set Ω via a partial differential equation. For more details on second order shape derivatives and their connection to the perturbation of identity, we refer the reader to [37, Sec. 6, Chap. 9] and [51, Chap. 5].

2.5.2 Structure theorem

In Hadamard's research on elastic plates [49] used normal deformation along the boundary to compute the shape derivative of the associated first eigenvalue and discovered that it is an integral over $\partial\Omega$ acting on the normal component of the shape perturbations for a smooth set Ω. This fundamental result of shape optimization was made rigorous later by J.-P. Zolésio in the *"structure theorem"*, where the integral representation is in general replaced by an distribution. When $dJ(\Omega)$ is of finite order and the domain Ω is smooth enough, one can often write the shape derivative as an integral over $\partial\Omega$, which is the canonical form in the shape optimization literature.

Theorem 2.38 (*structure theorem*). *Assume $\Gamma := \partial\Omega$ is compact and J is shape differentiable. Denote the associated distribution to the* shape derivative *by*

$$C_c^\infty(D, \mathbf{R}^d) \to \mathbf{R} : \ \theta \mapsto G(\theta) := dJ(\Omega)[\theta].$$

If G is of order $k \geq 0$ and Γ of class C^{k+1}, then there exists a continuous functional $g : C^k(\Gamma) \to \mathbf{R}$ such that

$$dJ(\Omega)(\theta) = g(\theta_{|\Gamma} \cdot n). \tag{2.16}$$

Proof. See [37, Thm. 3.6 and Corol. 1, pp. 479–481]. □

Remark 2.39. *In particular if $g \in L_1(\Gamma)$ in Theorem 2.38 then we have the typical boundary expression*

$$dJ(\Omega)(\theta) = \int_\Gamma g\, \theta \cdot n \, ds. \tag{2.17}$$

Remark 2.40 (Non-smooth domains). *When the domain Ω is not C^k, $k \geq 1$, then the struture theorem is not valid anymore as can be seen at the simple example*

$$J(\Omega) = \int_{\partial\Omega} dx$$

as demonstrated in [90]. In this case the shape derivative $dJ(\Omega)$ still exists when $\partial\Omega$ is only piecewise smooth, but it will depend not only on $\theta \cdot n$ but also on tangential parts of θ.

Remark 2.41 (Geometric property of g). *The function g appearing in (2.17) is in general neither an intrinsic quantity of the surface Γ (such as the Gauss curvature) nor can it be determined by the surface Γ alone. Usually, when J depends implicitly on some PDE (see e.g. Chapter 5 for several examples), then g involves gradients of functions that depend on functions defined in a neighborhood of Γ. Therefore, the main conclusion from the previous theorem is not that the shape derivative depends on the normal component on the boundary, but that $dJ(\Omega)[\theta]$ is supported in the boundary Γ.*

Remark 2.42 (Historical comment). *The credit of the previous theorem goes to J.-P.Zolésio. Although this result is usually referred to as Hadamard's structure theorem, it was J.-P.Zolésio who proved it in his 1979 thesis for C^{k+1}-domains ($k \geq 0$) and general shape functions. This result was extended to arbitrary domains in the paper [40] and the boundary representation was further refined in the recent paper [65]. In [49] J. Hadamard studied the shape sensitivity of the first eigenvalues of clamped elastic plates by using normal perturbations along a C^∞-boundary and found that the shape derivative has the form (2.17); cf. [37, Rem. 3.2, p. 481], [49] and the introduction.*

A theorem similar to the structure theorem mentioned previously can be established for the second order shape derivative and again we refer the reader to [37, Sec. 6, Chap. 9] for further details in this direction. Finally, we quote a version of *Reynolds' transport theorem* [37, Thm. 4.2, pp. 483–484], that will be used to compute the boundary expression of the shape derivative.

Theorem 2.43. *Let $\theta \in C_c^k(D, \mathbf{R}^d)$, $k \geq 1$, and fix $\tau > 0$. Moreover, suppose that $\varphi \in C([0,\tau], W^{1,1}_{loc}(\mathbf{R}^d)) \cap C^1([0,\tau], L^1_{loc}(\mathbf{R}^d))$ and an open bounded domain Ω with Lipschitz boundary Γ be given. The right sided derivative of the function $f(t) := \int_{\Omega_t} \varphi(t)\, dx$ at $t = 0$ denoted $f'(0^+) := \lim_{t\searrow 0}(f(t) - f(0))/t)$ is given by*

$$f'(0^+) = \int_\Omega \varphi'(0)\, dx + \int_\Gamma \varphi(0)\, \theta_n\, ds.$$

Chapter 3

Shape differentiability under PDE constraints

In this chapter, the following methods are used to prove the shape differentiability of a tracking type shape function constrained by semi-linear PDE: the material derivative method, the min-max formulation (theorem of Correa-Seeger), the rearrangement method and the min method. We present a modification of Céa's Lagrange method that allows a rigorous derivation of the shape derivative in the case of existence of material derivatives. Finally, we show how to derive the boundary expression (BE) of the shape derivative in two different ways.

3.1 The semi-linear model problem

Throughout this chapter, we consider the semi-linear *state equation*

$$-\Delta u + \varrho(u) = f \ \text{ in } \Omega, \quad u = 0 \ \text{ on } \Gamma \tag{3.1}$$

on a bounded domain $\Omega \subset \mathbf{R}^d$ with boundary $\Gamma := \partial\Omega$. The function $u : \Omega \to \mathbf{R}$ is called *state* and $f : D \to \mathbf{R}$ is a given function defined on a regular domain $D \subset \mathbf{R}^d$ containing Ω. Without loss of generality, we may assume $\varrho(0) = 0$ since otherwise consider $\tilde{\varrho}(x) := \varrho(x) - \varrho(0)$ with right hand side $\tilde{f}(x) := f(x) - \varrho(0)$. To simplify the exposition, we choose as objective function

$$J(\Omega) := \int_\Omega |u - u_r|^2 \, dx, \tag{3.2}$$

where u solves the above semi-linear equation on Ω and $|\cdot|$ denotes the absolute value. Let us start with some general assumptions:

Assumption (Data).

(i) Let $D \subset \mathbf{R}^d$ be a regular domain with boundary $\Sigma := \partial D$. Moreover, assume that $\Omega \subset D$ is open and has a Lipschitz boundary $\Gamma := \partial\Omega$.

(ii) The functions $u_r, f : D \to \mathbf{R}$ are continuously differentiable with bounded first derivative.[1]

(iii) Let θ belong to $C_c^2(D, \mathbf{R}^d)$ and denote by Φ_t its flow.

Unless stated otherwise, we assume that the previous assumption is satisfied.

[1]Therefore u_r and f are Lipschitz continuous on $\overline{D}$ and consequently belong to $W^1_\infty(D, \mathbf{R}^d)$.

3.2 Material derivative method

In order to derive the shape differentiability of J via material derivative method ϱ has to satisfy certain properties. Hence, additionally to Assumption (Data), we require:

Assumption ($\mathcal{M}$). *The function $\varrho : \mathbf{R} \to \mathbf{R}$ is continuously differentiable, bounded and nondecreasing.*

We call $u \in H^1_0(\Omega)$ a *weak solution* of (3.1) if

$$\int_\Omega \nabla u \cdot \nabla \psi \, dx + \int_\Omega \varrho(u)\, \psi \, dx = \int_\Omega f \psi \, dx \quad \text{for all } \psi \in H^1_0(\Omega). \tag{3.3}$$

The weak solution of the previous equation characterises the unique minimum of the energy $E(\Omega, \cdot) : H^1_0(\Omega) \to \mathbf{R}$ defined by

$$E(\Omega, \varphi) := \frac{1}{2} \int_\Omega |\nabla \varphi|^2 + \hat{\varrho}(\varphi)\, dx - \int_\Omega f \varphi \, dx,$$

where $\hat{\varrho}(s) := \int_0^s 2\, \varrho(s')\, ds'$. In the following, we denote by

$$\begin{aligned} d_\varphi E(\Omega, \varphi; \psi) &:= \lim_{t \searrow 0} \frac{E(\Omega, \varphi + t\,\psi) - E(\Omega, \varphi)}{t} \\ d^2_\varphi E(\Omega, \varphi; \psi, \tilde{\psi}) &:= \lim_{t \searrow 0} \frac{d_\varphi E(\Omega, \varphi + t\,\tilde{\psi}; \psi) - dE(\Omega, \varphi; \psi)}{t} \end{aligned}$$

the first and second order directional derivatives of E at φ in the direction ψ and $(\psi, \tilde{\psi})$, respectively. Then we may write (3.3) as $d_\varphi E(\Omega, u; \psi) = 0$, for all $\psi \in H^1_0(\Omega)$.

Lemma 3.1. *Assume that ϱ is continuously differentiable. Then the mapping*

$$s \mapsto \int_\Omega \varrho(\varphi + s\tilde{\varphi})\psi \, dx$$

is continuously differentiable on $\mathbf{R}$ for all $\varphi, \tilde{\varphi} \in L_\infty(\Omega)$ and $\psi \in H^1_0(\Omega)$.

Proof: *Let $\varphi, \tilde{\varphi} \in H^1_0(\Omega) \cap L_\infty(\Omega)$ and $\psi \in H^1_0(\Omega)$. We have to show that*

$$s \mapsto \int_\Omega \varrho(\varphi + s\tilde{\varphi})\psi \, dx$$

is continuously differentiable. Put $z^s(x) := \varrho(\varphi(x) + s\tilde{\varphi}(x))\psi(x)$. We have for almost all $x \in \Omega$

$$\begin{aligned} \frac{z^{s+h}(x) - z^s(x)}{h} \to &= \varrho'(\varphi(x) + s\tilde{\varphi}(x))\tilde{\varphi}(x)\psi(x) \quad \text{as } h \to 0, \\ \left| \frac{d}{ds} z^s(x) \right| &\le C|\psi(x)||\tilde{\varphi}(x)|. \end{aligned}$$

Then it holds

$$\begin{aligned} \left| \frac{z^{s+h}(x) - z^s(x)}{h} \right| &= \left| \frac{1}{h} \int_s^{s+h} \frac{d}{ds'} z^{s'}(x) ds' \right| \\ &\le C|\psi(x)||\tilde{\varphi}(x)| \frac{1}{h} \int_{s'}^{s'+h} ds' \\ &= C|\psi(x)||\tilde{\varphi}(x)|. \end{aligned}$$

Therefore applying Lebesgue's dominated convergence theorem we conclude

$$\frac{d}{ds} \int_\Omega z^s(x)\, dx = \int_\Omega \varrho'(\varphi(x) + s\tilde{\varphi}(x))\tilde{\varphi}(x)\psi(x)\, dx.$$

As a consequence of the previous lemma, we get the differentiability of $s \mapsto d_\varphi E(\Omega, \varphi + s\tilde{\varphi}, \psi)$. Moreover, we conclude by the monotonicity of ϱ

$$d_\varphi^2 E(\Omega, \varphi; \psi, \psi) = \int_\Omega |\nabla\psi|^2 + \varrho'(\varphi)\psi^2 \, dx \geq C\|\psi\|^2_{H_0^1(\Omega)}$$

for all $\varphi \in H_0^1(\Omega) \cap L_\infty(\Omega)$ and $\psi \in H_0^1(\Omega)$. We now want to calculate the shape derivative of (3.2). For this purpose, we consider the perturbed cost function $J(\Omega_t) = \int_{\Omega_t} |u_t - u_r|^2 \, dx$, where u_t denotes the weak solution of (3.3) on the domain $\Omega_t := \Phi_t(\Omega)$, that is, $u_t \in H_0^1(\Omega_t)$ solves

$$\int_{\Omega_t} \nabla u_t \cdot \nabla\hat{\psi} \, dx + \int_{\Omega_t} \varrho(u_t)\hat{\psi} \, dx = \int_{\Omega_t} f\hat{\psi} \, dx \quad \text{for all } \hat{\psi} \in H_0^1(\Omega_t). \tag{3.4}$$

It would be possible to compute the derivative of $u_t : \Omega_t \to \mathbf{R}$ pointwise by

$$du(x) := \lim_{t \searrow 0} \frac{u_t(x) - u(x)}{t} \quad \text{for all } x \in \left(\bigcap_{t\in[0,\tau]} \Omega_t \right) \cap \Omega.$$

In the literature this derivative is referred to as *local shape derivative of* u in direction θ; cf. [50]. Nevertheless, we go another way and use the change of variables $\Phi_t(x) = y$ to rewrite $J(\Omega_t)$ as

$$J(\Omega_t) = \int_\Omega \xi(t)|u^t - u_r \circ \Phi_t|^2 \, dx, \tag{3.5}$$

where $u^t := \Psi_t(u_t) : \Omega \to \mathbf{R}$ is a function on the fixed domain Ω. We introduce the mapping $\Psi_t(\varphi) := \varphi \circ \Phi_t$ with inverse $\Psi^t(\hat{\varphi}) := \Psi_t^{-1}(\hat{\varphi}) = \hat{\varphi} \circ \Psi_t^{-1}$. To study the differentiability of (3.5), we can study the function $t \mapsto u^t$. Notice that $u_0 = u^0 = u$ is nothing but the weak solution of (3.3).

The limit $\dot{u} := \lim_{t\searrow 0}(u^t - u)/t$ is called **strong material derivative** if we consider this limit in the norm convergence in $H_0^1(\Omega)$ and **weak material derivative** if we consider the weak convergence in $H_0^1(\Omega)$.

The crucial observation of [99, Theorem 2.2.2, p. 52] is that Ψ_t constitutes an isomorphism from $H^1(\Omega_t)$ into $H^1(\Omega)$. Hence using a change of variables in (3.4) shows that u^t satisfies

$$\int_\Omega A(t)\nabla u^t \cdot \nabla\psi \, dx + \int_\Omega \xi(t) \, \varrho(u^t)\psi \, dx = \int_\Omega \xi(t)f^t\psi \, dx \quad \text{for all } \psi \in H_0^1(\Omega), \tag{3.6}$$

where we used the notation from (2.6). The previous equation characterises the unique minimum of the convex energy $\tilde{E} : [0,\tau] \times H_0^1(\Omega) \to \mathbf{R}$[2]

$$\tilde{E}(t,\varphi) := \frac{1}{2}\int_\Omega \xi(t)|B(t)\nabla\varphi|^2 + \xi(t)\hat{\varrho}(\varphi) \, dx - \int_\Omega \xi(t)f^t\varphi \, dx. \tag{3.7}$$

By standard regularity theory (see e.g. [61]) it follows that $u^t \in C(\overline{\Omega})$ for all $t \in [0,\tau]$. Moreover, the proof of [22, Theorem 3.1] shows that there is a constant $C > 0$ such that

$$\|u^t\|_{C(\overline{\Omega})} + \|u^t\|_{H^1(\Omega)} \leq C \quad \text{for all } t \in [0,\tau].$$

[2]Here we mean convex with respect to φ for each $t \in [0,\tau]$.

As before using Lebesque's dominated convergence theorem it is easy to verify that for fixed $t \in [0,\tau]$ the second order directional derivative $d^2_\varphi \tilde{E}(t,\varphi;\psi,\eta)$ exists for all $\varphi \in L_\infty(\Omega)\cap H^1_0(\Omega)$ and $\psi,\eta \in H^1_0(\Omega)$. Taking into account Proposition 2.12, we see that

$$C\|\psi\|^2_{H^1(\Omega;\mathbf{R}^d)} \le d^2_\varphi \tilde{E}(t,\varphi;\psi,\psi) \quad \text{for all } \varphi \in L_\infty(\Omega)\cap H^1_0(\Omega), \psi \in H^1_0(\Omega) \text{ and all } t\in[0,\tau]. \tag{3.8}$$

Note that $d_\varphi \tilde{E}(t,\varphi;\psi)$ is also differentiable with respect to t and Lemma 2.14 shows:

$$\begin{aligned}\partial_t d_\varphi \tilde{E}(t,\varphi;\psi) &= \int_\Omega A'(t)\nabla\varphi\cdot\nabla\psi + \xi'(t)\varrho(\varphi)\,\psi\,dx - \int_\Omega (\xi'(t)f^t + \xi(t)B(t)\nabla f^t)\varphi\,dx \\ &\le C(1+\|\varphi\|_{H^1(\Omega)})\|\psi\|_{H^1(\Omega)},\end{aligned} \tag{3.9}$$

for all $t\in[0,\tau]$, where $C>0$ is a constant. By the coercivity property (3.8) of the second order derivative of $\tilde{E}$

$$\begin{aligned}C\|\nabla(u^t-u)\|^2_{L_2(\Omega;\mathbf{R}^d)} &\le \int_0^1 d^2_\varphi \tilde{E}(t,su^t+(1-s)u;u^t-u,u^t-u) &(3.10)\\ &= d_\varphi\tilde{E}(t,u^t;u^t-u) - d_\varphi\tilde{E}(t,u;u^t-u) &(3.11)\\ &= -(d_\varphi\tilde{E}(t,u;u^t-u) - d_\varphi\tilde{E}(0,u;u^t-u)) &(3.12)\\ &= -t\partial_t d_\varphi\tilde{E}(\eta_t\, t,u;u^t-u) &(3.13)\\ &\le C\,t\,\|\nabla(u^t-u)\|_{L_2(\Omega;\mathbf{R}^d)}. &(3.14)\end{aligned}$$

In step (3.10) to (3.11), we applied the mean value theorem in integral form, in step (3.11) to (3.12), we used that $d_\varphi\tilde{E}(t,u^t;u^t-u) = d_\varphi\tilde{E}(0,u;u^t-u)=0$, and in step from (3.12) to (3.13), we applied the mean value theorem which yields $\eta_t\in(0,1)$. In the last step (3.14), we employed the estimate (3.9). Finally, by the Poincaré inequality, we conclude that there is $c>0$ such that $\|u^t-u\|_{H^1(\Omega)}\le tc$ for all $t\in[0,\tau]$. From this estimate we deduce that for any real sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ as $n\to\infty$, the quotient $w^n := (u^{t_n}-u)/t_n$ converges weakly in $H^1_0(\Omega)$ to some element $\dot{u}$ and by compactness there is a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $(w^{n_k})_{k\in\mathbf{N}}$ converges strongly in $L_q(\Omega)$ to some v, where $0<q<\frac{2d}{d-2}$; (cf. [46, p.270, Theorem 6]).[3] Extracting a further subsequence we may assume that $w^{t_k}(x)\to\dot{u}(x)$ as $k\to\infty$ for almost every $x\in\Omega$. Notice that the limit $\dot{u}$ depends on the sequence $(t_{n_k})_{k\in\mathbf{N}}$. However, we will see that this limit is the same for any sequence $(t_n)_{n\in\mathbf{N}}$ converging to zero.

Subtracting (3.6) at $t>0$ and $t=0$ yields

$$\begin{aligned}\int_\Omega A(t)\nabla(u^t-u)\cdot\nabla\psi\,dx + \int_\Omega \xi(t)(\varrho(u^t)-\varrho(u))\,\psi\,dx &= -\int_\Omega (A(t)-I)\nabla u\cdot\nabla\psi\,dx \\ + \int_\Omega(\xi(t)-1)\,\varrho(u)\,\psi\,dx + \int_\Omega(\xi(t)-1)f^t\psi\,dx &+ \int_\Omega (f^t-f)\psi\,dx.\end{aligned} \tag{3.15}$$

We choose $t=t_{n_k}$ in the previous equation and want to pass to the limit $k\to\infty$. The only difficult term in (3.15) is

$$\int_\Omega \xi(t)\frac{\varrho(u^t)-\varrho(u)}{t}\,\psi\,dx = \int_\Omega \xi(t)\left[\int_0^1 \varrho'(u^t_s)\,ds\right]\left(\frac{u^t-u}{t}\right)\psi\,dx.$$

[3] When $d=2$ this means $H^1(\Omega)$ is compactly embedded into $L_p(\Omega)$ for arbitrary $p>1$. When $d=3$ we get that $H^1(\Omega)$ compactly embeds into $L_{6-\varepsilon}(\Omega)$ for any small $\varepsilon>0$.

From the strong convergence of $(u^{t_{n_k}} - u)/t_{n_k}$ to $\dot{u}$ in $L_2(\Omega)$ and the pointwise convergence $\xi(t_{n_k}) \to 1$ and $\varrho'(u_s^{t_{n_k}}) \to \varrho'(u)$, we infer that

$$\int_\Omega \xi(t_{n_k}) \frac{\varrho(u^{t_{n_k}}) - \varrho(u)}{t_{n_k}} \psi\, dx \longrightarrow \int_\Omega \varrho'(u)\, \dot{u}\, \psi\, dx \quad \text{as } k \to \infty.$$

Therefore, choosing $t = t_{n_k}$ in (3.15) and dividing by t_{n_k}, we may pass to the limit:

$$\begin{aligned} \int_\Omega \nabla \dot{u} \cdot \nabla \psi + \varrho'(u)\, \dot{u}\, \psi\, dx + \int_\Omega A'(0) \nabla u \cdot \nabla \psi\, dx + \int_\Omega \operatorname{div} \theta \varrho(u) \psi\, dx \\ = \int_\Omega \operatorname{div}(\theta) f \psi\, dx + \int_\Omega \nabla f \cdot \theta\, \psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega). \end{aligned} \tag{3.16}$$

The function $\dot{u}$ is the unique solution of (3.16). Hence for every sequence $(t_n)_{n\in\mathbf{N}}$ converging to zero there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $w^{t_k} \to \dot{u}$ as $k \to \infty$. Moreover, $\int_\Omega \xi(t)(\varrho(u^t) - \varrho(u)/t\, \psi\, dx \longrightarrow \int_\Omega \varrho'(u)\, \dot{u}\, \psi\, dx$ and $\int_\Omega A(t) \nabla(u^t - u)/t \cdot \nabla \psi\, dx \longrightarrow \int_\Omega \nabla \dot{u} \cdot \nabla \psi\, dx$ as $t \searrow 0$.

We now show that the strong material derivative exists. For this subtract (3.16) from (3.15) to obtain

$$\begin{aligned} &\int_\Omega A(t) \nabla \left(\frac{u^t - u}{t} - \dot{u} \right) \cdot \nabla \psi\, dx + \int_\Omega \xi(t) \left[\int_0^1 \varrho'(u_s^t)\, ds \right] \left(\frac{u^t - u}{t} - \dot{u} \right) \psi\, dx \\ &\quad = \int_\Omega (A(t) - I) \nabla \dot{u} \cdot \nabla \psi\, dx + \int_\Omega (\xi(t) - 1) \left[\int_0^1 \varrho'(u_s^t)\, ds \right] \dot{u}\, \psi\, dx \\ &\quad + \int_\Omega \left[\int_0^1 \varrho'(u_s^t) - \varrho'(u)\, ds \right] \dot{u}\, \psi\, dx - \int_\Omega \left(\frac{A(t) - I}{t} - A'(0) \right) \nabla u \cdot \nabla \psi\, dx \\ &\quad + \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) \varrho(u)\, \psi\, dx + \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) f^t \psi\, dx \\ &\quad + \int_\Omega \left(\frac{f^t - f}{t} - \nabla f \cdot \theta \right) \psi\, dx. \end{aligned}$$

Now we insert $\psi = w^t - \dot{u}$ as test function into the previous equation. Using Proposition 2.12 and the fact that $\xi(t) > 0$, $\varrho' \geq 0$ we get

$$\begin{aligned} \gamma_1 \|\nabla(w^t - \dot{u})\|^2_{L_2(\Omega)} \leq &\int_\Omega (A(t) - I) \nabla \dot{u} \cdot \nabla(w^t - \dot{u})\, dx + \int_\Omega (\xi(t) - 1) \int_0^1 \varrho'(u_s^t)\, ds\, \dot{u}\, (w^t - \dot{u})\, dx \\ &+ \int_\Omega \int_0^1 (\varrho'(u_s^t) - \varrho'(u)\, ds)\, \dot{u}\, (w^t - \dot{u})\, dx \\ &- \int_\Omega \left(\frac{A(t) - I}{t} - A'(0) \right) \nabla u \cdot \nabla(w^t - \dot{u})\, dx \\ &+ \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) (\varrho(u)\, (w^t - \dot{u}) + f^t (w^t - \dot{u}))\, dx \\ &+ \int_\Omega \left(\frac{f^t - f}{t} - \nabla f \cdot \theta \right) (w^t - \dot{u})\, dx. \end{aligned}$$

Using the convergences $A(t) \to I$, $(A(t) - I)/t - A'(0) \to 0$, $(f^t - f)/t - \nabla f \cdot \theta \to 0$, $\xi(t) \to 1$ and $(\xi(t) - 1)/t -$ div (θ) in $C(\overline{\Omega})$, and the uniform boundedness of $\|w^t - \dot{u}\|_{H^1(\Omega)}$ and $\|\dot{u}\|_{H^1(\Omega)}$ yields

$$\|w^t - \dot{u}\|_{H^1(\Omega)} \to 0 \quad \text{as } t \searrow 0.$$

We are now in the position to calculate the volume expression of the shape derivative. First, we differentiate (3.5) with respect to t

$$dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(\theta)|u-u_r|^2\,dx - \int_\Omega 2(u-u_r)\nabla u_r\cdot\theta\,dx + \int_\Omega 2(u-u_r)\dot{u}\,dx.$$

Note that for the previous calculation it was enough to have $\|u^t - u\|_{H^1(\Omega)} \le ct$ for all $t\in[0,\tau]$. This is sufficient to differentiate the L_2 cost function. Nevertheless, for a cost function involves gradients of u such as

$$\tilde{J}(\Omega) := \int_\Omega \|\nabla u - \nabla u_r\|^2\,dx,$$

this is not true anymore. Now in order to eliminate the material derivative in the last equation, the so-called adjoint equation is introduced

$$\text{Find } p\in H^1_0(\Omega): \quad d_\varphi E(\Omega,u;p,\psi) = -2\int_\Omega (u-u_r)\,\psi\,dx \quad \text{for all } \psi\in H^1_0(\Omega). \tag{3.17}$$

The function p is called *adjoint state*. Finally, testing the adjoint equation with $\dot{u}$ and the material derivative equation (3.16) with p, we arrive at the volume expression

$$\begin{aligned} dJ(\Omega)[\theta] &\overset{(3.17)}{=} \int_\Omega \operatorname{div}(\theta)|u-u_r|^2\,dx - \int_\Omega 2(u-u_r)\nabla u_r\cdot\theta\,dx - d_\varphi E(\Omega,u;p,\dot{u}) \\ &\overset{(3.16)}{=} \int_\Omega \operatorname{div}(\theta)|u-u_r|^2\,dx - \int_\Omega 2(u-u_r)\nabla u_r\cdot\theta\,dx \\ &\quad + \int_\Omega A'(0)\nabla u\cdot\nabla p + \operatorname{div}(\theta)\varrho(u)p\,dx - \int_\Omega \operatorname{div}(\theta f)p\,dx. \end{aligned} \tag{3.18}$$

Note that the volume expression already makes sense when $u,p\in H^1_0(\Omega)$. Assuming higher regularity of the state and adjoint (e.g. $u,p\in H^2(\Omega)\cap H^1_0(\Omega)$) would allow us to rewrite the previous volume expression into a boundary expression, that is, an integral over the boundary $\partial\Omega$.

3.3 Shape derivative method

Assuming that the solutions u,p and the boundary Γ are smooth, say C^2, we may transform the volume expression (3.18) into an integral over Γ. This can be accomplished by integration by parts or in the following described way. Instead of transporting the cost function back to Ω, one may directly differentiate $J(\Omega_t) = \int_{\Omega_t} |\Psi^t(u^t) - u_r|^2\,dx$ by invoking the transport Theorem 2.43, to obtain

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} |u-u_r|^2\theta\cdot n\,ds + \int_\Omega 2\,(u-u_r)(\dot{u} - \nabla u\cdot\theta)\,dx. \tag{3.19}$$

The function $u' := \dot{u} - \nabla u\cdot\theta$ is called *shape derivative* of u at Ω in direction θ associated with the parametrisation Ψ_t. It depends linearly on θ. Note that since $\Psi^0 = id_{H^1_0(\Omega)}$, we have $\Psi^t\circ\Psi^{-t} = \Psi^0 = id_{H^1_0(\Omega)}$ and $\Psi^{-t}\circ\Psi^t = \Psi^0 = id_{H^1_0(\Omega_t)}$. Setting $u^t := \Psi_t(u_t)$, we can write

$$u' = \frac{d}{dt}\Psi^t(u^t)|_{t=0} = \frac{d}{dt}(u^t\circ\Phi_t^{-1})|_{t=0}.$$

Therefore the shape derivative decomposes into two parts, namely

$$u' = \underbrace{\partial_t\Psi^t(u^t)_{|t=0}}_{\in L_2(\Omega)} + \underbrace{\Psi^0(\dot{u})}_{\in H^1_0(\Omega)},$$

where $\partial_t \Psi^t(u^t)|_{t=0} := \lim_{t\searrow 0}(\Psi^t(u^t) - \Psi^0(u^t))/t = -\nabla u \cdot \theta$. Assuming that the solution u belongs to $u \in H_0^1(\Omega) \cap H^2(\Omega)$, we get

$$u' = \underbrace{\partial_t \Psi^t(u^t)_{|t=0}}_{\in H^1(\Omega)} + \underbrace{\Psi^0(\dot{u})}_{\in H_0^1(\Omega)\cap H^2(\Omega)}$$

One may write the perturbed state equation (3.4) in the equivalent form

$$\int_{\Omega_t} \nabla(\Psi^t(u^t)) \cdot \nabla(\Psi^t(\varphi)) \;+\; \varrho(\Psi^t(u^t))\,(\Psi^t(\varphi))\,dx = \int_{\Omega_t} f\Psi^t(\varphi)\,dx \quad \text{ for all } \varphi \in H_0^1(\Omega).$$

Then by the previous discussion, we know that $u^t : [0,\tau] \to H^1(\Omega)$ is differentiable in 0. Hence by formally differentiating the last equation using the transport Theorem 2.43:

$$\begin{aligned} &\int_\Omega \nabla u' \cdot \nabla\varphi + \varrho'(u)u'\,\varphi\,dx - \int_\Omega \nabla u \cdot \partial_\theta\varphi + \varrho(u)\,\partial_\theta\varphi\,dx \\ &\qquad + \int_{\partial\Omega} (\nabla u \cdot \nabla\varphi + \varrho(u)\,p)\,\theta_n ds = \int_{\partial\Omega} f\varphi\,\theta_n ds - \int_\Omega f\partial_\theta\varphi\,dx \end{aligned} \tag{3.20}$$

for all $\varphi \in H^2(\Omega) \cap H_0^1(\Omega)$, where $\theta_n := \theta \cdot n$ and $\partial_\theta := \theta \cdot \nabla$. Note that adjoint state p vanishes on Γ. Notice that this equation can also be derived from (3.16) by partial integration.

Remark 3.2. *Note that u' does not belong to $H_0^1(\Omega)$, but only to $H^1(\Omega)$. As the shape derivative does not belong to the solution space of the state equation, it may lead to false or incomplete formulas for the boundary expression of the shape derivative.*

Remark 3.3. *Let $\gamma : [0,1] \to \Gamma$ be a smooth curve in the boundary with $\gamma(0) = x \in \Gamma$ and $\gamma'(0) = v$. Assume $u : \Omega \to \mathbf{R}$ admits an extension in a neighborhood of Γ, denoted also by u, then we compute $0 = \frac{d}{dt}(u(\gamma(t))|_{t=0} = \nabla u \cdot \gamma'(0) = \nabla_\Gamma u \cdot v + (\partial_n u)n \cdot v$. Note that v lies in the tangential plane at x, thus $v \cdot n = 0$. Since v was arbitrary, we conclude $u = 0$ on Γ implies that $\nabla_\Gamma u = 0$ on Γ.*

The remark shows that $\nabla u = (\partial_n u)n$. Then integrating by parts in (3.20) and using that u is a strong solution yields

$$\begin{aligned} \int_\Omega \nabla\dot{u} \cdot \nabla\varphi \;+\; \varrho'(u)\dot{u}\,\varphi\,dx = &\int_\Gamma (\partial_n u\,\partial_n\varphi - 2\,\partial_n u\,\partial_n\varphi)\,\theta_n\,ds \\ &+ \int_\Omega \partial_\theta u\,(-\Delta\varphi + \varrho'(u)\,\varphi)\,dx. \end{aligned} \tag{3.21}$$

Now, using the previous equation and the adjoint state equation one can eliminate $\dot{u}$ in (3.19)

$$\begin{aligned} dJ(\Omega)[\theta] &\overset{(3.17)}{=} \int_\Gamma |u - u_r|^2\,\theta_n\,ds + \int_\Omega \nabla\dot{u} \cdot \nabla p + \varrho'(u)\,\dot{u}\,p\,dx + \int_\Omega \nabla u \cdot \theta\,2(u - u_r)\,dx \\ &\overset{(3.21)}{=} \int_\Gamma |u - u_r|^2\,\theta_n\,ds - \int_\Gamma 2\partial_n u\,\partial_n p\,\theta_n ds \\ &\qquad + \int_\Omega (-\Delta p + \varrho'(u)\,p + 2(u - u_r))\nabla u \cdot \theta\,dx. \end{aligned}$$

Finally, assuming that p solves the adjoint equation in the strong sense, we get

$$dJ(\Omega)[\theta] = \int_\Gamma (|u - u_r|^2 - \partial_n u\,\partial_n p)\,\theta_n\,ds. \tag{3.22}$$

What we observe in the calculations above is that there is no material derivative $\dot{u}$ or shape derivative u' in the final expression (3.18) or (3.22). This suggests that there might be a way to obtain this formula without the computation of $\dot{u}$. In the next section, we get to know one possible way to avoid the material derivatives.

3.4 The min-max formulation of Correa and Seeger

In this section we want to discuss the minimax formulation of shape optimization problems and a theorem of Correa and Seeger ([30]). This theorem provides a powerful tool to differentiate a minimax function with respect to a parameter. The cost function for many optimal control problems can be rewritten as the min-max of a Lagrangian function $\mathcal{L}$, that is, a utility function plus the equality constraints, i.e.,

$$J(u) = \inf_{\varphi\in A} \sup_{\psi\in B} \mathcal{L}(u,\varphi,\psi).$$

Therefore, the directional differentiation of the cost function is equivalent to the differentiation of the inf-sup with respect to u. This method is in particular applicable to linear partial differential equations and convex cost functions.

3.4.1 Saddle points and their characterisation

For the convenience of the reader we recall here the definition of saddle points and their characterisation.

Definition 3.4. *Let A, B be sets and $G : A \times B \to \mathbf{R}$ a map. Then a pair $(u, p) \in A \times B$ is said to be a* saddle point *on $A \times B$ if*

$$G(u,\psi) \le G(u,p) \le G(\varphi,p) \quad \textit{for all } \varphi\in A, \quad \textit{for all } \psi \in B.$$

The result [44, Prop. 1.2, p. 167] provides a condition for (u, p) to be a saddle point.

Lemma 3.5. *A pair $(u, p) \in A \times B$ is a saddle point of $G(,)$ if and only if* [4]

$$\min_{\hat u\in A}\sup_{\hat p\in B} G(\hat u,\hat p) = \max_{\hat p\in B}\inf_{\hat u\in A} G(\hat u,\hat p),$$

and it is equal to $G(u, p)$, where u is the attained minimum and p the attained maximum, respectively.

For a convex-concave function G that is additionally Gaeuaux differentiable, one may check that $(u, p) \in A \times B$ is a saddle point by [44, Prop. 1.6, p. 169–170]:

Proposition 3.6. *Let E, F be two Banach spaces. Let us suppose that $A \subset E$ and $B \subset F$, A, B are closed, convex and non-empty. Moreover, let $G : E \times F \to \mathbf{R}$ be such that for all $p \in B$, the function $u \mapsto G(u, p)$ is lower semi-continuous, convex and Gaeuaux differentiable, and for all $u \in A$ the function $p \mapsto G(u, p)$ is upper semi-continuous, concave and Gaeuaux differentiable. Then $(\bar u, \bar p) \in A \times B$ is a saddle point if and only if*

$$\left\langle \frac{\partial G}{\partial u}(\bar u,\bar p), u-\bar u\right\rangle \ge 0 \quad \textit{for all } u\in A,$$

$$\left\langle \frac{\partial G}{\partial p}(\bar u,\bar p), p-\bar p\right\rangle \le 0 \quad \textit{for all } p\in B.$$

[4]Here the min and max indicate that the infimum and supremum is attained, respectively.

3.4.2 Min-max formulation for the semi-linear equation

The point of departure for the *min-max formulation* is the observation that

$$\boxed{J(\Omega) = \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega,\varphi,\psi),}$$

where the Lagrangian $\mathcal{L}$ is defined by

$$\mathcal{L}(\Omega,\varphi,\psi) := \int_\Omega |\varphi - u_r|^2\,dx + \int_\Omega \nabla\varphi\cdot\nabla\psi\,dx - \int_\Omega f\psi\,dx \quad (\varphi,\psi\in H_0^1(\Omega)).$$

This is true since for any $\varphi \in H_0^1(\Omega)$

$$\sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega,\varphi,\psi) = \begin{cases} J(\Omega) & \text{if } \varphi = u \text{ solves (3.3)} \\ +\infty & \text{else .}\end{cases}$$

In order to apply the *theorem of* Correa-Seeger to the Lagrangian $\mathcal{L}$, we have to show that it admits saddle points. Reasonable conditions to ensure the existence of saddle points for our specific example is to assume that $\mathcal{L}$ is convex and differentiable with respect to φ.

Assumption ($\mathcal{C}$). *The function ϱ is linear, i.e., $\varrho(x) = ax$, where $a\in\mathbf{R}$.*

Since for any open set $\Omega\subset\mathbf{R}^d$ the Lagrangian $\mathcal{L}$ is convex and differentiable with respect to φ, and concave and differentiable with respect to ψ, we know from [44, Prop. 1.6, p. 169–170] that the saddle points $(u,p)\in H_0^1(\Omega)\times H_0^1(\Omega)$ can be characterised by $\partial_\psi\mathcal{L}(\Omega,u,p)(\hat\psi) = 0$ for all $\hat\psi\in H_0^1(\Omega)$ and $\partial_\varphi\mathcal{L}(\Omega,u,p)(\hat\varphi) = 0$ for all $\hat\varphi\in H_0^1(\Omega)$. These last equations coincide with the state equation (3.3) and the adjoint equation (3.17). To compute the shape derivative of J, we consider for $t>0$

$$J(\Omega_t) = \min_{\hat\varphi\in H_0^1(\Omega_t)} \sup_{\hat\psi\in H_0^1(\Omega_t)} \mathcal{L}(\Omega_t,\hat\varphi,\hat\psi) = \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega_t,\Psi^t(\varphi),\Psi^t(\psi)), \tag{3.23}$$

where the saddle points of $\mathcal{L}(\Omega_t,\cdot,\cdot)$ are again given by the solutions of (3.3) and (3.17), but the domain Ω has to be replaced by Ω_t. By definition of a saddle point

$$\mathcal{L}(\Omega_t,u_t,\hat\psi) \le \mathcal{L}(\Omega_t,u_t,p_t) \le \mathcal{L}(\Omega_t,\hat\varphi,p_t) \quad \text{for all } \hat\psi,\hat\varphi\in H_0^1(\Omega_t). \tag{3.24}$$

Now, since $\Psi_t : H_0^1(\Omega_t)\to H_0^1(\Omega)$ is a bijection it is easily seen that the saddle points of $G(t,\varphi,\psi) := \mathcal{L}(\Omega_t,\Psi^t(\varphi),\Psi^t(\psi))$ are given by $u^t = \Psi_t(u_t)$ and $p^t = \Psi_t(p_t)$. It can also be verified that the function u^t solves (3.6) and applying the change of variables $\Phi_t(x) = y$ to (3.17) shows that p^t solves

$$\int_\Omega A(t)\nabla\psi\cdot\nabla p^t + \xi(t)\,\varrho'(u^t)\,p^t\,\psi\,dx = -2\int_\Omega \xi(t)(u^t - u_r^t)\psi\,dx \quad \text{for all } \psi\in H_0^1(\Omega). \tag{3.25}$$

Moreover, the functions u^t,p^t satisfy $G(t,u^t,\psi)\le G(t,u^t,p^t)\le G(t,\varphi,p^t)$ for all $\psi,\varphi\in H_0^1(\Omega)$. Applying the change of variables $\Phi_t(x) = y$ we can write the function G as

$$G(t,\varphi,\psi) = \int_\Omega \xi(t)|\varphi - u_r^t|^2\,dx + \int_\Omega A(t)\nabla\varphi\cdot\nabla\psi + \xi(t)\varrho(\varphi)\,\psi\,dx - \int_\Omega \xi(t)f^t\psi\,dx. \tag{3.26}$$

From Lemma 3.5 and the definition of a saddle point (u^t,p^t) of $G(t,\ ,\ )$, we conclude that

$$g(t) := \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} G(t,\varphi,\psi) = G(t,u^t,p^t).$$

Moreover, we have the relation $g(t) = G(t, u^t, \psi)$ for all $\psi \in H_0^1(\Omega)$, since u^t solves (3.6). In view of (3.23), the shape derivative $dJ(\Omega)[\theta]$ exists if the derivative of $g(t)$ at $t = 0$ from the right hand side exists. But since G is a Lagrangian, that is, the sum of a cost function plus a state equation, the differentiability of g is equivalent to the differentiability of $t \mapsto G(t, u^t, \psi)$ for any (and thus for all) $\psi \in H_0^1(\Omega)$. Notice that when the state equation has no unique solution the cost function is not well-defined in general, but the the function g is.

Theorem 3.9 below gives conditions, which allows to conclude the equality

$$dJ(\Omega)[\theta] = \partial_t G(0, u, p)$$

without employing the material derivative $\dot{u}$. Let us sketch the proof of this fundamental result when G is given by (3.26).

Proposition 3.7. *The function $t \mapsto G(t, u^t, \psi)$ is differentiable from the right side at 0. Moreover, we have*

$$\frac{d}{dt} G(t, u^t, \psi)|_{t=0} = \partial_t G(0, u, p) \tag{3.27}$$

for arbitrary $\psi \in H_0^1(\Omega)$. Here, $p \in H_0^1(\Omega)$ solves the adjoint equation (3.17).

Proof. Assume that $(u^t, p^t) \in H_0^1(\Omega) \times H_0^1(\Omega)$ is a saddle point. Then, by definition of a saddle point, we get the inequalities $G(t, u^t, p^t) \le G(t, u, p^t)$ and $G(0, u, p) \le G(0, u^t, p)$. Therefore setting $\Delta(t) := G(t, u^t, p^t) - G(0, u, p)$ gives

$$G(t, u^t, p) - G(0, u^t, p) \le \Delta(t) \le G(t, u, p^t) - G(0, u, p^t).$$

Using the mean value theorem, we find for each $t \in [0, \tau]$ constants $\zeta_t, \eta_t \in (0, 1)$ such that

$$t\partial_t G(t\zeta_t, u^t, p) \le \Delta(t) \le t\partial_t G(t\eta_t, u, p^t), \tag{3.28}$$

where the derivative of G with respect to t is given by

$$\begin{aligned} \partial_t G(t, \varphi, \psi) = &\int_\Omega \xi'(t)|\varphi - u_r^t|^2 - 2\xi(t)(\varphi - u_r^t)B(t)\nabla u_r^t \cdot \theta^t \, dx \\ &+ \int_\Omega A'(t)\nabla\varphi \cdot \nabla\psi + \xi'(t)\varrho(\varphi)\,\psi - \xi'(t)\, f^t\psi - B(t)\nabla f^t \cdot \theta^t \psi \, dx \end{aligned} \tag{3.29}$$

and the derivatives ξ' and A' are given by Lemma 2.14. It can be verified from this formula that $(t, \varphi) \mapsto \partial_t G(t, \varphi, p)$ is strongly continuous and $(t, \psi) \mapsto \partial_t G(t, u, \psi)$ is even weakly continuous. Moreover, from (3.6) and (3.25) it can be inferred that $t \mapsto u^t$ and $t \mapsto p^t$ are bounded in $H_0^1(\Omega)$. Therefore, for any sequence of non-negative numbers $(t_n)_{n \in \mathbf{N}}$ we get $u^{t_n} \rightharpoonup w$, $p^{t_n} \rightharpoonup v$ as $n \to \infty$ for two elements $w, v \in H_0^1(\Omega)$. Passing to the limit in (3.6) and (3.25) and taking Lemma 2.16 into account, we see that w solves the state equation and v the adjoint equation. By uniqueness of the state and adjoint equation we get $w = u$ and $v = p$. Selecting a further subsequence $(t_{n_k})_{k \in \mathbf{N}}$ yields that $u^{t_{n_k}}$ converges strongly in $L_2(\Omega)$. Thus we conclude from (3.28) $\liminf_{t \searrow 0} \Delta(t)/t \ge \partial_t G(0, u, p)$ and $\limsup_{t \searrow 0} \Delta(t)/t \le \partial_t G(0, u, p)$. Combining these estimates leads to $\limsup_{t \searrow 0} \Delta(t)/t = \liminf_{t \searrow 0} \Delta(t)/t$, which proves (3.27) and thus the shape differentiability of J. $\square$

Evaluating the derivative $\partial_t G(t,u,p)|_{t=0}$ leads to the formula (3.18). Note that we may extend u, p to global H^2 functions $\tilde{u}, \tilde{p} \in H^2(\mathbf{R}^d)$. Then the boundary expression may be obtained by applying Theorem 2.43 to $d/dt\mathcal{L}(\Omega_t, \Psi^t(\tilde{u}), \Psi^t(\tilde{p}))|_{t=0}$ to get

$$\begin{aligned} dJ(\Omega)[\theta] = &\int_\Gamma (|u-u_r|^2 + \nabla u\cdot\nabla p + \varrho(u)\,p)\theta_n\,ds + \int_\Omega \nabla\mathring{u}\cdot\nabla p + \varrho'(u)\,\mathring{u}\,p\,dx \\ &+ \int_\Omega (u-u_r)\mathring{u}\,dx + \int_\Omega \nabla u\cdot\nabla\mathring{p} + \varrho(u)\,\mathring{p}\,dx - \int_\Omega f\mathring{p}\,dx, \end{aligned}$$

where $\mathring{u} = \partial_t(\Psi^t(\tilde{u}))|_{t=0} = -\nabla u\cdot\theta$, $\mathring{p} = \partial_t(\Psi^t(\tilde{p}))|_{t=0} = -\nabla p\cdot\theta$. To rewrite the previous expression into an integral over Γ, we integrate by parts in the integrals over Ω to obtain

$$\begin{aligned} dJ(\Omega)[\theta] = &\int_\Gamma (|u-u_r|^2 + \nabla u\cdot\nabla p + \varrho(u)\,p)\,\theta_n\,ds + \int_{\partial\Omega} \mathring{u}\,\partial_n p\,ds + \int_{\partial\Omega} \partial_n u\,\mathring{p}\,ds \\ &- \int_\Omega \mathring{u}\left(-\Delta p + \varrho'(u)\,p + 2(u-u_r)\right)\,dx - \int_\Omega \mathring{p}\left(-\Delta u + \varrho(u) - f\right)\,dx. \end{aligned}$$

Finally, using the strong solvability of u and p, and taking Remark 3.3 into account, we arrive at (3.22).

Remark 3.8. *We point out that the first inequality in (3.24) is the key to avoid the material derivative. Nevertheless, without the assumption of convexity of G with respect to φ it is difficult to prove this inequality.*

3.4.3 A theorem of Correa-Seeger

Finally, we quote the improved version [37, Theorem 5.1, pp. 556–559] of the theorem of Correa-Seeger. This theorem also applies, roughly speaking, to situations when the state equation admits no unique solution and the Lagrangian admits saddle points. The proof is similar to the one of Proposition 3.7. Let a real number $\tau > 0$ and vector spaces E and F be given. We consider the mapping

$$G : [0,\tau]\times E\times F \to \mathbf{R}.$$

For each $t \in [0,\tau]$, we define

$$g(t) := \inf_{x\in E}\sup_{y\in F} G(t,x,y), \qquad h(t) := \sup_{y\in F}\inf_{x\in E} G(t,x,y)$$

and the associated sets

$$X(t) = \left\{\hat{x}\in E : \sup_{y\in F} G(t,\hat{x},y) = g(t)\right\} \tag{3.30}$$

$$Y(t) = \left\{\hat{y}\in F : \inf_{x\in E} G(t,x,\hat{y}) = h(t)\right\}. \tag{3.31}$$

For fixed t they comprise all those points in E (F) where the infimum respectively the supremum is attained with value $g(t)$ $(h(t))$. According to Lemma 3.6, we know that if $g(t) = h(t)$ then the set of saddle points is given by $S(t) := X(t)\times Y(t)$.

Theorem 3.9 (R. Correa and A. Seeger, [36]). *Let the function G and the vector spaces E,F be as before. Suppose the conditions:*

(HH1) For all $t\in[0,\tau]$ assume $S(t)\neq\emptyset$.

(HH2) *The partial derivative $\partial_t G(t,x,y)$ exists for all $(t,x,y) \in [0,\tau] \times E \times F$.*

(HH3) *For any sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ and an element $x_0 \in X(0)$, $x_{t_{n_k}} \in X(t_{n_k})$ such that for all $y \in Y(0)$*

$$\lim_{\substack{k\to\infty \\ t\searrow 0}} \partial_t G(t, x_{n_k}, y) = \partial_t G(0, x_0, y).$$

(HH4) *For any sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ and an element $y_0 \in Y(0)$, $y_{t_{n_k}} \in Y(t_{n_k})$ such that for all $x \in X(0)$*

$$\lim_{\substack{k\to\infty \\ t\searrow 0}} \partial_t G(t, x, y_{t_{n_k}}) = \partial_t G(0, x, y_0).$$

Then there exists $(x_0, y_0) \in X(0) \times Y(0)$ such that

$$\frac{d}{dt} g(t)|_{t=0} = \partial_t G(0, x_0, y_0).$$

3.5 Céa's classical Lagrange method and a modification

Let the function G be defined by (3.26). Assume that G is sufficiently differentiable with respect to t, φ and ψ. Additionally, assume that the strong material derivative $\dot{u}$ exists in $H_0^1(\Omega)$. Then we may calculate as follows

$$dJ(\Omega)[\theta] = \frac{d}{dt}(G(t,u^t,p))|_{t=0} = \underbrace{\partial_t G(t,u,p)|_{t=0}}_{\text{shape derivative}} + \underbrace{\partial_\varphi G(0,u,p)(\dot{u})}_{\text{adjoint equation}},$$

and due to $\dot{u} \in H_0^1(\Omega)$ it implies $dJ(\Omega)[\theta] = \partial_t G(t,u,p)|_{t=0}$. Therefore, we can follow the lines of the calculation of the previous section to obtain the boundary and volume expression of the shape derivative.

In the original work [23], it was calculated as follows

$$dJ(\Omega)[\theta] = \partial_\Omega \mathcal{L}(\Omega,u,p) + \partial_\varphi \mathcal{L}(\Omega,u,p)(u') + \partial_\psi \mathcal{L}(\Omega,u,p)(p'), \tag{3.32}$$

where $\partial_\Omega \mathcal{L}(\Omega,u,p) := \lim_{t\searrow 0}(\mathcal{L}(\Omega_t,u,p) - \mathcal{L}(\Omega,u,p))/t$. Then it was assumed that u' and p' belong to $H_0^1(\Omega)$, which has as consequence that $\partial_\varphi \mathcal{L}(\Omega,u,p)(u') = \partial_\psi \mathcal{L}(\Omega,u,p)(p') = 0$. Thus (3.32) leads to the wrong formula

$$dJ(\Omega)[\theta] = \int_\Gamma (|u-u_r|^2 + \partial_n u\, \partial_n p)\, \theta_n \, ds.$$

This can be fixed by noting that $u' = \dot{u} - \nabla u \cdot \theta$ and $p' = \dot{p} - \nabla p \cdot \theta$ with $\dot{u}, \dot{p} \in H_0^1(\Omega)$:

$$dJ(\Omega)[\theta] = \partial_\Omega \mathcal{L}(\Omega,u,p) - \partial_\varphi \mathcal{L}(\Omega,u,p)(\nabla u \cdot \theta) - \partial_\psi \mathcal{L}(\Omega,u,p)(\nabla p \cdot \theta),$$

which gives the correct formula. Note that for Maxwell's equations a different parametrisation than $v \mapsto v \circ \Phi_t$ of the function space is necessary since the differential operator is modified differently. This leads then to a different definition of the shape derivative (of the state) and also the formulas will be different. This is well known from the finite element analysis of Maxwell's equations; cf. [5, 20, 53, 74].

We would like to stress that we do not claim that the Lagrange method to calculate the volume or boundary expression is always applicable, but it is applicable under the described assumptions also for non-linear problems. For a particular problem one has to carefully check the assumptions. One example where the described method does not work for the p-Laplacian, where it is known that the material derivative only belongs to some weighted Sobolev space and not to the solution space of the PDE.

3.6 Rearrangement of the cost function

The rearrangement method introduced in [60] avoids the material derivative and is applicable to a wide class of elliptic problems. We describe the method at hand of our semi-linear example and write subsequently the perturbed cost function (3.5) as

$$J(\Omega_t) = \int_\Omega j(t, u^t)\, dx, \quad j(t,v) := \xi(t)|v - u_r^t|^2. \tag{3.33}$$

In order to derive the shape differentiability, we make the assumptions:

Assumption ($\mathcal{R}$). *Assume that $\varrho \in C^2(\mathbf{R}) \cap L_\infty(\mathbf{R})$, $\varrho'' \in L_\infty(\mathbf{R})$ and $\varrho'(x) \geq 0$ for all $x \in \mathbf{R}$.*

Instead of requiring the Lipschitz continuity of $t \mapsto u^t$, we claim that holds: there exist $c, \tau, \varepsilon > 0$ such that $\|u^t - u\|_{H_0^1(\Omega)} \leq ct^{1/2+\varepsilon}$ for all $t \in [0, \tau]$.

Theorem 3.10. *Let Assumption ($\mathcal{R}$) be satisfied and let $\theta \in C_c^2(D, \mathbf{R}^d)$. Then $J(\Omega_t)$ given by (3.33) is differentiable with derivative:*

$$dJ(\Omega)[\theta] = \partial_t G(0, u, p),$$

where u, p are solutions of the state and adjoint state equation.

Proof. The main idea is to rewrite the difference $J(\Omega_t) - J(\Omega)$ and use a first order expansions of the PDE and the cost function with respect to the unknown together with Hölder continuity of $t \mapsto u^t$. To be more precise, one writes

$$\begin{aligned} \frac{J(\Omega_t) - J(\Omega)}{t} &= \underbrace{\frac{1}{t}\int_\Omega (j(t,u^t) - j(t,u) - j'(t,u)(u^t - u))\, dx}_{B_1(t)} + \underbrace{\frac{1}{t}\int_\Omega (j(t,u) - j(0,u))\, dx}_{B_2(t)} \\ &+ \underbrace{\frac{1}{t}\int_\Omega (j'(t,u) - j'(0,u))(u^t - u)\, dx}_{B_3(t)} + \underbrace{\frac{1}{t}\int_\Omega j'(0,u)(u^t - u)\, dx}_{B_4(t)}, \end{aligned} \tag{3.34}$$

where $j' := \partial_u j$ and $u_s^t := su^t + (1-s)u$. Using the mean value theorem in integral form entails for some constant $C > 0$

$$\begin{aligned} \int_\Omega (j(t,u^t) - j(t,u) - j'(t,u)(u^t - u))\, dx &= \int_0^1 (1-s) j''(t, u_s^t)(u^t - u)^2\, dx \\ &\leq C\|u^t - u\|_{L_2(\Omega)}^2 \quad \text{for all } t \in [0,\tau]. \end{aligned}$$

Using that $\lim_{t\searrow 0} \|u^t - u\|_{H_0^1(\Omega)}/\sqrt{t} = 0$, we see that B_1 tends to zero as $t \searrow 0$. Let $\tilde{E}(t, \varphi)$ be defined by (3.7). Then the fourth term in (3.34) can be written by using the adjoint equation (3.17) as follows

$$\begin{aligned} \int_\Omega j'(0,u)(u^t - u)\, dx = {} & d_\varphi \tilde{E}(0, u^t; p) - d_\varphi \tilde{E}(0, u; p) - d^2\tilde{E}(0, u; u^t - u, p) \\ & + d\bar{E}(t, u^t; p) - d\bar{E}(t, u; p) - (d_\varphi \tilde{E}(0, u^t; p) - d_\varphi \tilde{E}(0, u; p)) \\ & + d_\varphi \tilde{E}(t, u; p) - d_\varphi \tilde{E}(0, u; p). \end{aligned} \tag{3.35}$$

By standard elliptic regularity theory (cf. [61]), we obtain $p \in H_0^1(\Omega) \cap L_\infty(\Omega)$. Therefore by virtue of Taylor's formula in Banach spaces (cf. [8, Thm. 5.8, p. 193]) the first line in (3.35) on the right hand side can be written as

$$d_\varphi \tilde{E}(0, u^t; p) - d_\varphi \tilde{E}(0, u; p) - d^2 \tilde{E}(0, u; u^t - u, p) = \int_0^1 (1-s) d_\varphi^3 \tilde{E}(0, u_s^t; u^t - u, u^t - u, p)\, ds,$$

where the remainder can be estimated as follows

$$\begin{aligned} \int_0^1 (1-s) d^3 \tilde{E}(0, u_s^t; u^t - u, u^t - u, p)\, ds &= \int_0^1 (1-s) \varrho''(u_s^t)(u^t - u)^2 p\, ds \\ &\le \frac{1}{2} \|p\|_{L_\infty(\Omega)} \|\varrho''\|_{L_\infty(\mathbf{R})} \|u^t - u\|_{L_2(\Omega)} \text{ for all } t \in [0, \tau]. \end{aligned}$$

Using $d_\varphi \tilde{E}(t, u^t; p) - d_\varphi \tilde{E}(0, u; p) = 0$, and the differentiability of $t \mapsto \tilde{E}(t, u)$ yields

$$\begin{aligned} \lim_{t \searrow 0} \frac{1}{t} (d_\varphi \tilde{E}(t, u^t; p) - d_\varphi \tilde{E}(t, u; p)) &= \lim_{t \searrow 0} \frac{1}{t} (d_\varphi \tilde{E}(0, u^t; p) - d_\varphi \tilde{E}(0, u; p)), \\ \lim_{t \searrow 0} \frac{1}{t} (d_\varphi \tilde{E}(t, u; p) - d_\varphi \tilde{E}(0, u; p)) &= \int_\Omega A'(0) \nabla u \cdot \nabla p - \operatorname{div}(\theta) f p - \nabla f \cdot \theta\, p\, dx. \end{aligned}$$

Thus from (3.35), we infer

$$\begin{aligned} \lim_{t \searrow 0} \frac{1}{t} \int_\Omega j'(0, u)(u^t - u)\, dx = \int_\Omega & A'(0) \nabla u \cdot \nabla p + \operatorname{div}(\theta) \varrho(u) p\, dx \\ & - \int_\Omega \operatorname{div}(\theta f) p\, dx. \end{aligned}$$

Therefore we may pass to the limit in (3.34) and obtain

$$\lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t} = \int_\Omega \partial_t j(0, u)\, dx + \partial_t d_\varphi \tilde{E}(0, u; p).$$

Altogether we have proved that $dJ(\Omega)[\theta] = \frac{d}{dt} G(t, u^t, \psi) = \partial_t G(0, u, p)$ for all $\psi \in H_0^1(\Omega)$. $\square$

3.7 Differentiability of energy functionals

If it happens that the cost function J is the energy of the PDE (3.1), that is,

$$J(\Omega) := \min_{\varphi \in H_0^1(\Omega)} E(\Omega, \varphi),$$

then it is easy to show the shape differentiability of J by using the result [37, Thm. 2.1, p. 524], see also [38, pp. 139]. First note that $J(\Omega_t) = \min_{\varphi \in H_0^1(\Omega)} \tilde{E}(t, \varphi)$. By definition of the minimum u^t of $\tilde{E}(t, \cdot)$ and u of $\tilde{E}(0, \cdot)$, respectively, we have

$$\tilde{E}(0, u^t) - \tilde{E}(0, u) \ge 0, \qquad \tilde{E}(t, u) - \tilde{E}(0, u) \le 0 \quad \text{for all } t \in [0, \tau]$$

and thus

$$\begin{aligned} J(\Omega_t) - J(\Omega) &= \tilde{E}(t, u^t) - \tilde{E}(0, u^t) + \tilde{E}(0, u^t) - \tilde{E}(0, u) \\ &\ge \tilde{E}(t, u^t) - \tilde{E}(0, u^t) \\ J(\Omega_t) - J(\Omega) &= \tilde{E}(t, u^t) - \tilde{E}(t, u) + \tilde{E}(t, u) - \tilde{E}(0, u) \\ &\le \tilde{E}(t, u) - \tilde{E}(0, u). \end{aligned}$$

Using the mean value theorem, we conclude the existence of constants $\eta_t, \zeta_t \in (0,1)$ such that

$$t\partial_t \tilde{E}(\eta_t\, t, u^t) \leq J(\Omega_t) - J(\Omega) \leq t\partial_t \tilde{E}(\zeta_t\, t, u).$$

Thus if

$$\tilde{E}(0,u) \geq \liminf_{\substack{t \searrow 0 \\ t>0}} \partial_t \tilde{E}(\eta_t\, t, u^t), \qquad \tilde{E}(0,u) \leq \limsup_{\substack{t \searrow 0 \\ t>0}} \partial_t \tilde{E}(\zeta_t\, t, u), \tag{3.36}$$

then we may conclude that J is shape differentiable by the squeezing lemma. We obtain

$$\lim_{t\searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t} = \partial_t \tilde{E}(0,u).$$

This result can be seen as a special case of Theorem 3.9. Note that in our example

$$\begin{aligned} \partial_t \tilde{E}(t,\varphi) = &\int_\Omega A'(t)\nabla\varphi \cdot \nabla\varphi + \xi'(t)\varrho(\varphi)\, dx \\ &- \int_\Omega \xi'(t) f^t \varphi\, dx + \int_\Omega \xi(t)\, B(t)\nabla f^t \cdot \varphi\, dx. \end{aligned}$$

From this identity, the convergence of $u^t \to u$ in $H_0^1(\Omega)$ and the smoothness of $A(t)$, $\xi(t)$ and $B(t)$, we infer that (3.36) are satisfied.

Chapter 4

Shape derivative via Lagrange method

This chapter represents the core of this thesis and presents a novel approach to the differentiability of a *minimax of a Lagrangian* that is a utility function plus a linear penalisation of the state equation. Its originality is to replace the usual adjoint state equation by an *averaged adjoint state equation*. When compared to the former theorems [36, Thm. 3, p. 842], [33, Thm. 3, p. 93] and [30], all the hypotheses are now verified for a Lagrangian functional without going to the dual problem and without any saddle point assumption. It relaxes the classical continuity assumptions on the derivative of the Lagrangian involving both the state and adjoint state to continuity assumptions that only involve the averaged adjoint state. Besides this new theorem, we propose different other theorems with stronger assumptions to prove the shape differentiability. Finally, we discuss in a quite general setting how the assumptions of the presented theorems can be satisfied.

4.1 An extension of the Theorem of Correa-Seeger

4.1.1 Preliminaries

Let E, F be linear vector spaces and fix $\tau > 0$. We consider a Lagrangian function

$$G : [0,\tau] \times E \times F \to \mathbf{R}, \quad (t,x,y) \mapsto G(t,x,y), \tag{4.1}$$

such that $y \mapsto G(t,x,y)$ is *affine* for all $(t,x) \in [0,\tau] \times F$. As a result there are functions $f : [0,\tau] \times E \to \mathbf{R}$ and $\mathfrak{e} : [0,\tau] \times E \times F \to \mathbf{R}$, where the latter is linear in y, such that

$$G(t,x,y) = f(t,x) + \mathfrak{e}(t,x,y).$$

Associated with this Lagrangian, we consider the real valued function

$$g(t) := \inf_{x\in E} \sup_{y\in F} G(t,x,y).$$

Subsequently, we discuss the differentiability of g under weak assumptions on the function G. Let

$$E(t) := \{x \in E |\ d_y G(t,x,0;\hat{y}) = 0 \quad \text{for all } \hat{y} \in F\}.$$

Moreover, we introduce the sets

$$X(t) = \left\{ \bar{x} \in E |\ \inf_{x\in E} \sup_{y\in F} G(t,x,y) = \sup_{y\in F} G(t,\bar{x},y) \right\}. \tag{4.2}$$

The two sets $E(t)$ and $X(t)$ are related to each other.

Lemma 4.1. *Assume that $E \neq \emptyset$ and $F \neq \emptyset$ and $t \in [0,\tau]$.*

(i) In general, we have for all $\bar{y} \in F$

$$\inf_{x\in E}\sup_{y\in F} G(t,x,y) = \sup_{y\in F}\inf_{x\in E(t)} G(t,x,y) = \inf_{x\in E(t)} G(t,x,\bar{y})$$

(ii) We have $g(t) = \infty$ if and only if $E(t) = \emptyset$.

(iii) Assume $g(t) < \infty$ for all $t \in [0,\tau]$. Then $x^t \in E(t)$ with

$$\inf_{x\in E(t)} G(t,x,y) = G(t,x^t,y) \quad \textit{for all } y \in F$$

if and only if $x^t \in X(t)$. In particular, we always have $X(t) \subset E(t)$ and $E(t) = X(t) = \{x^t\}$ if $E(t)$ is single-valued.

Proof. (i) Since $y \mapsto G(t,x,y)$ is affine for all $(t,x) \in [0,\tau]\times E$, we get

$$G(t,x,y) - G(t,x,0) = \partial_y G(t,x,0)(y),$$

and thus

$$\sup_{y\in F} G(t,x^t,y) = \sup_{y\in F}\big(G(t,x^t,0) + \partial_y G(t,x^t,0)(y)\big) = \begin{cases} G(t,x^t,0), & \text{if } x^t \in E(t) \\ \infty, & \text{else} \end{cases}.$$

Taking the infimum the first assertion follows.
(ii) That $E(t) = \emptyset$ implies $g(t) = \infty$ follows by the definition of the infimum. To prove the other direction suppose that $E(t) \neq \emptyset$. Then by (i)

$$g(t) = \inf_{x\in E(t)} G(t,x,0) \leq G(t,x^*,0) < \infty,$$

for any $x^* \in E(t)$, hence $g(t) = \infty$ implies $E(t) = \emptyset$.
(iii) "$\Leftarrow$": Assume $E(t) \neq \emptyset$ then it follows from (ii) that $g(t) < \infty$. Then for $x^t \in X(t)$

$$\sup_{y\in F} G(t,x^t,y) - G(t,x^t,0) = \sup_{y\in F} \partial_y G(t,x^t,0)(y)$$

and thus it follows from Definition 4.2 and the definition of $g(t)$

$$g(t) - G(t,x^t,0) = \sup_{y\in F} \partial_y G(t,x^t,0)(y).$$

By contradiction, we assume that $x^t \in E \setminus E(t)$. There exists a $0 \neq \hat{y} \in F$ with

$$\begin{aligned} g(t) - G(t,x,0) = \sup_{y\in F} \partial_y G(t,x,0)(y) &\geq \sup_{\lambda\in\mathbf{R}} \partial_y G(t,x,0)(\lambda\hat{y}) \\ &= \sup_{\lambda\in\mathbf{R}} (\lambda\, \partial_y G(t,x,0)(\hat{y})) = \infty, \end{aligned}$$

which is a contradiction since $g(t) < \infty$. Finally, since $x^t \in E(t)$

$$-\infty < G(t,x^t,y) \leq \sup_{y\in F} G(t,x^t,y) = g(t) = \inf_{x\in E(t)} G(t,x,y) \leq G(t,x^t,y).$$

"$\Rightarrow$": Conversely, assume that $x^t \in E(t)$ such that for all $\bar{y} \in F$

$$\inf_{x\in E(t)} G(t,x,\bar{y}) = G(t,x^t,\bar{y})$$

then from part (i) it follows that for all $\bar{y} \in F$

$$\inf_{x\in E}\sup_{y\in F} G(t,x,y) = \inf_{x\in E(t)} G(t,x,\bar{y}) = G(t,x^t,\bar{y}) = \sup_{y\in F} G(t,x^t,y)$$

□

We introduce the following hypothesis.

Assumption (H0). *For all $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ it holds:*

(i) For all $y \in F$ the mapping $[0,1] \to \mathbf{R}: \ s \mapsto G(t, sx^t + (1-s)x^0, y)$ is absolutely continuous. This implies that the derivative $d_xG(t, sx^t + (1-s)x^0, y; x^t - x^0)$ exists for almost all $s \in [0,1]$ and in particular

$$G(t,x^t,y) - G(t,x^0,y) = \int_0^1 d_xG(t, sx^t + (1-s)x^0, y; x^t - x^0)\, ds.$$

(ii) For all $\varphi \in E$ the map $s \mapsto d_xG(t, sx^t + (1-s)x^0, y; \varphi)$ belongs to $L_1(0,1)$.

(iii) For every $(x,t) \in E \times [0,\tau]$ the mapping $F \to \mathbf{R}: \ y \mapsto G(t,x,y)$ is affine-linear.

Introduce for $t \in [0,\tau]$, $x^t \in X(t)$ and $x^0 \in X(0)$ the following subset of F

$$Y(t,x^t,x^0) := \left\{ q \in F |\ \int_0^1 d_xG(t, sx^t + (1-s)x^0, q; \hat{\varphi})\, ds = 0 \quad \text{for all } \hat{\varphi} \in E \right\}. \tag{4.3}$$

For $t = 0$, we set $Y(0,x^0) := Y(0,x^0,x^0)$, which coincides with the usual adjoint equation

$$Y(0,x^0) = \left\{ q \in F |\ d_xG(0,x^0,q;\hat{\varphi}) = 0 \quad \text{for all } \hat{\varphi} \in E \right\}. \tag{4.4}$$

In the most general situation, we define for $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ the set

$$\overline{Y}(t,x^t,x^0) := \left\{ q \in F |\ G(t,x^t,q) - G(t,x^0,q) = 0 \right\}.$$

Note that under the Assumption (H0), we have $Y(t,x^t,x^0) \subset \overline{Y}(t,x^t,x^0)$ for all $t \in [0,\tau]$, $x^t \in E(t)$, $x^0 \in E(0)$. In particular, we have $\overline{Y}(0,x^0,x^0) = F$.

4.1.2 Lagrange method for non-linear problems

The following result extends a theorem of Correa-Seeger [37] in the case when the sets $X(t)$ and $Y(t,x^t,x^0)$, $x^t \in X(t)$, are single-valued and the function is a Lagrangian. The result is due to [91].

Theorem 4.2. *Let the linear vector spaces E and F, the real number $\tau > 0$, and the function*

$$G : [0,\tau] \times E \times F \to \mathbf{R}, \quad (t,\varphi,\psi) \mapsto G(t,\varphi,\psi),$$

be given. Let Assumption (H0) and the following conditions be satisfied.

(H1) For all $t \in [0,\tau]$ and all $(u,p) \in X(0) \times F$ the derivative $\partial_t G(t,u,p)$ exists.

(H2) For all $t \in [0,\tau]$, $X(t)$ is nonempty and single-valued. For all $t \in [0,\tau]$, $x^t \in X(t)$ and $x^0 \in X(0)$, the set $Y(t,x^t,x^0)$ is nonempty and single-valued.

(H3) Let $x^0 \in X(0)$ and $y^0 \in Y(0,x^0)$. For any sequence of non-negative real numbers $(t_n)_{n\in\mathbf{N}}$ converging to zero, there exist a subsequence $(t_{n_k})_{k\in\mathbf{N}}$, elements $x^{t_{n_k}} \in E(t_{n_k})$ and $y^{t_{n_k}} \in Y(t_{n_k}, x^{t_{n_k}}, x^0)$ such that

$$\lim_{\substack{k\to\infty\\ t\searrow 0}} \partial_t G(t, x^0, y^{t_{n_k}}) = \partial_t G(0, x^0, y^0).$$

We pick any $\psi \in F$. Then letting $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ and $y^0 \in Y(0,x^0)$, we conclude

$$\frac{d}{dt}(G(t, x^t, \psi))|_{t=0} = \partial_t G(0, x^0, y^0).$$

Proof. Step 1: Let $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ and $y^t \in Y(t, x^t, x^0)$, $y^0 \in Y(0,x^0)$ be given. We will show that there exist an $\eta_t \in (0,1)$ such that

$$G(t, x^t, \psi) - G(0, x^0, \psi) = t\partial_t G(\eta_t t, x^0, y^t), \tag{4.5}$$

for all $\psi \in F$. Write

$$\begin{aligned} G(t, x^t, \psi) - G(0, x^0, \psi) &= G(t, x^t, y^t) - G(0, x^0, y^0) \\ &= G(t, x^t, y^t) - G(t, x^0, y^t) + G(t, x^0, y^t) - G(0, x^0, y^t) \end{aligned} \tag{4.6}$$

for all $\psi \in F$, where we used $G(0, x^0, y^t) - G(0, x^0, y^0) = 0$, since $\psi \mapsto G(t, u, \psi)$ is affine-linear. By Hypothesis (H1), we find for each $t \in [0,\tau]$ a number $\eta_t \in (0,1)$ such that

$$G(t, x^0, y^t) - G(0, x^0, y^t) = t\partial_t G(\eta_t t, x^0, y^t). \tag{4.7}$$

Now using part (i) and (ii) of Hypothesis (H0), we see that $y^t \in \overline{Y}(t, x^t, x^0)$ and thus plugging (4.7) into (4.6), we recover (4.5).
Step 2: For arbitrary $\psi \in F$, we show that $\lim_{t\searrow 0} \delta(t)/t$ exists, where $\delta(t) := G(t, x^t, \psi) - G(0, x^0, \psi)$. To do so it is sufficient to show that $\liminf_{t\searrow 0} \delta(t)/t = \limsup_{t\searrow 0} \delta(t)/t$. By definition of the lim inf, there is a sequence $(t_n)_{n\in\mathbf{N}}$ such that

$$\lim_{n\to\infty} \delta(t_n)/t_n = \liminf_{t\searrow 0} \delta(t)/t =: \underline{d\delta}(0).$$

Now let $x^0 \in X(0)$ and $y^0 \in Y(0,x^0)$. Recall that $\delta(t)/t = \partial_t G(\eta_t t, x^0, y^t)$. Owing to (H3), for any sequence of non-negative real numbers $(t_n)_{n\in\mathbf{N}}$ converging to zero, i.e., $t_n \to 0$ as $n \to \infty$, there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$, elements $x^{t_{n_k}} \in E(t_{n_k})$ and $y^{t_{n_k}} \in Y(t_{n_k}, x^{t_{n_k}}, x^0)$ such that

$$\lim_{\substack{k\to\infty\\ t\searrow 0}} \partial_t G(t, x^0, y^{t_{n_k}}) = \partial_t G(0, x^0, y^0).$$

Thus we conclude

$$\begin{aligned} \underline{d\delta}(0) = \lim_{n\to\infty} \partial_t G(\eta_{t_n} t_n, x^0, y^{t_n}) &= \lim_{k\to\infty} \partial_t G(\eta_{t_{n_k}} t_{n_k}, x^0, y^{t_{n_k}}) \\ &= \partial_t G(0, x^0, y^0). \end{aligned} \tag{4.8}$$

Completely analogous, we may show for $\overline{d\delta}(0) := \limsup_{t\searrow 0} \delta(t)/t$ that

$$\overline{d\delta}(0) = \partial_t G(0, x^0, y^0) \tag{4.9}$$

Combining (4.8) and (4.9), we obtain $\overline{d\delta}(0) = \partial_t G(0, x^0, y^0) = \underline{d\delta}(0)$, which shows that

$$\lim_{t \searrow 0} \frac{\delta(t)}{t} = \partial_t G(0, x^0, y^0).$$

Since $\psi \in F$ was arbitrary, we finish the proof. □

Remark 4.3. *In concrete applications the conditions (H0)-(H3) have the following meaning.*

(i) Condition (H0) ensures that we can apply the fundamental theorem of calculus to G with respect to the primal variable. Condition (H1) allows an application of the mean value theorem with respect to t. Note that the assumption (H0) is much milder than Fréchet differentiability of $\varphi \mapsto G(t, \varphi, \psi)$.

(ii) Condition (H2) ensures that the state equation and the perturbed state equation has a unique solution. The set $Y(t, x^t, x^0)$ can be understood as the solution of some averaged adjoint state equation.

(iii) Condition (H3) can be verified by showing that y^t converges weakly to y^0 and that $(t, \psi) \mapsto G(t, x^0, \psi)$ is weakly continuous. Note that there is no assumption on the convergence of $x^t \in X(t)$ to $x^0 \in X(0)$, but in applications we need the convergence $x^t \to x^0$ to prove $y^t \to y^0$ in some topologies.

(iv) The set $X(t)$ corresponds to the solution of the state equation on the perturbed domain Ω_t pulled back to the fixed domain Ω.

Remark 4.4. *By definition of $y^t \in Y(t, x^t, x^0)$, we have for all $y \in F$*

$$G(t, x^t, y) = G(t, x^0, y^t) \quad \Leftrightarrow \quad f(t, x^t) - f(t, x^0) = \mathfrak{e}(t, x^0, y^t).$$

From the last equality, we get by the mean value theorem the existence of $\eta_t \in (0, 1)$ such that

$$\frac{f(t, x^t) - f(t, x^0)}{t} = \partial_t \mathfrak{e}(\eta_t\, t, x^0, y^t).$$

This means that the continuity of $(s, t) \mapsto \partial_t \mathfrak{e}(s, x^0, y^t)$ is directly related to the differentiability of $t \mapsto f(t, x^t)$. For applications this means that the differentiability of the cost function is connected with the continuity of linearised state equation.

4.1.3 Possible generalisations

We can consider a weaker averaged equation and thus weaken the condition (i),(ii) of Assumption (H0). We may write G as

$$G(t, x, y) = f(t, x) + \mathfrak{e}(t, x, y),$$

for two functions $f : [0, \tau] \times E \to \mathbf{R}$ and $\mathfrak{e} : [0, \tau] \times E \times F \to 0$, where the function $\mathfrak{e}$ is linear in y. Now it is sufficient to require that $\mathfrak{e}$ satisfies assumption (H0) (G replaced by $\mathfrak{e}$) and for f we need: for all $t \in [0, \tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ the function

$$[0, \tau] \to \mathbf{R} : \; s \mapsto f(t, sx^t + (1 - s)x^0)$$

is differentiable. Under these assumptions, we conclude by the mean value theorem that there exists $s' \in [0,\tau]$ depending on t such that

$$f(t,x^t) - f(t,x^0) = d_x f(t, s'x^t + (1-s')x^0; x^t - x^0) \tag{4.10}$$

and in particular

$$\begin{aligned} G(t,x^t,p) - G(t,x^0,p) = &\int_0^1 d_x \mathfrak{e}(t, sx^t + (1-s)x^0, p; x^t - x^0)\, ds \\ &+ d_x f(t, s'x^t + (1-s')x^0; x^t - x^0). \end{aligned}$$

Now assume that for all $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$, $s' \in (0,1)$ and for all $\hat{u} \in E$

$$d_x f(t, s'x^t + (1-s')x^0; \hat{u}) \quad \text{exists.}$$

Then instead of considering the averaged equation, we could consider the modified averaged equation: Find $y^t \in F$ such that

$$\int_0^1 d_x \mathfrak{e}(t, sx^t + (1-s)x^0, y^t; \hat{u})\, ds + d_x f(t, s'x^t + (1-s')x^0; \hat{u}) = 0 \tag{4.11}$$

for all $\hat{u} \in E$. Since s' (defined by (4.10)) depends on t, the set $Y(t,x^t,x^0)$ has to be replaced by

$$\widetilde{Y}(t,x^t,x^0) := \{q \in F : \ q \text{ solves (4.11) with } s' \text{ such that (4.10)}\}.$$

Then we can follow the lines of the proof of Theorem 4.2 with the mentioned changes. Since in applications f will be the cost function, this remark means that we only need the cost function to be directional differentiable without continuity. Nevertheless, to identify the limit y^0 we need some continuity to pass to the limit $t \searrow 0$ in (4.11). Using the Henstock–Kurzweil integral in (4.11) (see e.g. [15]), we may even weaken the absolute continuity of $s \mapsto \mathfrak{e}(t, sx^t + (1-s)x^0, y)$ ($y \in F$) to differentiability, since for this integral the fundamental theorem is satisfied for merely differentiable functions.

4.1.4 A modification of the single-valued case

Let E_1, E_2 and F_1, F_2 be Banach spaces. Consider a function

$$G : [0,\tau] \times E_1 \times E_2 \times F_1 \times F_2 \to \mathbf{R}, \quad (t,v,w,y,z) \mapsto G(t,v,w,y,z).$$

We make the following assumption for the function G.

Assumption (D0). *(i) For all $t \in [0,\tau]$, $v, \tilde{v} \in E_1, w, \tilde{w} \in E_2$, $y \in F_1, z \in F_2$*

$$\begin{aligned} [0,1] \to \mathbf{R} :\ s \mapsto G(t, v + s\tilde{v}, w, y, z) \\ [0,1] \to \mathbf{R} :\ s \mapsto G(t, v, w + s\tilde{w}, y, z) \end{aligned}$$

are absolutely continuous, which implies that

$$\begin{aligned} G(t, v+\tilde{v}, w, y, z) - G(t,v,w,y,z) &= \int_0^1 d_v G(t, v_s^t, w, y, z; v - \tilde{v})\, ds \\ G(t, v, w+\tilde{w}, y, z) - G(t,v,w,y,z) &= \int_0^1 d_w G(t, v, w_s^t, y, z; w - \tilde{w})\, ds, \end{aligned}$$

where $v_s^t := s\tilde{v} + (1-s)v$ and $w_s^t := s\tilde{w} + (1-s)w$.

(ii) *For all $v, \tilde{v}, \hat{v} \in E_1, w, \tilde{w}, \hat{w} \in E_2$, $y \in F_1, z \in F_2$*

$$s \mapsto dG(t, v + s\hat{v}, w, y, z; \tilde{w}) \quad \text{and} \quad s \mapsto dG(t, v, w + s\hat{w}, y, z; \tilde{w})$$

exist and belong to $L_1(0, 1)$.

(iii) *For all $v, \tilde{v}, \hat{v} \in E_1, w, \tilde{w}, \hat{w} \in E_2$, $y \in F_1, z \in F_2$ the mappings $\tilde{y} \mapsto G(t, v, w, \tilde{y}, z)$ and $\tilde{z} \mapsto G(t, v, w, y, \tilde{z})$ are affine-linear.*

For any $t \in [0, \tau]$, we consider the system of state equations

$$d_y G(t, v, w, y, z; \tilde{y}) = 0 \quad \text{for all } \tilde{y} \in F_1 \tag{4.12}$$
$$d_z G(t, v, w, y, z; \tilde{z}) = 0 \quad \text{for all } \tilde{z} \in F_2. \tag{4.13}$$

The set of all $(v, w) \in E_1 \times E_2$ satisfying (4.12),(4.13) is denoted by $\boldsymbol{E}(t)$. For any $t \in [0, \tau]$, $\boldsymbol{q}^t := (v^t, w^t) \in \boldsymbol{E}(t)$ and $\boldsymbol{q}^t := (v^0, w^0) \in \boldsymbol{E}(0)$, we consider the system

$$\int_0^1 d_v G(t, v_s^t, w^t, y^t, z^t; \tilde{y})\, ds = 0 \quad \text{for all } \tilde{y} \in F_1 \tag{4.14}$$
$$\int_0^1 d_w G(t, v^0, w_s^t, y^t, z^t; \tilde{z})\, ds = 0 \quad \text{for all } \tilde{z} \in F_2, \tag{4.15}$$

where $v_s^t := sv^t + (1-s)v^0$ and $w_s^t := sw^t + (1-s)w^0$. We introduce for $\boldsymbol{q}^t := (v^t, w^t) \in \boldsymbol{E}(t)$ the set

$$\mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0) := \big\{(y^t, z^t) \in F_1 \times F_2 |\ (y^t, z^t) \text{ solves } (4.14), (4.15)\big\}.$$

For $t = 0$ we set $\mathbf{Y}(0, \boldsymbol{q}^0) := \mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ which is the usual adjoint system. Note that under Assumption (D0), $(y^t, z^t) \in \mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ implies

$$G(t, v^t, w^t, y^t, z^t) - G(t, v^0, w^t, y^t, z^t) = 0 \tag{4.16}$$
$$G(t, v^0, w^t, y^t, z^t) - G(t, v^0, w^0, y^t, z^t) = 0. \tag{4.17}$$

Therefore, we may introduce a generalisation of the set $\mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ by

$$\overline{\mathbf{Y}}(t, \boldsymbol{q}^t, \boldsymbol{q}^0) := \{(y^t, z^t) \in F_1 \times F_2 |\ (y^t, z^t) \text{ satisfies } (4.16), (4.17)\ \}.$$

If (D0) is satisfied, we have $\mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0) \subset \overline{\mathbf{Y}}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ and $\overline{\mathbf{Y}}(0, \boldsymbol{q}^0, \boldsymbol{q}^0) = F_1 \times F_2$. Now we may prove the following theorem.

THEOREM 4.5. *Let the Banach spaces E_1, E_2 and F_1, F_2, the real number $\tau > 0$, and the function*

$$G : [0, \tau] \times E_1 \times E_2 \times F_1 \times F_2 \to \mathbf{R}, \quad (t, v, w, y, z) \mapsto G(t, v, w, y, z),$$

be given. Additionally to the Hypothesis (D0), let the following hypotheses be satisfied.

(D1) *For all $v \in E_1$, $w \in E_2$, $y \in F_1$ and $z \in F_2$*

$$[0, \tau] \to \mathbf{R} : t \mapsto G(t, v, w, y, z)$$

is differentiable.

(D2) *For all $t \in [0, \tau]$, we have $\mathbf{E}(t) \neq \emptyset$. For for all $t \in [0, \tau]$, $\boldsymbol{q}^t := (v^t, w^t) \in \mathbf{E}(t)$ and $\boldsymbol{q}^0 := (v^0, w^0) \in \mathbf{E}(0)$, the $\mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0) \neq \emptyset$ be non-empty. Moreover, $\mathbf{E}(t)$ is single-valued for all $t \in [0, \tau]$ and also $\mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ is single-valued for all $t \in [0, \tau]$, $\boldsymbol{q}^t \in \mathbf{E}(t)$ and $\boldsymbol{q}^0 \in \mathbf{E}(0)$.*

(D3) Let $\boldsymbol{q}^0 \in \boldsymbol{E}(0)$ and $\boldsymbol{p}^0 \in Y(0, \boldsymbol{q}^0)$. For any sequence of non-negative real numbers $(t_n)_{n\in\mathbf{N}}$ converging to zero, there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$, elements $\boldsymbol{q}^{t_{n_k}} \in \boldsymbol{E}(t_{n_k})$ and $\boldsymbol{p}^{t_{n_k}} = (z^{t_{n_k}}, y^{t_{n_k}}) \in Y(t_{n_k}, \boldsymbol{q}^{t_{n_k}}, \boldsymbol{q}^0)$ such that

$$\lim_{\substack{k\to\infty\\ t\searrow 0}} \partial_t G(t, \boldsymbol{q}^0, \boldsymbol{p}^{t_{n_k}}) = \partial_t G(0, \boldsymbol{q}^0, \boldsymbol{p}^0).$$

Then for all $\tilde{\boldsymbol{\psi}} := (\psi_1, \psi_2) \in F_1 \times F_2$

$$\frac{d}{dt}(G(t, \boldsymbol{q}^t, \tilde{\boldsymbol{\psi}})|_{t=0} = \partial_t G(0, \boldsymbol{q}^t, \boldsymbol{p}^0).$$

Proof. Let $t \in [0, \tau]$, $\boldsymbol{q}^t = (v^t, w^t) \in \mathbf{E}(t)$, $\boldsymbol{q}^0 := (v^0, w^0) \in \mathbf{E}(0)$ and $\boldsymbol{p}^t = (y^t, z^t) \in \mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$, $\boldsymbol{p}^0 = (y^0, z^0) \in \mathbf{Y}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$ be given.
Step 1: We first show that there exists $\eta_t \in (0, 1)$ such that

$$G(t, \boldsymbol{q}^t, \boldsymbol{\psi}) - G(0, \boldsymbol{q}^0, \boldsymbol{\psi}) = t\, \partial_t G(\eta_t t, \boldsymbol{q}^0, \boldsymbol{p}^t). \tag{4.18}$$

Write

$$\begin{aligned} G(t, v^t, w^t, \boldsymbol{\psi}) - G(0, x_1, x_2, \boldsymbol{\psi}) &= G(t, v^t, w^t, y^t, z^t) - G(0, x_1, x_2, y, z) \\ &= G(t, v^t, w^t, y^t, z^t) - G(t, v, w^t, y^t, z^t) \\ &+ G(t, v^0, w^t, y^t, z^t) - G(t, v^0, w^0, y^t, z^t) \\ &+ G(t, v^0, w^0, y^t, z^t) - G(0, v^0, w^0, y^t, z^t) \end{aligned} \tag{4.19}$$

for all $\boldsymbol{\psi} = (\psi_t, \psi_2) \in F_1 \times F_2$. By Hypotheses (D1), we find for each $t \in [0, \tau]$ a number $\eta_t \in (0, 1)$ such that

$$G(t, x_1, x_2, y^t, z^t) - G(0, x_1, x_2, y^t, z^t) = t\, \partial_t G(\eta_t t, x_1, x_2, y^t, z^t).$$

Therefore, plugging the previous equation into (4.19) and using $\boldsymbol{p}^t \in \overline{\mathbf{Y}}(t, \boldsymbol{q}^t, \boldsymbol{q}^0)$, we end up with (4.18).
Step 2: Let $\psi \in F_1 \times F_2$ be arbitrary and set $\delta(t) := G(t, x^t, \psi) - G(0, x, \psi)$. Proceeding now as in the proof of Theorem 4.2, we conclude

$$\underline{dg}(0) = \overline{dg}(0) = \lim_{t\searrow 0} \partial_t G(\eta_t t, x, y^t) = \partial_t G(0, x, y).$$

Since $\psi \in F_1 \times F_2$ was arbitrary we finish the proof. ☐

4.2 More theorems on the differentiability of Lagrangians

Now we present alternative theorems to prove the shape differentiability, which complement Theorem 4.2. We introduce several perturbed adjoint equations and exploit a first order expansion of the Lagrangian with respect to the unknown. The remainder of the expansion is assumed to vanish with order two. Still the result from the previous section turns out to have the lowest requirements. In the following let E and F be two Banach spaces.

4.2.1 A theorem using weak differentiability of the state

For $t \in [0, \tau]$, $\tau > 0$ let the sets $X(t)$ and $Y(0, x^0)$, $x^0 \in X(0)$ be defined as in (4.2), (4.4), respectively. The following theorem uses the weak differentiability of $t \mapsto x^t$.

THEOREM 4.6. *Let E and F be Banach spaces and assume that E is reflexive. Let Assumption (H0) and the following hypotheses be satisfied.*

(E2) There are constants $c > 0$ and $\tau > 0$ such that $\|x^t - x^0\|_E \leq ct$ for all $t \in [0, \tau]$.

(E3) For all $t \in [0, \tau]$, the sets $X(t)$ and $Y(t, x^0)$ are non-empty and single-valued.

(E4) Assume that for all $t \in [0, \tau]$ the set $X(t)$ is single-valued. Introduce for $t \in [0, \tau]$ and $x^t \in X(t)$, $x^0 \in X(0)$ the operator

$$\hat{x} \mapsto B(t, \hat{x}, y) := \int_0^1 d_x G(t, sx^t + (1-s)x^0, y; \hat{x})\, ds.$$

Let $(x_n)_{n \in \mathbf{N}}$ be an arbitrary weakly converging sequence in X with limit $\tilde{x}$. Then

$$\lim_{\substack{n \to \infty \\ t \searrow 0}} B(t, x_n, y) = B(0, \hat{x}, y).$$

Then letting $t \in [0, \tau]$, $x^t \in X(t)$, $x^0 \in X(0)$, $y^0 \in Y(0, x^0)$ and $y \in F$, it follows

$$\frac{d}{dt} G(t, x^t, y)|_{t=0} = \partial_t G(0, x^0, y^0).$$

Proof. Step 1:
For $y \in Y$, $x^t \in X(t)$ and $x^0 \in X(0)$, we write

$$G(t, x^t, y) - G(0, x^0, y) = G(t, x^t, y) - G(t, x^0, y) + G(t, x^0, y) - G(0, x^0, y). \tag{4.20}$$

Step 2:
We will show that

$$\lim_{t \searrow 0} \frac{G(t, x^t, y) - G(t, x^0, y)}{t} = 0. \tag{4.21}$$

Due to Assumption (H0), we have the following relation

$$G(t, x^t, y) - G(t, x^0, y) = \int_0^1 d_x G(t, sx^t + (1-s)x^0, y; x^t - x^0)\, ds.$$

By Assumption (E4), we get that the operator

$$\varphi \mapsto B(t, \varphi, y) := \int_0^1 d_x G(t, sx^t + (1-s)x^0, y; \varphi)\, ds$$

satisfies for any $y \in F$ and any weakly converging sequence $x_n \rightharpoonup \tilde{x}$ that

$$\lim_{\substack{n \to \infty \\ t \searrow 0}} B(t, x_n, y) = B(0, \tilde{x}, y).$$

We will show that $\liminf_{t \searrow 0} \tilde{\delta}(t)/t = \limsup_{t \searrow 0} \tilde{\delta}(t)/t$, where $\tilde{\delta}(t) := G(t, x^t, y) - G(t, x^0, y)$. By definition of $\liminf_{t \searrow 0}$, there exists a sequence $t_n \searrow 0$ such that $\lim_{n \to \infty} \tilde{\delta}(t_n)/t_n =$

$\liminf_{t\searrow 0}\tilde\delta(t)/t$. Now, by condition (E2) the sequence $(x^t-x^0)/t$ is bounded and we may pick a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ that is also converging to zero such that

$$(x^{t_{n_k}}-x^0)/t_{n_k}\rightharpoonup\tilde x$$

for some element $\tilde x\in E$. Thus, we get

$$\lim_{n\to\infty}B(t_{n_k},(x^{t_{n_k}}-x^0)/t_{n_k},y)=\lim_{\substack{n\to\infty\\ t\searrow 0}}B(t,(x^{t_{n_k}}-x^0)/t_{n_k},y)=B(0,\tilde x,y).$$

Due to Hypothesis (E4) the right hand side tends to zero as $k\to\infty$, therefore we get $\liminf_{t\searrow 0}\tilde\delta(t)/t=0$. In the same way, we may prove $\limsup_{t\searrow 0}\tilde\delta(t)/t=0$ and consequently we recover (4.21). Finally, dividing (4.20) by $t>0$ and using the previous equation, we finish the prove. □

4.2.2 Partially perturbed adjoint equation

In [33] a theorem is proved (Theorem 4 in the cited paper) that gives some criteria when a minimax function may be differentiated without saddle point assumption. Unfortunately, it is not directly applicable to Lagrange functions. We will present a version of this theorem that is well-suited for Lagrangians.

Let E and F be two Banach spaces and let the function G be defined as in (4.1). Introduce for $x^0\in X(0)$ and $t\in[0,\tau]$ the set

$$Y(t,x^0):=\{y^t\in F: d_xG(t,x^0,y^t;\hat x)=0,\quad\text{for all }\hat x\in E\}.$$

Note that $Y(0,x^0)$ coincides with the set introduced in (4.4) of Subsection 4.1.1.

Theorem 4.7. *Additionally to Assumption (H0) let the following hypotheses be satisfied.*

(G0) There exist $\tau>0$ and $C>0$ such that for all $t\in[0,\tau]$, for all $x^t\in X(t)$ and for all $y^t\in Y(t,x^0)$

$$|G(t,x^t,y^t)-G(t,x^0,y^t)|\le C\|x^t-x^0\|_E^2.$$

(G1) For all $t\in[0,\tau]$, the sets $X(t)$ and $Y(t,x^0)$ are non-empty and single-valued.

(G2) There exist constants $c>0$, $\varepsilon>0$ and $\tau>0$ such that $\|x^t-x^0\|_X\le ct^{1/2+\varepsilon}$ for all $t\in[0,\tau]$.

(G3) Let $x^0\in X(0)$ and $y^0\in Y(0,x^0)$. For any non-negative real sequence $(t_n)_{n\in\mathbf{N}}$ converging to zero, there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$, and there exists $y^{t_{n_k}}\in Y(t_{n_k},x^0)$ such that

$$\lim_{\substack{k\to\infty\\ t\searrow 0}}\partial_tG(t,x^0,y^{t_{n_k}})=\partial_tG(0,x^0,y^0).$$

Then it follows for any $y\in F$

$$\frac{d}{dt}G(t,x^t,y)|_{t=0}=\partial_tG(0,x^0,y^0),$$

where $x^t\in X(t)$ $(t\in[0,\tau])$, $x^0\in X(0)$ and $y^0\in Y(0,x^0)$.

Proof. Let $t \in [0,\tau]$, $x^t \in X(t)$, $x^0 \in X(0)$ and $y^t \in Y(t,x^0)$ be given. Then, we write

$$G(t,x^t,y^t) - G(t,x^t,y^t) = G(t,x^t,y^t) - G(t,x^0,y^t) + G(t,x^0,y^t) - G(0,x^0,y^t). \tag{4.22}$$

Due to Assumption (G0) and $y^t \in Y(t,x^0)$, we have the following expansion

$$|G(t,x^t,y^t) - G(t,x^0,y^t)| \leq C \|x^t - x^0\|_E^2.$$

Taking into account (G2), we get that

$$\lim_{t \searrow 0} \frac{G(t,x^t,y) - G(t,x^0,y)}{t} = 0.$$

Applying the mean value theorem to $s \mapsto G(st,x^0,y^t)$ on $(0,1)$, we get a number $\eta_t \in (0,1)$ such that

$$(G(t,x^0,y^t) - G(0,x^0,y^t))/t = \partial_t G(\eta_t t, x^0, y^t).$$

Put $\underline{d}g(0) := \liminf_{\substack{t\searrow 0\\ t>0}} \partial_t G(\eta_t t, x^0, y^t)$ and $\overline{d}g(0) := \liminf_{\substack{t\searrow 0\\ t>0}} \partial G(\eta_t t, x^0, y^t)$. Then taking a sequence $t_n \searrow 0$ such that $\underline{g}(0) = \lim_{n\to\infty} \partial_t G(\eta_{t_n} t_n, x^0, y^{t_n})$ and using (G3) it is easily seen that $\underline{d}g(0) = \partial_t G(0,x^0,y^0)$. In the same way we may prove $\overline{d}g(0) = \partial_t G(0,x^0,y^0)$ and thus $\underline{g}(0) = \overline{g}(0)$, which implies that $\lim_{t\searrow 0}(G(t,x^0,y^t) - G(0,x^0,y^t))/t = \partial_t G(0,x^0,y^0)$. Therefore, we may divide (4.22) by $t > 0$ and pass to the limit $t \searrow 0$ to obtain the desired result. □

4.3 Continuity and Lipschitz continuity of $t \mapsto x^t$

To study the behavior of $t \mapsto x^t$, $x^t \in X(t)$, we investigate the operators associated with the averaged adjoint and the usual adjoint equation. In general they will be bilinear forms on Banach spaces as can be easily seen by considering the p-Laplacian with $p \neq 2$.

Consider a family of continuous bilinear forms

$$(t,v,w) \mapsto a(t,v,w) : \ [0,\tau] \times H_1 \times H_2 \to \mathbf{R}$$

on two Hilbert spaces H_1 and H_2.

Assumption (L).

(i) There exists $L > 0$ such that

$$a(t,v,w) \leq L\|v\|_{H_1}\|v\|_{H_2} \quad \textit{for all } v \in H_1,\ w \in H_2, t \in [0,\tau].$$

(ii) For all $\hat{v} \in H_1$ and $\hat{w} \in H_2$ the functions

$$v \mapsto a(t,v,\hat{w}) \quad \textit{and} \quad w \mapsto a(t,\hat{v},w)$$

are linear functions.

(iii) Assume that there is a constant $\alpha > 0$ independent of $t \in [0,\tau]$ such that

$$\forall x \in H_1 : \ \alpha \|x\|_{H_1} \leq \sup_{\substack{w\in H_2\\ w\neq 0}} \frac{a(t,x,w)}{\|w\|_{H_2}}. \tag{4.23}$$

For given $f(t,\cdot) \in H_2'$ and $t \in [0,\tau]$, we are then interested in the question under which conditions there exists $u \in H_1$ such that

$$a(t,u,v) = f(t,v) \text{ for all } v \in H_2? \tag{4.24}$$

One answer is given by a theorem of Nečas. The following result is an equivalent version of [78, Thm. 3.3].

Theorem 4.8 (Nečas). *Let $a : H_1 \times H_2 \to \mathbf{R}$ be a continuous bilinear form and $f \in H_2'$ a continuous linear functional. Then the variational problem*

$$u \in H_1 : \quad a(u,v) = f(v) \quad \textit{for all } v \in H_2$$

admits a unique solution $u \in H_1$ and depends continuously on f if and only if

(C1) There exists $\alpha > 0$ such that

$$(SU) \qquad \forall\, v \in H_1 : \quad \sup_{\substack{w \in H_2 \\ w \neq 0}} \frac{a(v,w)}{\|w\|_{H_2}} \geq \alpha \, \|v\|_{H_1}.$$

(C2) For every $0 \neq w \in H_2$ there exists $v \in H_1$ such that $a(v,w) \neq 0$.

As a result, we conclude that the problem (4.24) admits for each $t \in [0,\tau]$ a unique solution $x^t \in H_2$ when Assumption (L) is satisfied. Moreover, it follows immediately

$$\alpha \, \|x^t\|_{H_1} \leq \sup_{\substack{w \in H_2 \\ w \neq 0}} \frac{a(t,x^t,w)}{\|w\|_{H_2}} = \sup_{\substack{w \in H_2 \\ w \neq 0}} f(t,w) = \|f(t)\|_{H_2'}.$$

Introducing the operator $\mathfrak{C}(t) : H_1 \to H_2'$ by $\langle \mathfrak{C}(t)u, v\rangle := a(t,u,v)$, $u \in H_1, v \in H_2$, we can rewrite the previous inequality as

$$\alpha \, \|x^t\|_{H_1} \leq \|\mathfrak{C}(t)x^t\|_{H_2'} = \|f(t)\|_{H_2'}.$$

4.3.1 Estimates of $\|x^t - x^0\|$ under saddle point assumption

Let H_1, H_2 be Hilbert spaces and $\tau > 0$ a real number. Throughout this paragraph we consider the Lagrangian $\mathfrak{L} : [0,\tau] \times H_1 \times H_2 \to \mathbf{R}$ given by

$$\mathfrak{L}(t,x,y) := \mathfrak{e}(t,x,y) + \frac{1}{2}\|x - x^0\|_{H_1}^2. \tag{4.25}$$

The function $\mathfrak{e}$ can be imagined as a perturbed PDE as described in the previous chapter. Let $g(t)$ and $h(t)$ be defined as Subsection 3.4.3, where E, F and G are replaced by H_1, H_2 and $\mathfrak{L}$. Then we define the sets (cf. (3.30),(3.31))

$$H_1(t) = \left\{ \hat{x} \in H_1 : \sup_{y \in H_1} \mathfrak{L}(t,\hat{x},y) = g(t) \right\}, \quad H_2(t) = \left\{ \hat{y} \in H_2 : \inf_{x \in H_1} \mathfrak{L}(t,x,\hat{y}) = h(t) \right\}.$$

According to Lemma 3.6, if $g(t) = h(t)$ then the set of saddle points of $\mathfrak{L}$ is given by

$$\tilde{S}(t) := H_1(t) \times H_2(t).$$

We start with the simpler case, where the state equation is convex-concave.

(S1) The Lagrangian $\mathfrak{L}(t,\cdot,\cdot)$ admits a unique saddle points for each $t \in [0,\tau]$.

(S2) Let $\mathfrak{L}$ satisfy Assumption (H0) (on page 49) and suppose that for all elements $y \in H_2$ the mapping $H_1 \to \mathbf{R} : x \mapsto \mathfrak{e}(t,x,y)$ is Gateaux differentiable.

(S3) There exist $C > 0$ and $\alpha \in (0,1]$ such that for $x^0 \in H_1(0)$ and $y^t \in H_2(t)$

$$|\mathfrak{e}(t,x^0,y^t) - \mathfrak{e}(0,x^0,y^t)| \le C\, t^\alpha\, \|y^t\|_{H_2}.$$

(S4) For all $t \in [0,\tau]$ and $x^t \in H_1(t)$ the operator $a(t,x,y) := d_x\mathfrak{e}(t,x^t,x;y)$ satisfies Assumption (L) and Hypotheses (C1) and (C2).

Before we proceed, we make the following observation which follows from Lemma 3.6. A saddle point $(x^t,y^t) \in \tilde{S}(t)$ satisfies for arbitrary $(\hat{x},\hat{y}) \in H_1 \times H_2$ and $s \in [0,1]$

$$\begin{aligned} \mathfrak{L}(t,x^t + s(x^t - x), y^t, \hat{x}) - \mathfrak{L}(t,x^t,y^t) \ge 0 \\ \mathfrak{L}(t,x^t,y^t + s(y^t - \hat{y})) - \mathfrak{L}(t,x^t,y^t)) \le 0. \end{aligned}$$

Thus dividing both equations by $s > 0$ and passing to the limit $s \to 0$ yield

$$\begin{aligned} d_x\mathfrak{e}(t,x^t,y^t,\hat{x}) = -(x^t - x^0,\hat{x})_{H_1} \quad \text{for all } \hat{x} \in \tilde{E}, \\ \mathfrak{e}(t,x^t,\hat{y}) = 0 \quad \text{for all } \hat{y} \in H_2 \end{aligned} \tag{4.26}$$

and hence $x^t \in X(t)$. Conversely, a solution of the system (4.26) is a saddle point if $\mathfrak{e}(t,x,y)$ is a convex-concave function. The following is a consequence of the previous considerations.

Proposition 4.9. *Let the Hilbert spaces H_1, H_2 and the Lagrangian $\mathfrak{L}$ as in (4.25) be given. Assume that the conditions (S1)-(S3) are satisfied. Then there are constants $C > 0$, $\tau > 0$ and $\alpha \in (0,1]$ such that*

$$\|x^t - x^0\|_{H_1} \le Ct^\alpha \quad \textit{for all } t \in [0,\tau].$$

Proof. By definition of a saddle point $(x^t,y^t) \in H_1 \times H_2$ and the definition of $\mathfrak{L}$

$$\mathfrak{L}(t,x^t,y^t) \le \mathfrak{L}(t,x^0,y^t), \quad \iff \quad \|x^t - x^0\|_{H_1}^2 \le \mathfrak{e}(t,x^0,y^t) - \mathfrak{e}(t,x^t,y^t).$$

Now from Hypothesis (S3) and the last inequality, we infer that there exist $C > 0$, $\tau > 0$ and $\alpha \in (0,1]$ such that $\|x^t - x^0\|_{H_1}^2 \le Ct^\alpha\, \|y^t\|_{H_2}$, for all $t \in [0,\tau]$. Further from (4.23) and $\sup_{\|v\|_{H_1} \le 1, v \ne 0}(x^t - x^0, v)_{H_2} = \|x^t - x^0\|_{H_2}$, we infer $\|x^t - x^0\|_{H_1} \le C\, t^\alpha$ for all $t \in [0,\tau]$. □

4.3.2 Estimates of $\|x^t - x^0\|$ using the averaged adjoint equation

Let H be a Hilbert space and F a Banach space. For $t \in [0,\tau], x^t \in X(t)$ and $x^0 \in X(0)$ (cf. (4.2) for the definition of $X(t)$), we consider the Lagrangian $\mathfrak{L} : [0,\tau] \times H \times F \to \mathbf{R}$ given by

$$\mathfrak{L}(t,x,y) := \frac{1}{2}\|x - x^0\|_H^2 + \mathfrak{e}(t,x,y).$$

Suppose that $\mathfrak{L}$ satisfies Assumption (H0) on page 49. Notice that $y^t \in Y(t,x^t,x^0)$ if and only if:

$$\boxed{\int_0^1 d_x\mathfrak{e}(t,sx^t + (1-s)x^0, y^t, \hat{x})\, ds = -(x^t - x^0,\hat{x})_H \quad \text{for all } \hat{x} \in H.} \tag{4.27}$$

It will be useful to introduce the operator $\mathfrak{D}(t, x^t, x^0) : F \to H'$ by

$$\langle \mathfrak{D}(t, x^t, x^0)y, z\rangle := \int_0^1 d_x\mathfrak{e}(t, sx^t + (1-s)x^0, y; z)\, ds, \quad y \in F,\ z \in H.$$

Then we may write (4.27) as

$$\mathfrak{D}(t, x^t, x^0)y^t = -(x^t - x^0) \quad \text{in } H'.$$

(T1) Let $\mathfrak{L}$ satisfy Assumption (H0) and suppose that for all $y \in F$ the mapping $H \to \mathbf{R} : x \mapsto \mathfrak{e}(t, x, y)$ is Gateaux differentiable.

(T2) There exist constants $\tau > 0$, $C > 0$ and $\alpha \in (0, 1]$ such that for $t \in [0, \tau]$, $x^0 \in X(0)$ and $y^t \in Y(t, x^t, x^0)$

$$|\mathfrak{e}(t, x^0, y^t) - \mathfrak{e}(0, x^0, y^t)| \le C\, t^\alpha\, \|y^0\|_F.$$

(T3) The bilinear form $a(t, y, z) := \langle \mathfrak{D}(t, x^t, x^0)y, z\rangle$ satisfies Hypotheses (L), (C1) and (C2).

Theorem 4.10. *Let the Hypotheses (T1)-(T3) be satisfied. Then there exist constants $C > 0, \tau > 0$ and $\alpha \in (0, 1]$ such that*

$$\|x^t - x^0\|_H \le Ct^\alpha \quad \textit{for all } t \in [0, \tau].$$

Proof. We get from the mean value theorem in integral form

$$\langle \mathfrak{D}(t, x^t, x^0)y^t, x^t - x^0\rangle = \mathfrak{e}(t, x^0, y^t) - \mathfrak{e}(t, x^t, y^t) \;\text{ for all } t \in [0, \tau].$$

Therefore using (T2) and $\mathfrak{e}(t, x^t, y) = 0$ for all $t \in [0, \tau]$, $y \in F$, we get for some constants $C > 0$, $\tau > 0$ and $\alpha \in [0, 1)$ the estimate

$$\begin{aligned}\|x^t - x^0\|_H^2 &= \mathfrak{e}(t, x^0, y^t) - \mathfrak{e}(t, x^t, y^t)\\ &= \mathfrak{e}(t, x^0, y^t) - \mathfrak{e}(0, x^0, y^t)\\ &\le Ct^\alpha\, \|y^t\|_F \quad \text{for all } t \in [0, \tau].\end{aligned}$$

Since the operator $\mathfrak{D}(t, x^t, x^0)$ is uniformly invertible, we obtain $\|y^t\|_F \le c\|x^t - x^0\|_H$ for all $t \in [0, \tau]$, which together with the previous equation yields the desired estimate. □

4.3.3 Weak differentiability of $t \mapsto x^t$ via Theorem 4.2

The following is a generalisation of an idea introduced by M.C. Delfour [1]. We introduce the auxillary Lagrangian $\mathfrak{L} : [0, \tau] \times E \times F \to \mathbf{R}$ by

$$\mathfrak{L}(t, x, y) := \mathfrak{e}(t, x, y) + \mathfrak{G}(x - x^0),$$

where E and F are reflexive Banach spaces and $\mathfrak{G} : E \to \mathbf{R}$ is a continuous functional on E. We assume again that $\mathfrak{e}$ satisfies Assumption (H0) on page 49. Note that $y^t \in Y(t, x^t, x^0)$ if and only if

$$\langle \mathfrak{D}(t, x^t, x^0)y^t, \hat{x}\rangle = -\mathfrak{G}(\hat{x}) \quad \text{for all } \hat{x} \in E. \tag{4.28}$$

The convergence of $x^t \in X(t)$ to $x := x^0$ does not depend on $\mathfrak{G}$. Thus if the hypotheses (H0)-(H3) of Theorem 4.2 are satisfied for any cost function then they will certainly be satisfied for $J(\hat{x}) := \mathfrak{G}(\hat{x} - x^0)$.

[1] M.C. Delfour is professor at the Université de Montréal in the Département de mathématiques et de statistique.

Assumption. *Assume that for any $\mathfrak{G} \in L(E;\mathbf{R})$ the Lagrangian*

$$\mathfrak{L}(t,x,y) := \mathfrak{e}(t,x,y) + \mathfrak{G}(x - x_0)$$

satisfies the Assumptions (H0)-(H3).

We have that

$$g(t) = \inf_E \sup_F \mathfrak{L}(t,x,y) = \mathfrak{G}(x^t - x^0)$$

and conclude from Theorem 4.2 that

$$\lim_{t \searrow 0} (g(t) - g(0))/t = \lim_{t \searrow 0} \mathfrak{G}\left(\frac{x^t - x^0}{t}\right)$$

exists for all $\mathfrak{G} \in L(E;\mathbf{R})$ and is equal to $\partial_t \mathfrak{L}(0,x^0,y^0) = \partial_t \mathfrak{e}(0,x^0,y^0)$. Note that y^0 depends on $\mathfrak{G}$ via (4.28). We introduce the canonical linear mapping from E' into $\mathbf{R}$ namely $L(E;\mathbf{R}) \to \mathbf{R} : f \mapsto \delta_x(f) = f(x)$. Put $\hat{x}^t := (x^t - x^0)/t$, then we see that $\delta_{\hat{x}^t} : L(E;\mathbf{R}) \to \mathbf{R}$ defines a family of continuous linear mappings such that

$$\sup_{t\in[0,\tau]} |\delta_{\hat{x}^t}(f)| = \sup_{t\in[0,\tau]} \left| f\left(\frac{x^t - x^0}{t}\right)\right| < \infty, \quad \text{for all } f \in E'.$$

From the Theorem of Banach-Steinhaus [96, Thm IV.2.1, p.141], we infer $\sup_{t\in[0,\tau]} \|\delta_{\hat{x}^t}\|_{E''} < \infty$, where $E'' := L(E',\mathbf{R})$ denotes the bi-dual of E. Now, by reflexivity of E, we obtain $\|x\|_E = \|\delta_x\|_{E''}$ and thus

$$C := \sup_{t\in[0,\tau]} \left\| \frac{x^t - x^0}{t} \right\|_E < \infty.$$

In particular $(x^t - x^0)/t$ stays bounded and

$$\|x^t - x^0\|_E \le C\, t \text{ for all } t \in [0,\tau].$$

Finally, note that for any sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ as $n \to \infty$, we may extract a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $(x^{t_{n_k}})_{k\in\mathbf{N}}$ converges weakly to some $v \in E$. But this v satisfies

$$\partial_t \mathfrak{e}(0,x^0,y^0) = \mathfrak{G}(v).$$

In fact, the weak limit v is characterised by x^0 and y^0 and the derivative of $\mathfrak{e}$ with respect to t.

Remark 4.11. *This result is quite remarkable and makes a statement about the Lagrangian approach in general. Leaving aside the Assumptions (H0)-(H3) of Theorem 4.2, we see that if the Lagrangian approach works for simple cost functions, then, roughly spoken, it implies that the weak material derivative exists. For problems like the p-Laplacian it has to be checked if it is applicable, because if yes then we get a posteriori the weak differentiability of $t \mapsto x^t$, which cannot be established by the implicit function theorem.*

4.3.4 A comparison of the adjoint equation

Let the function $G(t,x,y)$ be such that Assumption (H0) of page 49 is satisfied. So far we introduced three types of adjoint equations to prove the shape differentiability

$$\begin{aligned}
d_x G(t,x^t,\bar{y}^t;\varphi) &= 0 \quad \text{for all } \varphi \in E \quad \rightsquigarrow \text{ Correa-Seeger}\\
d_x G(t,x^0,\tilde{y}^t;\varphi) &= 0 \quad \text{for all } \varphi \in E \quad \rightsquigarrow \text{ partial perturbed adjoint}\\
\int_0^1 d_x G(t,sx^t + (1-s)x^0,y^t;\varphi) &= 0 \quad \text{for all } \varphi \in E \quad \rightsquigarrow \text{ averaged adjoint.}
\end{aligned}$$

We pick any $x^t \in X(t)$, $x^0 \in X(0)$ and $y^t \in Y(t, x^t, x^0)$. Then, assuming that Hypothesis (G0) is valid, we get

$$\begin{aligned} G(t,x^t,y^t) - G(t,x^0,y^t) - d_xG(t,x^0,y^t,x^t-x^0) &= |d_xG(t,x^0,y^t,x^t-x^0)| \\ &= \mathcal{O}(\|x^t-x^0\|_E^2). \end{aligned}$$

Assume that $\|x^t - x^0\|_E \leq Ct$ for all $[0,\tau]$, where $C > 0$ is a constant. Then $\tilde{y}^t \in Y(t,x^t,x^0)$ solves

$$d_xG(t,x^0,y^t;x^t-x^0) = \mathcal{O}(t^2).$$

If $(x^t,\bar{y}^t)$ is a saddle point of $G(t,x,y)$ then $G(t,x^t,\bar{y}^t) \leq G(t,x^0,\bar{y}^t)$ for all $t \in [0,\tau]$. Thus

$$\begin{aligned} -d_xG(t,x^0,\bar{y}^t,x^t-x^0) &\leq G(t,x^t,\bar{y}^t) - G(t,x^0,\bar{y}^t) - d_xG(t,x^0,\bar{y}^t,x^t-x^0) \\ &= \mathcal{O}(\|x^t-x^0\|_E^2). \end{aligned}$$

Since $d_xG(t,x^0,\bar{y}^t,x^t-x^0) \leq 0$ it follows

$$d_xG(t,x^0,\bar{y}^t;x^t-x^0) = O(t^2).$$

Finally, by definition of $\hat{y}^t \in Y(t,x^0)$, we have

$$d_xG(t,x^0,\hat{y}^t;x^t-x^0) = 0.$$

Chapter 5

Applications to transmission problems

Transmission problems naturally arise in many applications such as the *electrical impedance tomography*, *magneto induction tomography* or the classical *Stefan problem*. For the regularity analysis of linear transmission problems in smooth domains, we refer the reader to [31]. The main difficulty in the analysis of shape optimization problems is the discontinuity of the derivative of the PDE over the interface on which usually interface conditions are imposed.

In the present chapter, we apply Theorem 4.2 to a *semi-linear problem* (Section 5.1), a linear *transmission problem in elasticity* (Section 5.2), an *electrical impedance problem* (Section 5.3) and a *quasi-linear scalar transmission problem* (Section 5.4). For the latter three problems we discuss the existence of optimal shapes using the techniques introduced in Section 2.4.

5.1 The semi-linear model problem

5.1.1 The problem from Chapter 3

In this section we revisit the example (3.1),(3.2) from Chapter 3. To demonstrate the efficiency of Theorem 4.2, we apply it to this simple model problem. For convenience, we recall the cost function

$$J(\Omega) := \int_\Omega |u - u_r|^2\, dx, \tag{5.1}$$

and the weak formulation of (3.1)

$$\int_\Omega \nabla u \cdot \nabla \psi \, dx + \int_\Omega \varrho(u)\, \psi \, dx = \int_\Omega f\psi \, dx \quad \text{for all } \psi \in H^1_0(\Omega). \tag{5.2}$$

Suppose in the following that the assumptions on the data f, u_r and Ω introduced in the beginning of Subsection 3.2 is satisfied. We want to prove the shape differentiability of (5.1) under the following conditions:

Assumption $(\mathcal{S})$. *The function $\varrho : \mathbf{R} \to \mathbf{R}$ is continuously differentiable and satisfies:*

$$\forall x, y \in \mathbf{R} : \quad (\varrho(x) - \varrho(y))(x - y) \geq 0.$$

For $t \in [0, \tau], (\tau > 0)$ let $X(t)$, $Y(0, u^0)$ and $Y(t, u^t, u^0)$ $(u^t \in X(t), u^0 \in X(0))$ be the sets defined in (4.2), (4.4) and (4.3), respectively. Recall from Chapter 3 that the equation

(5.2) on the domain $\Phi_t(\Omega)$ transported back to Ω by $y = \Phi_t(x)$ reads

$$\int_\Omega A(t)\nabla u^t \cdot \nabla\psi\, dx + \int_\Omega \xi(t)\varrho(u^t)\psi\, dx = \int_\Omega \xi(t) f^t \psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega). \tag{5.3}$$

This equation characterises the unique minimum of the convex energy (3.7). For details, we refer the reader to Chapter 3. Recall the definition of the Lagrangian associated to the problem

$$G(t,\varphi,\psi) = \int_\Omega \xi(t)|\varphi - u_r^t|^2\, dx + \int_\Omega A(t)\nabla\varphi\cdot\nabla\psi + \xi(t)\varrho(\varphi)\,\psi\, dx - \int_\Omega \xi(t) f^t\psi\, dx. \tag{5.4}$$

THEOREM 5.1. *Let Assumption ($\mathcal{S}$) be satisfied. The shape derivative of J defined in (5.1) exists and is given by*

$$dJ(\Omega)[\theta] = \partial_t G(0, u^0, p^0),$$

where $p^0 \in Y(0,u^0)$.

Proof. Let us verify the conditions (H0)-(H3) for the function G given by (5.4).
(H0) This has already been proven in Section 3.2.
(H1) This is an easy consequence of $\theta \in C_c^2(D,\mathbf{R}^d)$ and Lemma 2.16. The derivative is given by (3.29).
(H2) Note that for all $t \in [0,\tau]$, we have $X(t) = \{u^t\}$, where u^t solves (5.3). Moreover, $p^t \in Y(t,u^t,u^0)$ if and only if

$$\int_\Omega A(t)\nabla\psi\cdot\nabla p^t + \xi(t)k(u,u^t)\,\psi\, dx = -\int_\Omega \xi(t)(u^t + u - 2u_r^t)\psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega), \tag{5.5}$$

where $k(u,u^t) := \int_0^1 \varrho'(u_s^t)\, ds$ and $u_s^t := su^t + (1-s)u$. Due to the Lemma of Lax-Milgram the previous equation has a unique solution $y^t \in H_0^1(\Omega)$. Note that the strong formulation of the averaged adjoint on the moved domain, namely, $p_t := p^t\circ\Phi_t^{-1}$ on Ω_t satisfies

$$\begin{aligned} -\Delta p_t + k(u\circ\Phi_t^{-1}, u_t)p_t &= -(u_t - u\circ\Phi_t^{-1} - 2u_r) \quad \text{in } \Omega_t\\ p_t &= 0 \quad \text{on } \partial\Omega_t, \end{aligned}$$

where $k(u\circ\Phi_t^{-1}, u^t\circ\Phi_t^{-1}) := \int_0^1 \varrho'(u_s^t\circ\Phi_t^{-1})\, ds = \int_0^1 \varrho'(su_t + (1-s)u\circ\Phi_t^{-1})\, ds$.
(H3) We already know that Assumption ($\mathcal{S}$) implies that $t\mapsto u^t$ is continuous as a map from $[0,\tau]$ into $H_0^1(\Omega)$. But this is actually not necessary as we will show now. Suppose that we do not know that $t\mapsto u^t$ is continuous. Then by inserting $\psi = u^t$ in the state equation (5.3), we obtain $\|u^t\|_{H^1(\Omega)} \le C$ for all $t\in[0,\tau]$, where $C>0$ is a constant after an application of Hölder's inequality. For any sequence of non-negative real numbers $(t_n)_{n\in\mathbf{N}}$ converging to zero there exists a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $u^{t_{n_k}} \rightharpoonup z$ as $k\to\infty$. Setting $t = t_{n_k}$ in the state equation and passing to the limit $k\to\infty$ shows $z = u$. Moreover, inserting $\psi = y^t$ into (5.5) as test function and using Hölder's inequality yields for some constant $C > 0$

$$\|y^t\|_{H_0^1(\Omega)} \le C\|u^t + u - 2u_r^t\|_{L_2(\Omega)} \qquad \text{for all } t\in[0,\tau].$$

Therefore again for any sequence $(t_n)_{n\in\mathbf{N}}$ there exists a subsequence $(t_{n_k})_{n\in\mathbf{N}}$ such that $y^{t_{n_k}} \rightharpoonup q$ as $k\to\infty$ for some $q\in H_0^1(\Omega)$. Selecting $t = t_{n_k}$ in (5.5), we would like to pass to the limit $k\to\infty$ by using Lebesgue's dominated convergence theorem. It suffices to show that $w^k(x) := \int_0^1 \varrho'(u_s^{t_{n_k}}(x))\, ds$ is bounded in $L_\infty(\mathbf{R}^d)$ independently of k and that this sequence convergences pointwise almost everywhere in Ω to $\varrho'(u)$. The boundedness of w^k follows from the continuity of u^t on $\overline{\Omega}$ and the continuity of ϱ'. The pointwise convergence

$w^k(x) \to \varrho'(u(x))$ as $k \to \infty$ (possibly a subsequence) follows from the fact that ϱ is continuous and $u^{t_{n_k}}$ converges pointwise to u as $k \to \infty$. Therefore there is a sequence $t_n \searrow 0$ such that we may pass to the limit $n \to \infty$ in (5.5), after inserting $t = t_n$. By uniqueness we conclude $q = y \in Y(0, u^0)$. Finally note that $(t, \psi) \mapsto \partial_t G(t, u, \psi)$ is weakly continuous. All conditions (H0)-(H3) are satisfied and we finish the proof. □

5.1.2 A semi-linear optimal control problem

We consider the cost function

$$J(y) := \int_\Omega |u(y) - u_r|^2 \, dx + \alpha \int_\Omega y^2 \, dx, \quad (\alpha > 0)$$

where $u = u(y)$ satisfies

$$\boxed{\begin{aligned} -\Delta u + \varrho(u) &= y \;\text{ in } \Omega \\ u &= 0 \;\text{ on } \partial\Omega. \end{aligned}}$$

The weak formulation of the previous equation reads

$$\int_\Omega \nabla u \cdot \nabla \psi \, dx + \int_\Omega \varrho(u) \, \psi \, dx = \int_\Omega y\psi \, dx \;\text{ for all } \psi \in H_0^1(\Omega).$$

We want to calculate the directional derivative of J at y_0 in direction $\hat{y}$, where $\hat{y}, y_0 \in L_2(\Omega)$. For this we consider the weak formulation of the semi-linear equation with right-hand side $y_0 + t\hat{y}$

$$\int_\Omega \nabla u^t \cdot \nabla \psi \, dx + \int_\Omega \varrho(u^t) \, \psi \, dx = \int_\Omega (y_0 + t\hat{y})\psi \, dx \;\text{ for all } \psi \in H_0^1(\Omega). \tag{5.6}$$

Note that $u^t = u(y_0 + t\hat{y})$. We define the Lagrangian

$$\begin{aligned} G(t, \varphi, \psi) := &\int_\Omega |\varphi - u_r|^2 \, dx + \int_\Omega \alpha(y_0 + t\hat{y})^2 \, dx \\ &+ \int_\Omega \nabla \varphi \cdot \nabla \psi \, dx + \int_\Omega \varrho(\varphi) \, \psi \, dx - \int_\Omega (y_0 + t\hat{y})\psi \, dx. \end{aligned}$$

We will apply again Theorem 4.2 to prove the following theorem.

THEOREM 5.2. *Let Assumption ($\mathcal{S}$) from the previous subsection be satisfied. The cost function J has a directional derivative at all y_0 in all directions $\hat{y}$, where $\hat{y}, y_0 \in L_2(\Omega)$. Moreover, the derivative is given by*

$$dJ(y_0; \hat{y}) = \int_\Omega (2\alpha y_0 - p) \, \hat{y} \, dx, \tag{5.7}$$

where $p \in H_0^1(\Omega)$ solves:

$$\int_\Omega \nabla \varphi \cdot \nabla p \, dx + \int_\Omega \varrho'(u) \, p \, \varphi \, dx = -\int_\Omega 2(u - u_r) \, \psi \, dx$$

Proof. We check conditions (H0)-(H3) of Theorem 4.2.
(H0) As in the previous example it is easily verified that for all $\varphi, \tilde{\varphi}, \psi \in H_0^1(\Omega)$

$$s \mapsto G(t, \varphi + s\tilde{\varphi}, \psi)$$

is continuously differentiable on $\mathbf{R}$.
(H1) The differentiability of $G(t,\varphi,\psi)$ with respect to t is obvious.
(H2) Note that $X(t) = \{u^t\}$, where $u^t \in H_0^1(\Omega)$ solves (5.6). Moreover, $p^t \in Y(t,u^t,u^0)$ if and only if

$$\int_\Omega \nabla\varphi \cdot \nabla p^t\,dx + \int_\Omega \left(\int_0^1 \varrho'(u_s^t)\,ds\right) p^t\,\varphi\,dx = -\int_\Omega (u^t + u - 2u_r)\,\psi\,dx \qquad (5.8)$$

for all $\varphi \in H_0^1(\Omega)$, where $u_s^t := su^t + (1-s)u$. The function p^t solves in the strong sense

$$\begin{aligned} -\Delta p^t + k(u,u^t)p^t &= -(u_t + u - 2u_r) \quad \text{ in } \Omega_t \\ p^t &= 0 \quad \text{ on } \partial\Omega_t. \end{aligned}$$

where $k(u,u^t) := \int_0^1 \varrho'(u_s^t)\,ds$. Due to Assumption $(\mathcal{S})$, we have $\varrho'(x) \geq 0$ for all $x \in \mathbf{R}$, i.e. $k(u,u^t) \geq 0$ and thus by the Lemma of Lax-Milgram the previous equation has a unique solution $p^t \in H_0^1(\Omega)$.
(H3) Testing (5.8) with p^t and using Hölder's inequality, we get for some $C > 0$ the estimate $\|p^t\|_{H_0^1(\Omega)} \leq C$ for all $t \in [0,\tau]$. Therefore, we obtain $p^{t_n} \rightharpoonup \tilde{p}$ for some sequence $t_n \searrow 0$ and some element $\tilde{p} \in H_0^1(\Omega)$. Passing to the limit $t_n \searrow 0$ in (5.8) (compare the proof of Theorem 5.1 for a justification), entails that $\tilde{p} = p$, where p solves

$$\int_\Omega \nabla\varphi \cdot \nabla p\,dx + \int_\Omega \varrho'(u)\,p\,\varphi\,dx = -\int_\Omega 2(u-u_r)\,\varphi\,dx,$$

for all $\varphi \in H_0^1(\Omega)$. This finishes the proof of condition (H3) and we may apply Theorem 4.2 to obtain (5.7). □

5.2 A transmission problem in elasticity

Distortion refers to undesired alterations in the size and shape of a workpiece. Such unwanted deformations occur as side effects at some stage in the manufacturing chain, and they are often connected to a thermal treatment of a workpiece. Usually, in order to eliminate distortions, the manufacturing chain is augmented by an additional mechanical finishing step. The inferred cost, however, leads to severe economic losses within the machine, automotive, or transmission industry [94]. In order to overcome this adverse situation, recently a new strategy has been developed, which allows the elimination of distortions already during the heat treatment [87], thus rendering the additional finishing step unnecessary.

Alterations in form of geometry changes in a process involving thermal treatment of the workpiece can often be attributed to the occurrence of a solid-solid phase transition, which leads to a microstructure consisting of phases with different densities. As a result, internal stresses along phase boundaries build up. In addition, macroscopic geometry changes are relevant as well. *Distortion compensation* then seeks to find a desired phase mixture such that the resulting internal stresses and accompanying changes in geometry compensate the distortion and hence lead to the desired size and shape of the workpiece, respectively.

Assuming that no rate effects occur during cooling, i.e., neglecting transformation-induced plasticity [25], one can tackle this problem mathematically by a two-step hybrid approach. In the first step the optimal microstructure for distortion compensation is computed by solving a shape design problem subject to a stationary mechanical equilibrium problem. In the second step an optimal cooling strategy is computed to realise this microstructure. While the latter has been studied extensively, see, e.g., [58, 59], the goal of this paper is to develop a novel approach for the first step by computing an optimal microstructure or phase mixture in order to compensate for distortion.

Mathematically, here we assume that the domain occupied by the workpiece is denoted by $D \subset \mathbf{R}^d$ and consists of a microstructure with two phases in the domains $\Omega \subset D$ and $D \setminus \overline{\Omega}$, which are separated by a sharp interface. This is in contrast to [26], where a phase-field approach to distortion compensation is taken. In our situation, one might think of these two phases as if they emerged from one parent phase during a heat treatment. In order to distinguish between the associated sub-domains we introduce the characteristic function $\chi = \chi_\Omega$ of the set Ω, which equals 1 for $x \in \Omega$ and 0 otherwise.

When the workpiece is in equilibrium, then the stress tensor σ satisfies

$$\boxed{\begin{aligned} -\operatorname{div}\sigma &= 0 \quad \text{in } D \\ \sigma n &= 0 \quad \text{in } \Sigma_N \\ \mathbf{u} &= 0 \quad \text{in } \Sigma_0, \end{aligned}} \tag{5.9}$$

with $\bar{\Gamma}^N \cup \bar{\Gamma}_0 = \partial D$. According to Hooke's law only elastic strains contribute to the stress. Hence, in the case of small deformations we have $\sigma = A(\varepsilon(\mathbf{u}) - \tilde{\varepsilon})$, where A represents the stiffness tensor, $\tilde{\varepsilon}$ the internal strain, and $\varepsilon(\mathbf{u}) = \frac{1}{2}(\partial\mathbf{u} + (\partial\mathbf{u})^*)$ the linearised overall strain. In general, the stiffness may be different in both sub-domains. This leads to the ansatz

$$A = A_\chi(x) := \chi(x)A_1 + (1 - \chi(x))A_2, \tag{5.10}$$

with A_1 denoting the stiffness in the material domain $\Omega^+ \subset D$, and A_2 the stiffness in $\Omega^- := D \setminus \overline{\Omega^+}$. These different densities A_i are the main reason for the presence of internal stresses. Thus we invoke an analogous mixture ansatz for the internal strain, i.e., we assume $\tilde{\varepsilon} = \tilde{\varepsilon}_\chi(x) := \chi(x)\tilde{\varepsilon}_1 + (1 - \chi(x))\tilde{\varepsilon}_2$. In an isotropic situation, which we assume from now on, we have $A_i\tilde{\varepsilon}_i = \beta_i(x)I$, where I is the identity matrix. Consequently, the constitutive relation reads

$$\sigma_\chi(x) = A_\chi\varepsilon(\mathbf{u}) - \beta_\chi I,$$

with

$$\beta_\chi(x) := \chi(x)\beta_1 + (1 - \chi(x))\beta_2. \tag{5.11}$$

As a motivation of our modeling assumptions, one might view (5.9) as describing the steady state of an isotropic homogeneous linear thermoelastic body after cooling from a reference temperature θ_{ref} to an asymptotic temperature θ_∞. In that case the internal stress corresponds to the asymptotic linear thermoelastic stress, which can be described as $\varepsilon^{th} = \delta(\theta_\infty - \theta_{ref})I$, where δ denotes the thermal expansion.

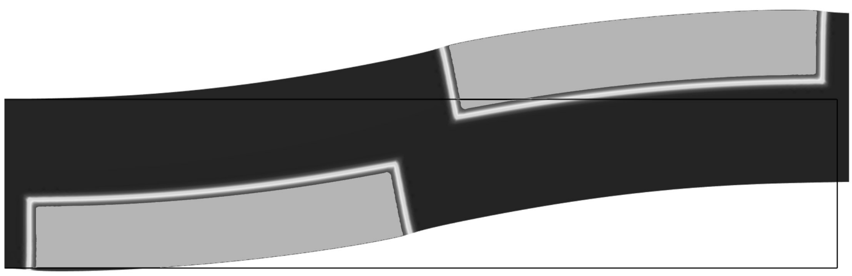

Figure 5.1: Deformation of a rectangular reference domain caused by sub-domains with different densities (black and wight).

Figure 5.1 demonstrates the effect of sub-domains with different densities for the mechanical equilibrium shape. The goal of this paper is to utilise this effect by finding an optimal mixture of sub-domains $\Omega := \Omega^+$ and its complement in D (denoted by Ω^-), such that the workpiece attains a desired equilibrium shape. This distortion compensation is achieved by minimizing the objective (or cost) function

$$J(\chi, \mathbf{u}) = \int_{\tilde{\Sigma}} \|\mathbf{u} - \mathbf{u}_d\|^2 ds + \alpha \hat{P}_D(\chi),$$

where $\tilde{\Sigma} \subset \Sigma_N$ and $\mathbf{u}_d \in H^1(\mathbf{R}^d, \mathbf{R}^d)$ are fixed. The first term of the cost functional aims at locating the workpiece near a desired equilibrium shape encoded in $\mathbf{u}_d$. It is well-known that minimizing solely this geometric part would lead to homogenised or laminated microstructures [6]. Thus, in order to avoid this scenario, the perimeter of Ω is penalised through the presence of $\hat{P}_D(\chi)$ in J with a positive weight α. Note that if the boundary is C^2, then the perimeter corresponds to the total surface area of the boundary in three-dimensional problems, and to the total arc length of the boundary in two-dimensions.

The optimal shape design problem to be studied in this section reads

$$\begin{aligned}
&\text{minimise} \quad J(\chi, \mathbf{u}) \quad \text{over } (\chi, \mathbf{u}) \\
&\text{subject to } \mathbf{u} = \mathbf{u}(\Omega) = \mathbf{u}(\chi) \text{ solves (5.9)}.
\end{aligned}$$

Subsequently, we will study the shape differentiability of the previous shape function and obtain results for scalar transmission problems derived in [4, 82].

5.2.1 Notation

Let the following assumption be satisfied.

Assumption 5.3. *Suppose that $D \subset \mathbf{R}^d$ is a regular domain in the sense of Definition 2.3 with boundary $\Sigma = \partial D$. Let $\Omega \subset D$ be a measurable subset and denote its associated characteristic function by $\chi := \chi_\Omega$. We put $\Omega^+ := \Omega$, $\Omega^- := D \setminus \overline{\Omega}$ and defined the* interface *by $\Gamma = \partial\Omega^- \cap \partial\Omega^+$. We assume that Σ_N and Σ_0 are disjoint parts of the boundary Σ, where the set Σ_0 has positive surface measure, i.e. $\mathcal{H}^{d-1}(\Sigma_0) > 0$ ($\mathcal{H}^{d-1}$ denotes the $d-1$ dimensional Hausdorff measure). We assume that both Σ_0 and Σ_N consist of finitely many connected components.*

An example of a regular domain D with subset $\Omega^+ \subset D$ is depicted in Figure 5.2. Recall that the set of characteristic functions χ_Ω with Lebesgue measurable $\Omega \subset D$ is denoted by $X(D)$.

5.2.2 The problem setting

The equations (5.9) and (5.10)–(5.11) lead to the following interface model constituting the *state system*:

$$\boxed{\begin{aligned}
-\operatorname{div}(A_1 \varepsilon(\mathbf{u}^+)) &= 0 && \text{in} \quad \Omega^+ \\
-\operatorname{div}(A_2 \varepsilon(\mathbf{u}^-)) &= 0 && \text{in} \quad \Omega^- \\
-A_2 \varepsilon(\mathbf{u}^-) n_D &= 0 && \text{on} \quad \Sigma_N \\
\mathbf{u}^- &= 0 && \text{on} \quad \Sigma_0
\end{aligned}} \tag{5.13}$$

including the *transmission boundary condition*

$$\boxed{(A_1 \varepsilon(\mathbf{u}^+) - A_2 \varepsilon(\mathbf{u}^-)) n = (\beta_1 - \beta_2) n \quad \text{on } \Gamma.} \tag{5.14}$$

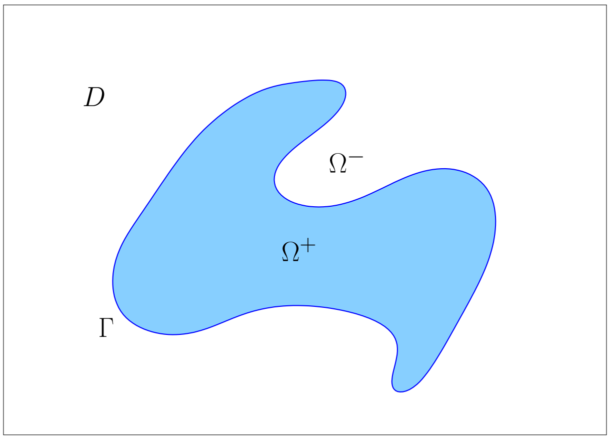

Figure 5.2: Domain D which contains Ω^+ and Ω^-, where Γ is the boundary of Ω^+.

Here, the *displacement field* $\mathbf{u} : \overline{D} \to \mathbf{R}^d$ is the unknown function, and n and n_D are the outward unit normal fields along $\partial\Omega$ and ∂D, respectively. Given a function $\varphi : D \to \mathbf{R}^d$, we define its restriction to Ω^i by $\varphi^i := \varphi_{|\Omega^i} : \Omega^i \to \mathbf{R}^d$, where $i \in \{+, -\}$. The bracket

$$[\varphi]_\Gamma := \varphi^+_{|\Gamma} - \varphi^-_{|\Gamma}$$

denotes the jump of a function φ across Γ, where $|_\Gamma$ indicates the trace operator. The material is assumed to be *isotropic* and *homogeneous* in each phase. Hence, the stiffness tensor takes the form

$$A_i(\Theta) := 2\mu_i\Theta + \lambda_i \mathrm{tr}(\Theta)I, \quad \Theta \in \mathbf{R}^{d,d},\ \mu_i, \lambda_i > 0,\ i = 1, 2.$$

Mathematically, the distribution of the material contained in Ω is denoted by χ, which serves as the control variable in our minimisation problem for optimally compensating unwanted distortions. For this purpose and as motivated in the introduction, we consider the cost functional

$$\hat{J}(\chi) := \int_{\tilde{\Sigma}} \|\mathbf{u}(\chi) - \mathbf{u}_d\|^2 ds + \alpha \hat{P}_D(\chi), \qquad \text{for fixed } \alpha > 0, \tag{5.15}$$

where $\tilde{\Sigma} \subset \Sigma \setminus \Sigma_0$. The function $\mathbf{u}(\chi)$ is the solution of (5.13)–(5.14), and $\mathbf{u}_d \in H^1_{\Sigma_0}(D, \mathbf{R}^3)$ describes the desired shape of the body.

We seek for optimal solutions in the set $\mathfrak{B}(D)$ defined in (2.12), which leads us to the study of the following problem:

$$\text{minimise} \quad \hat{J}(\chi) \quad \text{ over } \chi \in \mathfrak{B}(D). \tag{5.16}$$

Below, we prove that this problem admits at least one solution.

5.2.3 Analysis of state system

In this section we analyse the state system and prove existence of a solution to (5.12). For each $\chi \in X(D)$ let we associate to the problem (5.13),(5.14) a bilinear form

$$a_\chi : H^1(D; \mathbf{R}^d) \times H^1(D; \mathbf{R}^d) \to \mathbf{R} : \ (\boldsymbol{\varphi}, \boldsymbol{\psi}) \mapsto \int_D A_\chi \varepsilon(\boldsymbol{\varphi}) : \varepsilon(\boldsymbol{\psi})\, dx.$$

Note that the tensor A_χ is positive definite with constant $k := \min\{2\,\mu_1, 2\,\mu_2\}$

$$A_\chi(x)\tau : \tau \geq k|\tau|^2 \quad \text{for all } \tau \in \mathbf{R}^{d,d},\ x \in \overline{D}.$$

The weak formulation of the interface problem (5.13) reads: Find $\mathbf{u}(\chi) = \mathbf{u} \in H^1_{\Sigma_0}(D;\mathbf{R}^d)$ such that

$$a_\chi(\mathbf{u}, \boldsymbol{\psi}) = \int_D \beta_\chi \operatorname{div}(\boldsymbol{\varphi})\,dx \quad \text{for all } \boldsymbol{\varphi} \in H^1_{\Sigma_0}(D;\mathbf{R}^d). \tag{5.17}$$

Considering the previous equation for the characteristic function $\chi_{\Phi_t(\Omega)}$ and applying the change of variables $\Phi_t(x) = y$ yields

$$a^t(\mathbf{u}^t, \boldsymbol{\psi}) = b^t(\boldsymbol{\psi}) \quad \text{for all } \boldsymbol{\psi} \in H^1_{\Sigma_0}(D;\mathbf{R}^d), \tag{5.18}$$

where $(C(t) := \partial\Phi_t^{-1})$

$$\begin{aligned} a^t(\boldsymbol{\varphi}, \boldsymbol{\psi}) &:= \int_D \xi(t) A_\chi \mathcal{S}(\partial\boldsymbol{\varphi}\, C(t)) : \mathcal{S}(\partial\boldsymbol{\psi}\, C(t))\,dx \\ b^t(\boldsymbol{\psi}) &:= \int_D \xi(t)\, \beta_\chi \partial\Phi_t^\top : \partial\boldsymbol{\psi}\,dx. \end{aligned}$$

We refer to the previous equation as the perturbed state equation. We have the following result concerning existence and uniqueness of the state equation and perturbed state equation.

Theorem 5.4. *Let Assumption 5.3 be satisfied.*

(i) For given $\chi \in X(D)$ and for all $t \in [0,\tau]$ the equation (5.18) has exactly one weak solution $\mathbf{u}^t(\chi)$ and we have the following a priori bound

$$\|\mathbf{u}^t(\chi)\|_{H^1(D;\mathbf{R}^d)} \leq C \quad \textit{for all } \chi \in X(D), \quad \textit{for all } t \in [0,\tau].$$

Additionally, if the interface Γ is C^2 and the distance between Ω and the boundary ∂D is at least $\epsilon > 0$, i.e. $d_{\partial D}(x) := \inf_{y\in\partial D}|x - y| > \epsilon$ for all $x \in \Omega$, then we have $\mathbf{u}^t(\chi)|_{\Omega^+} \in H^2(\Omega^+;\mathbf{R}^d)$, $\mathbf{u}^t(\chi)|_{\hat\Omega^-} \in H^2(\hat\Omega^-;\mathbf{R}^d)$, for each $\hat\Omega^- \subset \Omega^-$ such that $d_{\partial D}(x) > 0$ for all $x \in \hat\Omega^-$.

(ii) There exists $\tau > 0$ such that

$$\|\mathbf{u}^t - \mathbf{u}\|_{H^1(D;\mathbf{R}^d)} \leq ct \quad \textit{for all } t \in [0,\tau].$$

Proof. (i) The higher regularity result is a direct consequence of [31, Thm 5.3.8]. For the existence of a solution consider the family of energies $E : [0,\tau] \times H^1_{\Sigma_0}(D;\mathbf{R}^d) \to \mathbf{R}$

$$E(t,\boldsymbol{\varphi}) := \frac{1}{2} a^t(\boldsymbol{\varphi},\boldsymbol{\varphi}) - \int_D \beta_\chi \operatorname{div}(\boldsymbol{\varphi})\,dx.$$

We show that this energy is strictly convex in $H^1_{\Sigma_0}(D;\mathbf{R}^d)$ and

$$dE^2(t,\boldsymbol{\varphi};\boldsymbol{\psi},\boldsymbol{\psi}) \geq k\|\boldsymbol{\psi}\|^2_{H^1(D;\mathbf{R}^d)} \quad \text{for all } \boldsymbol{\psi} \in H^1_{\Sigma_0}(D;\mathbf{R}^d), \quad \text{for all } t \in [0,\tau].$$

It is sufficient to show that the perturbed bilinear form a^t is uniformly coercive, i.e., there is a constant $C > 0$ such that

$$C\|\boldsymbol{\varphi}\|^2_{H^1(D;\mathbf{R}^d)} \leq a^t(\boldsymbol{\varphi},\boldsymbol{\varphi}) \quad \text{for all } \boldsymbol{\varphi} \in H^1_{\Sigma_0}(D;\mathbf{R}^d), \tag{5.19}$$

since $dE^2(t,\boldsymbol{\varphi};\boldsymbol{\psi},\boldsymbol{\psi}) = a^t(\boldsymbol{\psi},\boldsymbol{\psi})$. To see this note that Korn's inequality implies that there is a constant $C>0$ such that $C\|\boldsymbol{\varphi}\|^2_{H^1(D;\mathbf{R}^d)} \leq a_\chi(\boldsymbol{\varphi},\boldsymbol{\varphi})$ for all $\boldsymbol{\varphi}\in H^1_{\Sigma_0}(D;\mathbf{R}^d)$ and for all $\chi\in X(D)$. In particular this constant is independent of χ, but it depends on D. The change of variables $\Phi_t(x)=y$ yields

$$C\left(\int_D \xi(t)\,(|\partial_x\boldsymbol{\varphi}\partial_x\Phi_t^{-1}|^2 + |\boldsymbol{\varphi}|^2)\,dx\right) \leq a^t(\boldsymbol{\varphi},\boldsymbol{\varphi}) \quad \text{for all } \boldsymbol{\varphi}\in H^1(D;\mathbf{R}^d)$$

and, moreover, we have the following estimate $|\partial_x\boldsymbol{\varphi}| = |\partial_x\boldsymbol{\varphi}\partial_x\Phi_t^{-1}\partial_x\Phi_t| \leq |\partial_x\Phi_t|\,|\partial_x\boldsymbol{\varphi}\partial_x\Phi_t^{-1}|$. Thus using that $\xi(t)\geq c_1$ and $\|\partial_x\Phi_t\|\leq c_2$ for $t>0$ small, we obtain the desired inequality (5.19). Therefore the energy $\varphi\mapsto E(t,\varphi)$ has for each $t\in[0,\tau]$ a unique minimiser which is characterised by

$$dE(t,\boldsymbol{\varphi};\boldsymbol{\psi}) = 0 \quad \text{for all } \boldsymbol{\psi}\in H^1_{\Sigma_0}(D;\mathbf{R}^d),$$

which is the equation (5.17). Finally, let $\chi\subset X(D)$ and $\mathbf{u}^t_\chi$ the corresponding solutions to (5.18). We compute

$$c\|\mathbf{u}^t_\chi\|^2_{H^1(D;\mathbf{R}^d)} \leq a^t(\mathbf{u}^t,\mathbf{u}^t) = b^t(\mathbf{u}^t) \leq C\|\mathbf{u}^t\|_{H^1(D;\mathbf{R}^d)},$$

where C depends only on $\beta_1,\beta_2,m^d(D),d$ and c, where m^d is the Lebesgue measure.
(ii) Note that $a^t(\mathbf{u}^t-\mathbf{u},\hat{\boldsymbol{\varphi}}) = a^0(\mathbf{u},\hat{\boldsymbol{\varphi}}) - b^0(\hat{\boldsymbol{\varphi}}) - (a^t(\mathbf{u},\hat{\boldsymbol{\varphi}}) - b^t(\hat{\boldsymbol{\varphi}}))$, and thus by the mean value theorem there is a constant $\eta=\eta(t,\hat{\boldsymbol{\varphi}})\in(0,1)$ such that

$$a^t(\mathbf{u}^t-\mathbf{u},\hat{\boldsymbol{\varphi}}) = -\partial_t(a^{\eta_t t}(\mathbf{u},\hat{\boldsymbol{\varphi}}) - b^{\eta_t t}(\hat{\boldsymbol{\varphi}})),$$

where

$$\begin{aligned}\partial_t a^t(\mathbf{u},\hat{\boldsymbol{\varphi}})|_{t=0} = &-\int_D A_\chi\mathcal{S}(\partial_x\mathbf{u}\,\bar{\partial}_x\theta^t) : \partial_x\hat{\boldsymbol{\psi}}\,\partial\Phi_t^{-1}\,dx\\ &-\int_D A_\chi\mathcal{S}(\partial_x\mathbf{u}\,\partial\Phi_t^{-1}) : (\partial_x\hat{\boldsymbol{\psi}}\,\bar{\partial}_x\theta^t)\,dx,\end{aligned}$$

$\bar{\partial}_x\theta^t := \partial\Phi_t^{-1}\partial_x\theta^t\partial_x\Phi_t^{-1}$. From this and (5.19) we infer

$$\begin{aligned}C\|\mathbf{u}^t-\mathbf{u}\|^2_{H^1(D;\mathbf{R}^d)} &\leq -\partial_t(a^{\eta_t t}(\mathbf{u},\mathbf{u}^t-\mathbf{u}) - b^{\eta_t t}(\mathbf{u}^t-\mathbf{u}))\\ &\leq c(1+\|\mathbf{u}\|_{H^1(D;\mathbf{R}^d)})\,\|\mathbf{u}^t-\mathbf{u}\|_{H^1(D;\mathbf{R}^d)}, \quad \text{for all } t\in[0,\tau].\end{aligned}$$

□

5.2.4 Existence of an optimal shape

In order to obtain optimal shapes, we first show the continuity of $\chi\mapsto J(\chi)$ in an appropriate function space. We begin with the following Lipschitz continuity of the mapping $\chi\mapsto\mathbf{u}(\chi)\in H^1_{\Sigma_0}(D;\mathbf{R}^d)$, considered as function from $L_1(D)\to H^1_{\Sigma_0}(D;\mathbf{R}^d)$.

Lemma 5.5. *There exists a constant $C>0$ such that*

$$\forall\chi_1,\chi_2\in X(D):\ \|\mathbf{u}(\chi_1)-\mathbf{u}(\chi_2)\|_{H^1(D;\mathbf{R}^d)} \leq C\|\chi_1-\chi_2\|_{L_1(D)},$$

where $\mathbf{u}(\chi_1),\mathbf{u}(\chi_2)$ are solutions of (5.17).

Proof. Let $\chi_1, \chi_2 \in X(D)$ be two characteristic functions. Put $\mathbf{u}_i := \mathbf{u}(\chi_i)$, $i = 1, 2$, and $\mathbf{u} := \mathbf{u}(\chi)$, then we estimate

$$\begin{aligned}
c\|\mathbf{u}_1 - \mathbf{u}_2\|^2_{H^1(D;\mathbf{R}^d)} \leq & \int_D A_{\chi_1}\varepsilon(\mathbf{u}_1 - \mathbf{u}_2) : \varepsilon(\mathbf{u}_1 - \mathbf{u}_2)\, dx \\
= & \int_D (\beta_{\chi_1} - \beta_{\chi_2}) \operatorname{div}(\mathbf{u}_1 - \mathbf{u}_2)\, dx \\
& + \int_D (A_{\chi_2} - A_{\chi_1})\varepsilon(\mathbf{u}_2) : \varepsilon(\mathbf{u}_1 - \mathbf{u}_2)\, dx \\
\leq & \|\chi_1 - \chi_2\|_{L_2(D)}\|\mathbf{u}_1 - \mathbf{u}_2\|_{H^1(D;\mathbf{R}^d)} \\
& + \||A_{\chi_2} - A_{\chi_1}|\,|\varepsilon(\mathbf{u}_2)|\|_{L_2(D)}\|\mathbf{u}_1 - \mathbf{u}_2\|_{H^1(D;\mathbf{R}^d)}.
\end{aligned}$$

Now from [52] we know that $\varepsilon(\mathbf{u}) \in L_{2+\gamma}(D; \mathbf{R}^{d,d})$ for some $\gamma > 0$ and that there is a constant $C > 0$ dependent of the domain D such that $\|\varepsilon(\mathbf{u})\|_{L_{2+\gamma}(D;\mathbf{R}^{d,d})} \leq C$. Therefore dividing the above inequality by $\|\mathbf{u}_1 - \mathbf{u}_2\|_{H^1(D;\mathbf{R}^d)}$ and estimating the right-hand side with the Hölder inequality with $q = \frac{2+\gamma}{2}$ and $q' := \frac{q}{q-1} = \frac{2}{\gamma} + 1$, we obtain

$$\|\mathbf{u}_1 - \mathbf{u}_2\|_{H^1(D;\mathbf{R}^d)} \leq C(\|\beta_{\chi_1} - \beta_{\chi_2}\|_{L_2(D)} + \|A_{\chi_2} - A_{\chi_1}\|_{L_{2q'}(D)}\|\varepsilon(\mathbf{u}_2)\|_{L_{2q}(D)}).$$

Note that $|A_{\chi_1} - A_{\chi_2}| \leq |\chi_1 - \chi_2|(|A_1| + |A_2|)$ and $|\beta_{\chi_1} - \beta_{\chi_2}| \leq |\chi_1 - \chi_2|(|\beta_1| + |\beta_2|)$. Moreover, using Hölder's inequality and the boundedness of D it follows that for any $\varepsilon > 0$ there exists $C > 0$ depending on $m(D)$ such that $\|\chi_2 - \chi_1\|_{L_{2q'}(D)} \leq C\|\chi_2 - \chi_1\|_{L_1(D)}$ for all $\chi_1, \chi_2 \in X(D)$. □

Corollary 5.6. *Let us denote by Φ_t the flow generated by $\theta \in C^1_c(D, \mathbf{R}^d)$ and set $\Omega_t := \Phi_t(\Omega)$. Denote by $\mathbf{u}_t = \mathbf{u}(\chi_{\Omega_t})$ the solution of (5.17) with characteristic function $\chi = \chi_{\Omega_t}$. Then $\mathbf{u}_t \circ \Phi_t : [0, \tau] \to H^1(D; \mathbf{R}^d)$ and $\mathbf{u}_t : [0, \tau] \to H^1(D; \mathbf{R}^d)$ are continuous in 0 and*

$$\lim_{t\searrow 0} \|\mathbf{u}_t - \mathbf{u}\|_{H^1(D;\mathbf{R}^d)} = 0, \qquad \lim_{t\searrow 0} \|\mathbf{u}_t \circ \Phi_t - \mathbf{u}\|_{H^1(D;\mathbf{R}^d)} = 0.$$

Proof. The continuity of $\mathbf{u}_t : [0, \tau] \to H^1(D; \mathbf{R}^d)$ follows directly from the previous lemma by setting $\chi_1 := \chi_\Omega$ and $\chi_2 = \chi_{\Omega_t} = \chi_\Omega \circ \Phi_t^{-1}$

$$\|\mathbf{u}(\chi_\Omega) - \mathbf{u}(\chi_{\Omega_t})\|_{H^1(D;\mathbf{R}^d)} \leq C\|\chi_\Omega - \chi_\Omega \circ \Phi_t^{-1}\|_{L_q(D)},$$

and the right-hand side tends to zero as $t \to 0$ due to Lemma 2.16 item (i). Now the continuity of $\mathbf{u}_t \circ \Phi_t$ follows from Lemma 2.16 item (iv). □

After the preparations of the last section, we are ready to study the optimization problem (5.16).

Theorem 5.7. *For each $\alpha > 0$ the problem (P_χ) with the cost function (5.15) admits at least one solution.*

Proof. By Lemma 5.5 we know that the mapping $\chi \mapsto \mathbf{u}(\chi)$ is continuous from $X(D)$ equipped with δ_1 metric into $H^1(D, \mathbf{R}^d)$. Therefore the cost function $\hat{J}(\chi)$ is continuous from $(X(D), \delta_{1+\varepsilon})$ into $\mathbf{R}$ and the result follows from Theorem 2.25. □

Remark 5.8. *If we replace the perimeter by the Gagliardo semi-norm $P^{\bar{s}}_D(\cdot) = |\cdot|_{W^s_p}$, we obtain with Theorem 2.29 optimal sets in $\mathfrak{W}^{\bar{s}}(D)$, where $\bar{s} := ps$.*

5.2.5 Shape derivatives

In this section we utilise Theorem 4.2 to prove the shape differentiability of the cost function $J(\Omega) := \hat{J}(\chi_\Omega)$, where $\hat{J}$ is given by (5.15).

THEOREM 5.9. *Let $\Omega \subset D$ be an open set. Then the shape derivative of (5.21) exists for all $\theta \in C^2_c(D, \mathbf{R}^d)$ and is given by*

$$\begin{aligned} dJ(\Omega)[\theta] = & \int_D \operatorname{div}(\theta) A_\chi \varepsilon(\mathbf{u}) : \varepsilon(\boldsymbol{p})\, dx - \int_D A_\chi \mathcal{S}(\partial \mathbf{u}\, \partial\theta) : \varepsilon(\boldsymbol{p})\, dx \\ & - \int_D A_\chi \varepsilon(\mathbf{u}) : \mathcal{S}(\partial \boldsymbol{p}\, \partial\theta)\, dx + \int_D \beta_\chi \operatorname{div}(\theta) \operatorname{div}(\boldsymbol{p})\, dx \\ & - \int_D \beta_\chi (\partial\theta)^\top : \partial\boldsymbol{p}\, dx + \alpha \int_\Gamma \operatorname{div}_\Gamma(\theta)\; ds, \end{aligned}$$

where $\mathcal{S}(A) := \frac{1}{2}(A + A^\top)$. If the interface Γ is C^2, we obtain the following formula ($\theta_n := \theta \cdot n$)

$$\begin{aligned} dJ(\Omega)[\theta] = & \int_\Gamma [A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I) : \varepsilon(\boldsymbol{p})]_\Gamma\, \theta_n\, ds - \int_\Gamma [A_\chi \varepsilon(\boldsymbol{p}) n \cdot \partial_n \mathbf{u}]_\Gamma\, \theta_n\, ds \\ & - \int_\Gamma \left[(A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I) n) \cdot \partial_n \boldsymbol{p}\right]_\Gamma \theta_n\, ds + \alpha \int_\Gamma \kappa\, \theta_n\, ds. \end{aligned} \tag{5.20}$$

Here, $\mathbf{u}$ is the solution of the state equation (5.17) and $\boldsymbol{p} \in H^1_{\Sigma_0}(D; \mathbf{R}^d)$ solves the following adjoint state equation

$$a_\chi(\boldsymbol{\varphi}, \boldsymbol{p}) + 2\int_{\tilde{\Sigma}} (\mathbf{u}^+ - \mathbf{u}_d)\boldsymbol{\varphi}^+\, ds = 0, \quad \text{for all } \boldsymbol{\varphi} \in H^1_{\Sigma_0}(D; \mathbf{R}^d).$$

Proof. For the further considerations we introduce

$$J(\Omega, \boldsymbol{\varphi}) := \int_{\tilde{\Sigma}} |\boldsymbol{\varphi} - \mathbf{u}_d|^2\, ds + \alpha P_D(\Omega). \tag{5.21}$$

Since the perimeter is shape differentiable, we set $\alpha = 0$ in the following. Note that $\hat{J}(\Omega) = J(\Omega, \mathbf{u}(\Omega))$ for the solution $\mathbf{u} = \mathbf{u}(\Omega)$ of (5.17). Let

$$\mathcal{L}(\Omega, \boldsymbol{\varphi}, \boldsymbol{\psi}) := J(\Omega, \boldsymbol{\varphi}) + a_\chi(\boldsymbol{\varphi}, \boldsymbol{\psi}) - \int_D \beta_\chi \operatorname{div}(\boldsymbol{\psi})\, dx$$

be the associated Lagrangian of the minimisation problem. We are going to apply Theorem 4.2 to the function $G(t, \boldsymbol{\varphi}, \boldsymbol{\psi}) := \mathcal{L}(\Phi_t(\Omega), \boldsymbol{\varphi} \circ \Phi_t^{-1}, \boldsymbol{\psi} \circ \Phi_t^{-1})$ with $E = F = H^1_{\Sigma_0}(D; \mathbf{R}^d)$. The function G reads explicitly

$$\begin{aligned} G(t, \boldsymbol{\varphi}, \boldsymbol{\psi}) = & \int_{\tilde{\Sigma}} |\boldsymbol{\varphi}^- - \mathbf{u}_d|^2\, ds + \int_D \xi(t) A_\chi \mathcal{S}(\partial\boldsymbol{\varphi}\, C(t)) : \mathcal{S}(\partial\boldsymbol{\psi}\, B^*(t))\, dx \\ & + \int_D \beta_\chi B^*(t) : \partial\boldsymbol{\psi}\, dx. \end{aligned}$$

(H0) & (H1) The function G is C^1 with respect to t and C^∞ (in the sense of Fréchet) with respect to the other arguments. The derivative of G with respect to t reads

$$
\begin{aligned}
\partial_t G(t,\boldsymbol{\varphi},\boldsymbol{\psi}) = &\int_D \xi(t)\,\mathrm{div}\,(\theta^t) A_\chi \mathcal{S}(\partial\boldsymbol{\varphi}\, C(t)) : \mathcal{S}(\partial\boldsymbol{\psi}\, C(t))\, dx \\
&- \int_D \xi(t) A_\chi \mathcal{S}(\partial\boldsymbol{\varphi} C(t)\partial\theta^t C(t)) : \mathcal{S}(\partial\boldsymbol{\psi} C(t))\, dx \\
&- \int_D \xi(t) A_\chi \mathcal{S}(\partial\boldsymbol{\varphi} C(t)) : \mathcal{S}(\partial\boldsymbol{\psi} C(t)\partial\theta(t) C(t))\, dx \\
&+ \int_D \xi(t)\,\mathrm{div}\,(\theta^t)\beta_\chi (\partial\Phi_t)^\top : \partial\boldsymbol{\psi}\, dx \\
&+ \int_D \xi(t)\beta_\chi (\partial\Phi_t)^{-\top}(\partial\theta^t)^\top (\partial\Phi_t)^\top : \partial\boldsymbol{\psi}\, dx
\end{aligned}
$$

where we use the notation $\theta^t := \theta(\Phi_t(x))$. By the choice of $\theta \in C^2_c(D,\mathbf{R}^d)$ we have that $t \mapsto \theta(\Phi_t(x))$, $t \mapsto \partial\theta(t)$, $t \mapsto \partial\Phi_t(x)$ and $t \mapsto (\partial\Phi_t(x))^{-1}$ are continuous on the interval $[0,\tau]$.
(H2) Note that $(\mathbf{u}^t, \boldsymbol{p}^t) \in X(t) \times Y(t,\mathbf{u}^t,\mathbf{u})$ if and only if

$$
\begin{aligned}
d_{\boldsymbol{\psi}} G(t,\mathbf{u}^t,\boldsymbol{p}^t;\hat{\boldsymbol{\psi}}) = 0 &\quad \text{for all } \hat{\boldsymbol{\psi}} \in H^1_{\Sigma_0}(D;\mathbf{R}^d) \\
\int_0^1 d_{\boldsymbol{\varphi}} G(t, s\mathbf{u}^t + (1-s)\mathbf{u}, \boldsymbol{p}^t;\hat{\boldsymbol{\varphi}})\, ds = 0 &\quad \text{for all } \hat{\boldsymbol{\varphi}} \in H^1_{\Sigma_0}(D;\mathbf{R}^d)
\end{aligned}
$$

which is nothing but

$$
\begin{aligned}
a^t(\mathbf{u}^t,\hat{\boldsymbol{\psi}}) = b^t(\boldsymbol{\psi}) &\quad \text{for all } \hat{\boldsymbol{\psi}} \in H^1_{\Sigma_0}(D;\mathbf{R}^d) \\
a^t(\hat{\boldsymbol{\varphi}},\boldsymbol{p}^t) = \bar{b}^t(\hat{\boldsymbol{\varphi}}) &\quad \text{for all } \hat{\boldsymbol{\varphi}} \in H^1_{\Sigma_0}(D;\mathbf{R}^d),
\end{aligned}
\tag{5.22}
$$

where we introduced

$$
\bar{b}^t(\boldsymbol{\psi}) := -\int_D \xi(t)(\mathbf{u}^t + \mathbf{u} - 2\mathbf{u}^t_d)\boldsymbol{\psi}\, dx.
$$

Note that since $\mathrm{supp}(\theta) \subset D$ is compactly contained in D we have that Φ_t equals the identity near the boundary and therefore the integral $\int_{\tilde{\Sigma}}(\boldsymbol{\varphi}-\mathbf{u}_d)\boldsymbol{\varphi}^-\, ds$ is independent of t. It is easily checked that the equations (5.22) admit a unique solution.
(H3) Inserting $\boldsymbol{\psi} = \boldsymbol{p}^t$ as test function in (5.22), we obtain by using Hölder's inequality $\|\boldsymbol{p}_t\|_{H^1(D)} \le c$ for all $t \in [0,\tau]$ and thus for every sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ as $n \to \infty$, we get $\boldsymbol{p}^{t_n} \rightharpoonup \boldsymbol{q}$ as $n \to \infty$. Taking into account Lemma 2.16 and Lemma 5.5 we may pass to the limit in (5.22) and obtain by uniqueness $\boldsymbol{p}^{t_n} \rightharpoonup \boldsymbol{p}$, where $\boldsymbol{p}$ solves

$$
a(\boldsymbol{\varphi},\boldsymbol{p}) = -\int_{\tilde{\Sigma}} 2(\mathbf{u}-\mathbf{u}_d)\boldsymbol{\varphi}\, dx \quad \text{for all } \boldsymbol{\varphi} \in H^1_{\Sigma_0}(D;\mathbf{R}^d). \tag{5.23}
$$

By testing the adjoint equation (5.23) with appropriate functions, we get the strong formulation

$$
\boxed{
\begin{aligned}
-\mathrm{div}\,(A_1\varepsilon(\boldsymbol{p}^+)) = 0 &\quad \text{in } \Omega^+ \\
-\mathrm{div}\,(A_2\varepsilon(\boldsymbol{p}^-)) = 0 &\quad \text{in } \Omega^- \\
-A_2\varepsilon(\boldsymbol{p}^-)n_D = -2(\mathbf{u}^- - \mathbf{u}_d) &\quad \text{on } \Sigma \\
\boldsymbol{p}^- = 0 &\quad \text{on } \Sigma_0 \\
-A_2\varepsilon(\boldsymbol{p}^-)n_D = 0 &\quad \text{on } \partial D \setminus (\Sigma \cup \Sigma_0)
\end{aligned}
}
$$

complemented by the transmission conditions

$$
\boxed{A_1\varepsilon(\boldsymbol{p}^+)n = A_2\varepsilon(\boldsymbol{p}^-)n \quad \text{and} \quad \boldsymbol{p}^+ = \boldsymbol{p}^- \quad \text{on } \Gamma.} \tag{5.24}
$$

The previous considerations show that $\lim_{t\searrow 0}\partial_t G(t,\mathbf{u},\boldsymbol{p}^t) = \partial_t G(0,\mathbf{u},\boldsymbol{p})$, and therefore (H3) is satisfied. Therefore, we may apply Theorem 4.2 and we obtain the shape differentiability of J. $\square$

5.2.6 Boundary integrals

In order to derive the boundary expression of $dJ(\Omega)[\theta]$, we differentiate the function $j(t) = \mathcal{L}(\Omega_t, \boldsymbol{\varphi}\circ\Phi_t^{-1}, \boldsymbol{\psi}\circ\Phi_t^{-1})$, where $\boldsymbol{\varphi},\boldsymbol{\psi}\in H^1_{\Sigma_0}(D;\mathbf{R}^d)$. We have

$$
\begin{aligned}
j(t) :=& \frac{1}{2}\int_{\tilde\Sigma}\|\boldsymbol{\varphi}^{t,-}-\mathbf{u}_d\|^2\,ds + \int_{\Omega_t} A_1\varepsilon(\boldsymbol{\varphi}^{t,+}) : \varepsilon(\boldsymbol{\psi}^{t,+})\,dx + \int_{\Phi_t(D\setminus\overline{\Omega})} A_2\varepsilon(\boldsymbol{\varphi}^{t,-}) : \varepsilon(\boldsymbol{\psi}^{t,-})\,dx \\
&- \beta_1\int_{\Omega_t}\operatorname{div}(\boldsymbol{\psi}^{t,+})\,dx - \beta_2\int_{\Phi_t(D\setminus\overline{\Omega})}\operatorname{div}(\boldsymbol{\psi}^{t,-})\,dx + \alpha P_D(\Omega_t).
\end{aligned}
$$

Due to the mixed boundary conditions we have just $\mathbf{u}^-,\boldsymbol{p}^-\in H^2_{loc}(D\setminus\overline{\Omega};\mathbf{R}^d)$ and $\mathbf{u}^+,\boldsymbol{p}^+\in\mathcal{H}^2(\Omega;\mathbf{R}^d)$. Thus the only problematic terms could be the integrals over $\Phi_t(D\setminus\overline{\Omega})$. However, since $\operatorname{supp}(\theta)\subset D$, Φ_t is the identity in the vicinity of ∂D, hence these terms give no contribution to the derivative. We define $\hat\Omega = \operatorname{supp}(\theta)\cap(D\setminus\Omega)$ and apply the transport theorem to obtain $j'(0) = dJ(\Omega)[\theta]$ with

$$
\begin{aligned}
dJ(\Omega)[\theta] = &\sum_{\varsigma\in\{+,-\}}\int_{\Omega^\varsigma} A_\varsigma\varepsilon(\mathring{\mathbf{u}}^\varsigma) : \varepsilon(\boldsymbol{p}^\varsigma) + A_\varsigma\varepsilon(\mathbf{u}^\varsigma) : \varepsilon(\mathring{\boldsymbol{p}}^\varsigma)\,dx \\
&+ \int_\Gamma \left[(A_\chi(\varepsilon(\mathbf{u})-\delta_\chi I) : \varepsilon(\boldsymbol{p})\right])\,\theta_n\,ds + \int_\Gamma \kappa\,\theta_n\,ds,
\end{aligned}
\tag{5.25}
$$

where we used the definitions $\mathring{\mathbf{u}}^i = \frac{d}{dt}(\mathbf{u}^i\circ\Phi_t^{-1})_{t=0} = -\partial\mathbf{u}^i\cdot\theta$ and $\mathring{\boldsymbol{p}}^i = \frac{d}{dt}(\boldsymbol{p}^i\circ\Phi_t^{-1})_{t=0} = -\partial\boldsymbol{p}^i\cdot\theta$ $(i\in\{+,-\})$. We defined δ_i by $\beta_i I = \delta_i A_i I$ for $i=1,2$. The last line in (5.25) has already the right form but the other terms are still volume integrals. From now on we use the fact that $\mathbf{u}^i,\boldsymbol{p}^i\in\mathcal{H}^2_{loc}(\Omega_i;\mathbf{R}^d)$ $(i\in\{+,-\})$ at least and they satisfy the equations in the strong sense. We start with the first and second line in (5.25) by applying Gauss and using that $\mathbf{u}^i,\boldsymbol{p}^i$ are strong solutions in the respective domains $(i=1,2)$

$$
\int_{\Omega^i} A_i(\varepsilon(\mathbf{u}^i)-\delta_i I) : \varepsilon(\mathring{\boldsymbol{p}}^i)\,dx = -\int_\Gamma A_i(\varepsilon(\mathbf{u}^i)-\delta_i I)\,\mathring{\boldsymbol{p}}^i\cdot n^i\,ds \tag{5.26}
$$

$$
\int_{\Omega^i} A_i\varepsilon(\mathring{\mathbf{u}}^i) : \varepsilon(\boldsymbol{p}^i)\,dx = -\int_\Gamma (A_i\varepsilon(\boldsymbol{p}^i)\mathring{\mathbf{u}}^i)\cdot n^i\,ds. \tag{5.27}
$$

Therefore using (5.26) and (5.27) in (5.25) we get

$$
\begin{aligned}
dJ(\Omega)[\theta] = &\int_\Gamma \left[(A_\chi(\varepsilon(\mathbf{u})-\delta_\chi I) : \varepsilon(\boldsymbol{p})\right]_\Gamma \theta_n\,ds + \int_\Gamma \kappa\,\theta_n\,ds \\
&+ \sum_{\varsigma\in\{+,-\}}\int_\Gamma A_\varsigma(\varepsilon(\mathbf{u}^\varsigma)-\delta_\varsigma I)\mathring{\boldsymbol{p}}^\varsigma\cdot n^\varsigma + (A_\varsigma\varepsilon(\boldsymbol{p}^\varsigma)\mathring{\mathbf{u}}^\varsigma)\cdot n^\varsigma\,ds
\end{aligned}
$$

The last two lines are not following the structure theorem, but we can rewrite this by decomposing $\partial\mathbf{u}|_\Gamma = \partial_\Gamma\mathbf{u} + (\partial_n\mathbf{u})\otimes n$ into normal and tangential part. We have $((\partial_n\mathbf{u})\otimes n)n = \partial_n\mathbf{u}$ and $((\partial_n\mathbf{u})\otimes n)T = 0$. Here n is the normal vector along Γ and T such that $n\cdot T = 0$. Similarly, we define $\theta_\Gamma := \theta - \theta_n n$, where $\theta_n = \theta\cdot n$. We have on Γ:

$\mathring{\mathbf{u}}_i = -\partial_\Gamma \mathbf{u}^i\,\theta_\Gamma - \theta_n\,\partial_n \mathbf{u}^i$ and $\mathring{\boldsymbol{p}}_i = -\partial_\Gamma \boldsymbol{p}^i\,\theta_\Gamma - \theta_n\,\partial_n \boldsymbol{p}^i$, and thus we conclude (note that from $\mathbf{u}^+ = \mathbf{u}^-$ it follows $\partial_\Gamma \mathbf{u}^+ = \partial_\Gamma \mathbf{u}^-$)

$$\sum_{\varsigma\in\{+,-\}} \int_\Gamma A_\varsigma(\varepsilon(\mathbf{u}^\varsigma) - \delta_\varsigma I)\mathring{\boldsymbol{p}}^\varsigma \cdot n^\varsigma\, ds = -\sum_{\varsigma\in\{+,-\}} \int_\Gamma A_\varsigma(\varepsilon(\mathbf{u}^\varsigma) - \delta_\varsigma I)n^\varsigma) \cdot \partial_n \boldsymbol{p}^\varsigma \theta_n^\varsigma\, ds$$
$$-\int_\Gamma \underbrace{\big[(A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I)n))\big]_\Gamma}_{=0 \text{ cf. },(5.14)} \cdot (\partial_\Gamma \boldsymbol{p}\theta_\Gamma)\, ds = -\int_\Gamma \big[A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I)n) \cdot \partial_n \boldsymbol{p}\big]_\Gamma \theta_n\, ds,$$

and similarly using (5.24)

$$\sum_{\varsigma\in\{+,-\}} \int_\Gamma (A_\varsigma \varepsilon(\boldsymbol{p}^\varsigma)\mathring{\mathbf{u}}^\varsigma) \cdot n^\varsigma\, ds = -\int_\Gamma \big[(A_\chi \varepsilon(\boldsymbol{p})n) \cdot \partial_n \mathbf{u}\big]_\Gamma \theta_n\, ds.$$

Thus we obtain the formula (5.20).

Remark 5.10. *Note that* (5.20) *can be rewritten as*

$$dJ(\Omega)[\theta] = \int_\Gamma \left([A_\chi \varepsilon(\mathbf{u}) : \varepsilon(\boldsymbol{p})]_\Gamma - [(A_\chi \varepsilon(\mathbf{u}))n \cdot \partial_n \boldsymbol{p}]_\Gamma - [(A_\chi \varepsilon(\boldsymbol{p}))n \cdot \partial_n \mathbf{u}]_\Gamma\right) \theta_n\, ds$$
$$+[\beta]_\Gamma \int_\Gamma \operatorname{div}_\Gamma(\boldsymbol{p})\,\theta_n\, ds + \int_\Gamma \kappa\,\theta_n\, ds.$$

It is interesting to compare this expression with formula (4.1) in [16], where a phase fields approach is used and the formal sharp limit of the optimality conditions is derived. They derived for the optimal set Ω^+ on the interface $\Gamma := \partial\Omega^+$ the condition

$$0 = \gamma\kappa\sigma - [A\varepsilon(\mathbf{u}) : \varepsilon(\boldsymbol{p})]_\Gamma + [A\varepsilon(\mathbf{u})n \cdot \partial_n \boldsymbol{p}]_\Gamma + [A\varepsilon(\boldsymbol{p})n \cdot \partial_n \mathbf{u}]_\Gamma + \lambda_1 - \lambda_2$$

The constants $\lambda_1 = |\Omega^+|, \lambda_2 = |\Omega^-|$ arise from a volume constraint and would occur in our derivative if we had a term of the form $\int_{\Omega^+} \lambda_1\, dx + \int_{\Omega^-} \lambda_2\, dx$ in the cost function. Here, γ, σ are real numbers.

Lemma 5.11. *In the case $A := A_1 = A_2$ we have $\boldsymbol{p} \in H^2(K; R^d)$ for each $K \Subset D$ and the shape derivative* (5.20) *reduces to*

$$dJ(\Omega)[\theta] = (\beta_2 - \beta_1) \int_\Gamma \operatorname{div}(\boldsymbol{p})\,\theta_n\, ds.$$

Proof. Since $A := A_1 = A_2$ the adjoint $\boldsymbol{p}$ is more regular across the interface, i.e. $\partial \boldsymbol{p}^+ = \partial \boldsymbol{p}^-$ on Γ and in particular $\partial_n \boldsymbol{p}^+ = \partial_n \boldsymbol{p}^-$. Using the transmission condition (5.14), we get

$$\big[(A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I)n) \cdot \partial_n \boldsymbol{p}\big]_\Gamma = \big[(A_\chi(\varepsilon(\mathbf{u}) - \delta_\chi I)n)\big]_\Gamma \cdot \partial_n \boldsymbol{p} = 0$$

Moreover, for the remaining terms in (5.20)

$$\begin{aligned} \big[A(\varepsilon(\mathbf{u}) - \delta_\chi I) : \varepsilon(\boldsymbol{p})\big]_\Gamma &= \big[A(\varepsilon(\mathbf{u})) : \varepsilon(\boldsymbol{p})\big]_\Gamma - \big[\beta_\chi\big]_\Gamma \operatorname{div} \boldsymbol{p} \\ \big[A\varepsilon(\mathbf{u}) : \varepsilon(\boldsymbol{p})\big]_\Gamma &= \big[\partial_\Gamma \mathbf{u}\big]_\Gamma : A\varepsilon(\boldsymbol{p}) + \big[\partial_n \mathbf{u}\big] \otimes n : A\varepsilon(\boldsymbol{p}) \end{aligned} \tag{5.28}$$

since $\partial_\Gamma \mathbf{u}^+ = \partial_\Gamma \mathbf{u}^-$ on Γ. Note we have for all $v, w \in \mathbf{R}^d$ and all $B \in \mathbf{R}^{d,d}$ the identity $v \otimes w : B = Bw \cdot v$ and thus

$$\big[A\varepsilon(\mathbf{u}) : \varepsilon(\boldsymbol{p})\big]_\Gamma = A\varepsilon(\boldsymbol{p})n \cdot \big[\partial_n \mathbf{u}\big]_\Gamma. \tag{5.29}$$

Inserting (5.28) and (5.29) in (5.20) gives the desired formula. □

5.3 Electrical impedance tomography

We consider an application to a typical and important interface problem: the inverse problem of electrical impedance tomography (EIT) also known as the inverse conductivity or Calderón's problem [21] in the mathematical literature. It is an active field of research with an extensive literature; cf. the survey papers [18, 27] as well as [75] and the references therein. We consider the particular case where the goal is to reconstruct a piecewise constant conductivity σ which amounts to determine an interface Γ between some inclusions and the background. We refer the reader to [28, 54, 55, 63] for more details on this approach.

5.3.1 The problem setting

Subsequently, we use the same notations and setting as in Assumption 5.3 of Subsection 5.2.1. Let $\sigma = \sigma^+\chi_{\Omega^+} + \sigma^-\chi_{\Omega^-}$ where $\sigma^\pm$ are constants and $f = f^+\chi_{\Omega^+} + f^-\chi_{\Omega^-}$ where $f^+ \in H^1(\Omega^+), f^- \in H^1(\Omega^-)$. Consider the variational problems: find $u_N \in H^1_{\Sigma_0}(D)$ and $u_D \in H^1_{\Sigma_0,\Sigma_N}(D)$ such that

$$\int_D \sigma\nabla u_N \cdot \nabla z\, dx = \int_D fz + \int_{\Sigma_N} gz\, dx \quad \text{for all} \quad z \in H^1_{\Sigma_0}(D) \tag{5.30}$$

$$\int_D \sigma\nabla u_D \cdot \nabla z\, dx = \int_D fz\, dx \quad \text{for all} \quad z \in H^1_0(D) \tag{5.31}$$

where

$$\begin{aligned} H^1_{\Sigma_0}(D) &:= \{v \in H^1(D) \mid v = 0 \text{ on } \Sigma_0\}, \\ H^1_{\Sigma_0,\Sigma_N}(D) &:= \{v \in H^1(D) \mid v = 0 \text{ on } \Sigma_0 \text{ and } v = h \text{ on } \Sigma_N\}, \\ H^1_0(D) &:= \{v \in H^1(D) \mid v = 0 \text{ on } \Sigma\} \end{aligned}$$

and $g \in H^{-1/2}(\Sigma_N)$ represents the *input*, in this case the electric current applied on the boundary and $h \in H^{1/2}(\Sigma_N)$ is the *measurement* of the potential on Σ_N, or the other way around, i.e. h can be the input and g the measurement. Notice that u_N and u_D depend on χ_{Ω^+}. Define the space of piecewise Sobolev functions on D

$$PH^k(D) := \{u = u^+\chi_{\Omega^+} + u^-\chi_{\Omega^-} \mid u^+ \in H^k(\Omega^+),\ u^- \in H^k(\Omega^-)\}.$$

Consider the following assumption:

Assumption 5.12. *The domains D, Ω^+, Ω^- are of class C^k, $f \in PH^{\max(k-2,1)}(D)$, $g \in H^{k-\frac{3}{2}}(D)$ and $h \in H^{k-\frac{1}{2}}(D)$ for $k \geq 2$.*

Applying Green's formula under Assumption 5.12, equations (5.30) and (5.31) are equivalent to the following transmission problems where $u_N = u_N^+\chi_{\Omega^+} + u_N^-\chi_{\Omega^-}$ and $u_D = u_D^+\chi_{\Omega^+} + u_D^-\chi_{\Omega^-}$:

$$\boxed{\begin{aligned} -\sigma^+\Delta u_N^+ &= f \quad \text{in } \Omega^+ \quad -\sigma^-\Delta u_N^- = f \quad \text{in } \Omega^- && (5.32)\\ u_N^- &= 0 \quad \text{on } \Sigma_0 && (5.33)\\ \sigma^-\partial_n u_N^- &= g \quad \text{on } \Sigma_N + && (5.34) \end{aligned}}$$

$$\boxed{\begin{aligned} -\sigma^+\Delta u_D^+ &= f \quad \text{in } \Omega^+ \quad -\sigma^-\Delta u_D^- = f \quad \text{in } \Omega^- && (5.35)\\ u_D^- &= 0 \quad \text{on } \Sigma_0 \\ u_D^- &= h \quad \text{on } \Sigma_N && (5.36) \end{aligned}}$$

with the transmission conditions

$$\boxed{\begin{array}{rlrl} \sigma^+\partial_n u_N^+ = \sigma^-\partial_n u_N^- & \quad \sigma^+\partial_n u_D^+ = \sigma^-\partial_n u_D^- & \quad \text{on } \Gamma \\ u_N^+ = u_N^- & \quad u_D^+ = u_D^- & \quad \text{on } \Gamma. \end{array}}$$

On Σ_0 we impose homogeneous Dirichlet conditions, meaning that the voltage is fixed and no measurement is performed. One may take $\Sigma_0 = \emptyset$, in which case (5.30) becomes a pure Neumann problem and additional care must be taken for the uniqueness and existence of a solution. The situation $\Sigma_0 \neq \emptyset$ corresponds to partial measurements. Alternatively, it is also possible to consider functions u_N and u_D which have both the boundary conditions (5.34) and (5.36) on different parts of the boundary. Several measurements can be made by choosing a set of functions g or h. The result for several measurements can be straightforwardly deduced from the case of one measurement by summing the cost functions corresponding to each measurement, therefore we stick to the case of one measurement g for simplicity.

The problem of electrical impedance tomography reads:

$$\text{(EIT): Given } \{g_k\}_{k=1}^K \text{ and } \{h_k\}_{k=1}^K, \text{ find } \sigma \text{ such that } u_D = u_N \text{ in } D.$$

Note that $u_N = u_N(\Omega^+)$ and $u_D = u_D(\Omega^+)$ actually depend on Ω^+ through σ, however we often write u_N and u_D for simplicity.

The notion of well-posedness due to Hadamard requires the existence and uniqueness of a solution and the continuity of the inverse mapping. The severe ill-posedness of EIT is well-known: uniqueness and continuity of the inverse mapping depend on the regularity of σ, the latter being responsible for the instability of the reconstruction process. Additionally, partial measurements often encountered in practice render the inverse problem even more ill-posed. We refer to the reviews [18, 27] and the references therein for more details. A standard cure against the ill-posedness is to regularise the inverse mapping. In this example the regularisation is achieved by considering smooth perturbations of the domains Ω^+.

To solve the EIT problem, we use an optimization approach by considering the shape functions

$$\begin{aligned} J_1(\Omega^+) &= \frac{1}{2}\int_D (u_D(\Omega^+) - u_N(\Omega^+))^2\,dx \\ J_2(\Omega^+) &= \frac{1}{2}\int_{\Sigma_N} (u_N(\Omega^+) - h)^2\,ds. \end{aligned} \tag{5.37}$$

Since $u_D, u_N \in H^1(\Omega)$ and $h \in H^{1/2}(\Sigma_N)$, J_1 and J_2 are well-defined. Note that J_1 and J_2 are redundant for the purpose of the reconstruction but our aim is to provide an efficient way of computing the shape derivative of two functions which are often encountered in the literature. To compute these derivatives we follow the new Lagrangian approach from [91]. It is convenient to introduce

$$F_1(\varphi_D, \varphi_N) := \frac{1}{2}\int_D (\varphi_D - \varphi_N)^2\,dx \quad \text{ and } \quad F_2(\varphi_N) := \frac{1}{2}\int_{\Sigma_N} (\varphi_N - h)^2\,ds.$$

Note that $J_1(\Omega^+) = F_1(u_D(\Omega^+), u_N(\Omega^+))$ and $J_2(\Omega^+) = F_2(u_N(\Omega^+))$. Next consider $\Xi \subset 2^D$ and the Lagrangian $\mathcal{L} : \Xi \times H^1_{\Sigma_0} \times H^1_{\Sigma_0} \times H^1_{\Sigma_0} \times H^1_{\Sigma_0} \times H^{1/2}(\Sigma_N) \to \mathbf{R}$ given by

$$\begin{aligned} \mathcal{L}(\Omega^+, \boldsymbol{\varphi}, \boldsymbol{\psi}, \lambda) :=& \alpha_1 F_1(\varphi_D, \varphi_N) + \alpha_2 F_2(\varphi_N) \\ &+ \int_D \sigma\nabla\varphi_D \cdot \nabla\psi_D - f\psi_D + \int_{\Sigma_N} \lambda(\varphi_D - h)\,dx \\ &+ \int_D \sigma\nabla\varphi_N \cdot \nabla\psi_N - f\psi_N - \int_{\Sigma_N} g\psi_N\,dx, \end{aligned}$$

where $\boldsymbol{\varphi} := (\varphi_D, \varphi_N)$ and $\boldsymbol{\psi} := (\psi_D, \psi_N)$. The adjoint variable λ is used to enforce the boundary condition (5.36); see (5.41). Introduce the objective function

$$J(\Omega^+) := \alpha_1 J_1(\Omega^+) + \alpha_2 J_2(\Omega^+). \tag{5.38}$$

Convention. *When we want to make the dependence on the characteristic function explicit, we shall write $J(\Omega^+)$ as $\hat{J}(\chi_{\Omega^+})$.*

In order to compute the shape derivative for this linear transmission problem we shall employ Theorem 4.5, but before this we need some preparations.

5.3.2 State and adjoint equations

Let us denote $\mathbf{u} := (u_D, u_N)$. The equations $\partial_{\psi_D}\mathcal{L}(\Omega^+, \mathbf{u}, 0, \lambda)(\hat{\psi}_D) = 0$ for all $\hat{\psi}_D \in H^1_0(D)$ and $\partial_{\psi_N}\mathcal{L}(\Omega^+, \mathbf{u}, \boldsymbol{p}, \lambda)(\hat{\psi}_N) = 0$, for all $\hat{\psi}_N \in H^1_{\Sigma_0}(D)$ are the variational equations (5.30),(5.31). Under Assumption 5.12, we get $u_D \in PH^k(D)$, $k \geq 2$, and applying Green's formula to (5.31) in Ω^+ and Ω^- separately with $\hat{\psi}^+_D \in C^\infty_c(\Omega^+)$ and $\hat{\psi}^-_D \in C^\infty_c(\Omega^-)$ as test function, respectively, we get back to the strong formulation (5.35). Similarly, assuming $u_N \in PH^k(D)$, $k \geq 2$, yields by using Green's formula that the solution u_N of the previous variational equation is the solution of (5.32) and (5.33).

Now by solving $\partial_\lambda \mathcal{L}(\Omega^+, \mathbf{u}, \boldsymbol{p}, \lambda)(\hat{\lambda}) = 0$ for all $\hat{\lambda} \in H^{1/2}(\Sigma_N)$, we obtain

$$\int_{\Sigma_N} \hat{\lambda}(u_D - h) = 0 \quad \text{ for all } \hat{\lambda} \in H^{1/2}(\Sigma_N),$$

which gives $u_D = h$ and the boundary condition (5.36) is satisfied.

Solving the equation $\partial_{\varphi_D}\mathcal{L}(\Omega^+, \mathbf{u}, \boldsymbol{p}, \lambda)(\hat{\varphi}_D) = 0$, for all $\hat{\varphi}_D \in H^1_{\Sigma_0}(D)$, leads to the variational formulation for the adjoint state p_D, i.e.

$$\alpha_1 \int_D (u_D - u_N)\hat{\varphi}_D \, dx + \int_D \sigma \nabla p_D \cdot \nabla \hat{\varphi}_D \, dx + \int_{\Sigma_N} \lambda \hat{\varphi}_D \, dx = 0 \quad \text{ for all } \hat{\varphi}_D \in H^1_{\Sigma_0}(D)$$

for all $\hat{\varphi}_D \in H^1_{\Sigma_0}(D)$. This yields the following variational formulation when test functions are restricted to $H^1_0(D)$:

$$\alpha_1 \int_D (u_D - u_N)\widetilde{\varphi}_D \, dx + \int_D \sigma \nabla p_D \cdot \nabla \widetilde{\varphi}_D \, dx = 0 \quad \text{ for all } \widetilde{\varphi}_D \in H^1_0(D). \tag{5.39}$$

Under Assumption 5.12, we get $p_D \in PH^k(D)$ and applying Green's formula to the domains Ω^+ and Ω^- separately with test functions $\hat{\varphi}^+_D \in C^\infty_c(\Omega^+)$ and $\hat{\varphi}^-_D \in C^\infty_c(\Omega^-)$, respectively, we obtain

$$-\operatorname{div}(\sigma \nabla p_D) = -\alpha_1(u_D - u_N) \text{ in } \Omega^+ \text{ and } \Omega^-. \tag{5.40}$$

Now using Green's formula in Ω^+ and Ω^- for all $\hat{\varphi}_D \in H^1_{\Sigma_0}(D)$ yields

$$\begin{aligned}
&\int_{\Omega^+ \cup \Omega^-} \alpha_1(u_D - u_N)\hat{\varphi}_D \, dx - \operatorname{div}(\sigma \nabla p_D)\hat{\varphi}_D \, dx \\
&+ \int_\Gamma [\sigma \partial_n p_D]_\Gamma \hat{\varphi}_D \, ds + \int_{\Sigma_N} (\sigma \partial_n p_D + \lambda)\hat{\varphi}_D \, ds = 0.
\end{aligned}$$

where $[\sigma \partial_n p_D]_\Gamma = \sigma^+ \partial_n p^+_D - \sigma^- \partial_n p^-_D$ is the jump of $\sigma \partial_n p_D$ across Γ. Using (5.40), we obtain

$$\begin{aligned}
\lambda &= -\sigma^- \partial_n p_D \quad \text{ on } \Sigma_N \\
p_D &= 0 \quad \text{ on } \Gamma \\
\sigma^+ \partial_n p^+_D &= \sigma^- \partial_n p^-_D \quad \text{ on } \Gamma.
\end{aligned} \tag{5.41}$$

Having determined λ we consider a new Lagrangian, using the same notation for simplicity:

$$\mathcal{L}(\Omega^+, \boldsymbol{\varphi}, \boldsymbol{\psi}) := \mathcal{L}(\Omega^+, \boldsymbol{\varphi}, \boldsymbol{\psi}, -\sigma^- \partial_n \psi_D)$$

for which we have the relation $J(\Omega^+) = \mathcal{L}(\Omega^+, \mathbf{u}, \boldsymbol{\psi})$, for all $\boldsymbol{\psi} \in H^1_{\Sigma_0}(D) \times H^1_{\Sigma_0}(D)$, where $\mathbf{u} = (u_D, u_N)$. Finally solving $\partial_{\varphi_N} \mathcal{L}(\Omega^+, \mathbf{u}, \boldsymbol{p})(\hat{\varphi}_N) = 0$, for all $\hat{\varphi}_N \in H^1_{\Sigma_0}(D)$, leads to the variational formulation

$$\int_D -\alpha_1(\varphi_D - \varphi_N)\hat{\varphi}_N + \sigma \nabla \psi_N \cdot \nabla \hat{\varphi}_N \, dx + \int_{\Sigma_N} \alpha_2(\varphi_N - h)\hat{\varphi}_N \, ds = 0 \tag{5.42}$$

for all $\hat{\varphi}_N \in H^1_{\Sigma_0}(D)$. Under Assumption 5.12, we get $p_N \in PH^k(D)$, $k \geq 2$, and again applying Green's formula to Ω^+ and Ω^- separately with $\hat{\varphi}_N^+ \in C_c^\infty(\Omega^+)$ and $\hat{\varphi}_N^- \in C_c^\infty(\Omega^-)$ as test function, respectively, we obtain

$$-\operatorname{div}(\sigma \nabla p_N) = \alpha_1(u_D - u_N) \quad \text{ in } \Omega^+ \cup \Omega^-.$$

Using Green's formula in Ω^+ and Ω^- for all $\hat{\varphi}_N \in H^1_{\Sigma_0}(D)$ and $\varphi_N = 0$ on Σ_0 yields

$$\begin{aligned} &\int_{\Omega^+ \cup \Omega^-} -\alpha_1(u_D - u_N)\hat{\varphi}_N - \operatorname{div}(\sigma \nabla p_N)\hat{\varphi}_N \, dx \\ &+ \int_\Gamma [\sigma \partial_n p_N]_\Gamma \, dx + \int_{\Sigma_N} (\sigma \partial_n p_N + \alpha_2(u_N - h))\hat{\varphi}_N \, ds = 0. \end{aligned}$$

This gives the boundary conditions for the adjoint:

$$\begin{aligned} \sigma \partial_n p_N &= -\alpha_2(u_N - h) \text{ on } \Sigma_N \\ p_N &= 0 \text{ on } \Sigma_0 \end{aligned}$$

with the transmission conditions $\sigma^+ \partial_n p_N^+ = \sigma^- \partial_n p_N^-$ and $p_N^+ = p_N^-$ on Γ. Summarizing, under Assumption 5.12, we obtain the system for p_N:

$$\boxed{\begin{array}{llll} -\sigma^+ \Delta p_N^+ = \alpha_1(u_D^+ - u_N^+) & \text{in } \Omega^+ & -\sigma^- \Delta p_N^- = \alpha_1(u_D^- - u_N^-) & \text{in } \Omega^- \\ \sigma^- \partial_n p_N^- = -\alpha_2(u_N^- - h^-) & \text{on } \Sigma_N & & \\ p_N^- = 0 & \text{on } \Sigma_0 & & \\ p_N^+ = p_N^- \text{ on } \Gamma & & \sigma^+ \partial_n p_N^+ = \sigma^- \partial_n p_N^- \text{ on } \Gamma & \end{array}}$$

5.3.3 Existence of optimal shapes

We would like to study the minimisation of J given by (5.38) with the penalisation methods introduced in Section 2.4. In a similar fashion as Lemma 5.5, we may prove the following.

Lemma 5.13. *Denote by u_D resp. u_N the weak solution of (5.31) resp. (5.30). There exist constants $c_1, c_2 > 0$ such that*

$$\begin{aligned} \forall \chi_1, \chi_2 \in X(D) : \|u_D(\chi_1) - u_D(\chi_2)\|_{H^1(D)} &\leq c_1 \|\chi_1 - \chi_2\|_{L_2(D)}, \\ \|u_N(\chi_1) - u_N(\chi_2)\|_{H^1(D)} &\leq c_2 \|\chi_1 - \chi_2\|_{L_2(D)}. \end{aligned}$$

Proof. The result may be derived in the same manner as Lemma 5.5. Compare also the proof of Lemma 5.21. □

Corollary 5.14. *Let J be given by (5.38) and $\omega_0 \subset D$ and open and smooth subset. Let $p \in (1,\infty), 0 < s < 1/p, \alpha > 0$ and $\bar s := sp$. Then we define the cost functions*

$$\begin{aligned}\mathcal{J}_1(\chi_\Omega) &:= \hat J(\chi_\Omega) + \alpha \hat P_D^{\bar s}(\chi_\Omega)\\ \mathcal{J}_2(\chi_\Omega) &:= \hat J(\chi_\Omega) + \alpha \hat P_D(\chi_\Omega)\end{aligned}$$

Then the following minimisation problems have at least one solution

$$\min_{\chi\in\mathfrak{B}(D)} \mathcal{J}_1(\chi), \qquad \min_{\chi\in\mathfrak{W}^{\bar s}(D)} \mathcal{J}_2(\chi).$$

Proof. This is an easy consequence of Theorems 2.25,2.29. □

5.3.4 Shape derivatives

Let us consider a transformation Φ_t^θ defined by $\theta \in C_c^1(D,\mathbf{R}^d)$. We use the notation $\Omega_t^+ := \Phi_t^\theta(\Omega^+)$. Our aim is to show the shape differentiability of $J(\Omega^+)$ with the help of Theorem 4.2. For this purpose, introduce

$$G(t,\boldsymbol{\varphi},\boldsymbol{\psi}) := \mathcal{L}(\Omega_t^+, \boldsymbol{\varphi}\circ\Phi_t^{-1}, \boldsymbol{\psi}\circ\Phi_t^{-1}),$$

which reads after the change of variables $\Phi_t(x) = y$

$$\begin{aligned} G(t,\boldsymbol{\varphi},\boldsymbol{\psi}) =& \frac{\alpha_1}{2}\int_D (\varphi_D - \varphi_N)^2 \xi(t)\,dx + \frac{\alpha_2}{2}\int_{\Sigma_N} (\varphi_N - h)^2\,ds\\ &+ \int_D \sigma A(t)\nabla\varphi_D\cdot\nabla\psi_D - f\circ\Phi_t\psi_D\xi(t)\,dx - \int_{\Sigma_N} g\psi_N\,ds\\ &+ \int_D \sigma A(t)\nabla\varphi_N\cdot\nabla\psi_N - f\circ\Phi_t\psi_N\xi(t)\,dx - \int_{\Sigma_N}\sigma^{-1}\partial_n\psi_D(\varphi_D - h)\,ds,\end{aligned} \tag{5.43}$$

where the Jacobian $\xi(t)$ and $A(t)$ are as before. In the previous expression (5.43), one should note that the integrals on Γ are unchanged since $\Phi_t^{-1} = I$ on Γ. Thus we have $\Phi_t^\theta(\Omega) = \Omega$, however the terms inside the integrals on Ω are modified by the change of variable since $\Phi_t^{-1} \neq I$ inside Ω. Note that

$$J(\Omega_t^+) = G(t,\mathbf{u}^t,\boldsymbol{\psi}),\ \text{ for all } \boldsymbol{\psi}\in H^1_{\Sigma_0}(D)\times H^1_{\Sigma_0}(D),$$

where $\mathbf{u}^t = (u_N^t, u_D^t) := (u_{N,t}\circ\Phi_t, u_{D,t}\circ\Phi_t)$ and $u_{N,t}, u_{D,t}$ solve (5.30),(5.31), respectively, with the domain Ω^+ replaced by Ω_t^+. As one can verify by applying a change of variables to (5.30) and (5.31) on the domain Ω_t^+ the functions u_N^t, u_D^t satisfy

$$\int_D \sigma A(t)\nabla u_N^t\cdot\nabla\hat\psi_N\,dx = \int_D f\hat\psi_N\,dx + \int_{\Sigma_N} g\hat\psi_N\,dx \quad \text{for all } \hat\psi_N\in H^1_{\Sigma_0}(D) \tag{5.44}$$

and

$$\int_D \sigma A(t)\nabla u_D^t\cdot\nabla\hat\psi_D\,dx = \int_D f\hat\psi_D\,dx \quad \text{for all } \hat\psi_D\in H^1_0(D) \tag{5.45}$$

Testing equation (5.44) with $\hat\psi_D = u_D^t$ and equation (5.45) with $\hat\psi_N = u_N^t$, we infer the existence of constants $C_1, C_2 > 0$ and $\tau > 0$ such that for all $t\in[0,\tau]$:

$$\|u_D^t\|_{H^1(D)} \le C_1 \quad\text{and}\quad \|u_N^t\|_{H^1(D)} \le C_2. \tag{5.46}$$

From these estimates, we get $u_D^t \rightharpoonup w_1$ and $u_N^t \rightharpoonup w_2$ in $H^1(\Omega)$ as $t \to 0$. Passing to the limit in (5.44) and (5.45) yields $w_1 = u_D$ and $w_2 = u_N$ by uniqueness.

Let us now check the conditions (D0)-(D3) of Theorem 4.5 for the function G given by (5.43) and the Banach spaces $E_1 = F_1 = E_2 = F_2 = H^1_{\Sigma_0}(D)$.

(D0)&(D1) These conditions are automatically satisfied by construction since the function G is affine linear with respect to φ_D and φ_N, and linear with respect to ψ_D and ψ_N. Moreover, it is clear that this function is differentiable with respect to the variable t.

(D3) Note that $\mathbf{E}(t) = \{\mathbf{u}^t = (u_N^t, u_D^t)\}$. We have $\boldsymbol{p}^t = (p_N^t, p_D^t) \in \mathbf{Y}(t, \mathbf{u}^t, \mathbf{u}^0)$ if and only if they solve

$$\int_D \sigma A(t)\nabla p_D^t \cdot \nabla \hat{\varphi}_D \, dx + \alpha_1 \int_D \xi(t)(u_D^t + u_D - u_N^t)\hat{\varphi}_D + \int_{\Sigma_N} \partial_n p_D^t \hat{\varphi}_D \, dx = 0, \tag{5.47}$$

$$\int_D \sigma A(t)\nabla p_N^t \cdot \nabla \hat{\varphi}_N \, dx - \alpha_1 \int_D \xi(t)(u_D - (u_N^t + u_N))\hat{\varphi}_N \, dx \tag{5.48}$$
$$+ \alpha_2 \int_{\Sigma_N} (u_N - h)\partial_n \hat{\varphi}_N \, ds = 0$$

for all $\hat{\varphi}_D$, $\hat{\varphi}_N$ in $H^1_{\Sigma_0}(D)$. Thanks to the Lax-Milgram's lemma, we check that both equations (5.47) and (5.48) have a unique solution. Testing (5.47) with $\hat{\varphi}_D = p_D^t$ and (5.48) with $\hat{\varphi}_N = p_N^t$, we conclude by an application of Hölder's inequality together with (5.46) the existence of constants C_1, C_2 and $\tau > 0$ such that for all $t \in [0, \tau] : \ \|p_D^t\|_{H^1(D)} \le C_1$ and $\|p_N^t\|_{H^1(D)} \le C_2$. We get $p_D^t \rightharpoonup q_1$ and $p_N^t \rightharpoonup q_2$ for two elements $q_1, q_2 \in H^1(\Omega)$. Passing to the limit in (5.47) and (5.48) yields $q_1 = p_D$ and $q_2 = p_N$ by uniqueness, where p_D and p_N are solutions of the adjoint equations. Finally, differentiating G with respect to t yields

$$\begin{aligned}\partial_t G(t, \boldsymbol{\varphi}, \boldsymbol{\psi}) =& \frac{\alpha_1}{2} \int_D (\varphi_D - \varphi_N)^2 \xi(t) \operatorname{tr}(\partial\theta^t \partial\Phi_t^{-1}) \, dx \\ &+ \int_D \sigma A'(t)\nabla\varphi_D \cdot \nabla\psi_D - f \circ \Phi_t \psi_D \xi(t) \operatorname{tr}(\partial\theta^t \partial\Phi_t^{-1}) - \psi_D \nabla f \circ \Phi_t \cdot \theta_t \xi(t) \, dx \\ &+ \int_D \sigma A'(t)\nabla\varphi_N \cdot \nabla\psi_N - f \circ \Phi_t \psi_N \xi(t) \operatorname{tr}(\partial\theta^t \partial\Phi_t^{-1}) - \psi_N \nabla f \circ \Phi_t \cdot \theta_t \xi(t) \, dx.\end{aligned}$$

where $\theta_t = \theta \circ \Phi_t$. In view of $\theta \in C_c^1(D, \mathbf{R}^d)$, the functions $t \mapsto \partial\theta^t$ and $t \mapsto \operatorname{tr}(\partial\theta^t \Phi_t^{-1})$ are continuous on $[0, T]$. Moreover $\varphi_D, \varphi_N, \psi_D, \psi_N$ are in $H^1(\Omega)$, $f \in PH^1(\Omega)$ so that $\partial_t G(t, \boldsymbol{\varphi}, \boldsymbol{\psi})$ is well-defined for all $t \in [0, T]$. Further it follows from the above formula that $(t, \boldsymbol{\psi}) \mapsto \partial_t G(t, \mathbf{u}^0, \boldsymbol{\psi})$ is weakly continuous and therefore

$$\lim_{\substack{k \to \infty \\ t \searrow 0}} \partial_t G(t, \mathbf{u}^0, \boldsymbol{p}^{n_k}) = \partial_t G(0, \mathbf{u}^0, \boldsymbol{p}^0).$$

Using Theorem 4.5 one concludes

$$dJ(\Omega^+)[\theta] = \frac{d}{dt} G(t, \mathbf{u}^t, \boldsymbol{\psi})|_{t=0} = \partial_t G(0, \mathbf{u}^0, \boldsymbol{p}^0) \ \text{ for all } \boldsymbol{\psi} \in H^1_{\Sigma_0}(D) \times H^1_{\Sigma_0}(D),$$

and therefore we have proven the following Proposition.

Proposition 5.15 (volume expression). *Let $\Omega \subset \mathbf{R}^d$ be a Lipschitz domain, $\theta \in C_c^1(D, \mathbf{R}^d)$, $f \in PH^1(\Omega)$, $g \in H^{-1/2}(\Sigma_N)$, $h \in H^{1/2}(\Sigma_N)$, $\Omega^+ \subset \Omega$ is an open set, then the shape derivative of $J(\Omega^+)$ is given by*

$$\begin{aligned}dJ(\Omega^+)[\theta] = \int_D \Big(\frac{\alpha_1}{2}(u_D - u_N)^2 - f(p_N + p_D)\Big) \operatorname{div}\theta \, dx + \int_D -(p_D + p_N)\nabla f \cdot \theta \, dx \\ + \int_D \sigma A'(0)(\nabla u_D \cdot \nabla p_D + \nabla u_N \cdot \nabla p_N) \, dx,\end{aligned} \tag{5.49}$$

where $A'(0) = (\operatorname{div}\theta)I - \partial\theta^\top - \partial\theta$*,* u_N, u_D *are solutions of the variational inequalities* (5.30),(5.31) *and* p_N, p_D *of* (5.42),(5.39)*.*

It is remarkable that the volume expression of the shape gradient in Proposition 5.15 corresponding to point (i) of Theorem 2.38 has been obtained without any regularity assumption on Ω^+. In order to obtain a boundary expression on the interface Γ as in of Theorem 2.38 (iii) we need more regularity of the domain Ω^+ provided by Assumption 5.12.

Remark 5.16. *Note that* (5.49) *can be rewritten in a canonical form as*

$$dJ(\Omega^+)[\theta] = \int_D \mathbb{S} : \partial\theta + \mathfrak{S}\cdot\theta\, dx,$$

where

$$\begin{aligned}\mathbb{S} =& -\sigma(\nabla u_D \otimes \nabla p_D + \nabla p_D \otimes \nabla u_D + \nabla u_N \otimes \nabla p_N + \nabla p_N \otimes \nabla u_N)\\ &+ \sigma(\nabla u_D\cdot\nabla p_D + \nabla u_N\cdot\nabla p_N)I + \left(\frac{\alpha_1}{2}(u_D - u_N)^2 - f(p_N + p_D)\right) I,\\ \mathfrak{S} =& -(p_D + p_N)\nabla f.\end{aligned}$$

The tensor $\mathbb{S}$ *can be seen as a generalisation of the Eshelby energy momentum tensor in continuum mechanics introduced in [45].*

Under Assumption 5.12 we can show similar to the previous section that the following proposition is true. Since the technique to derive the boundary formula is the same as for the previous section it will be omitted here. A detailed calculation may be found in [67].

Proposition 5.17 (boundary expression). *Under Assumption 5.12 and* $\theta \in C^1_c(D, \mathbf{R}^d)$ *the shape derivative of* $J(\Omega^+)$ *is given by*

$$\begin{aligned}dJ(\Omega^+)[\theta] =& \int_\Gamma [\sigma(-\partial_n u_D \partial_n p_D - \partial_n u_N \partial_n p_N)]_\Gamma\, \theta\cdot n\, ds\\ &+ \int_\Gamma [\sigma]_\Gamma (\nabla_\Gamma u_D\cdot\nabla_\Gamma p_D + \nabla_\Gamma u_N\cdot\nabla_\Gamma p_N)\,\theta\cdot n\, ds.\end{aligned}$$

Note that our results cover and generalise several results that can be found in the literature of shape optimization approaches for EIT, including [3, 54]. For instance when taking $\alpha_2 = 1$, $\alpha_1 = 0$ we get $p_D \equiv 0$ and consequently

$$dJ(\Omega^+)[\theta] = \int_\Gamma ([-\sigma\partial_n u_N \partial_n p_N]_\Gamma + [\sigma]_\Gamma \nabla_\Gamma u_N\cdot\nabla_\Gamma p_N)\theta\cdot n. \tag{5.50}$$

Formula (5.50) is the same as the one obtained in [3, pp. 533] (under the name $DJ_{DLS}(\omega).V$) by computing the shape derivative of u_N and u_D. The adjoint is given by

$$\begin{aligned}-\operatorname{div}(\sigma\nabla p_N) &= 0,\\ \sigma\partial_n p_N &= -(u_N - h).\end{aligned}$$

According to Proposition 5.15 we have obtained the following more general volume expression which is valid for any open set Ω^+:

$$dJ(\Omega^+)[\theta] = \int_D \sigma A'(0)\nabla u_N\cdot\nabla p_N - f p_N \operatorname{div}\theta - p_N\nabla f\cdot\theta\, dx. \tag{5.51}$$

The two formulas (5.50) and (5.51) are equal when Assumption 5.12 is satisfied.

Note also that from a numerical point of view, the boundary expression in Proposition 5.17 is delicate to compute compared to the volume expression in Proposition 5.15 for which the gradients of the state and adjoint states can be straightforwardly computed at grid points when using the finite element method for instance. The boundary expression, on the other hand, needs here the computation of the normal vector and the interpolation of the gradients on the interface Γ which requires a precise description of the boundary and introduce an additional error.

5.4 A quasi-linear transmission problem

We investigate a non-linear transmission problem and compute the shape derivative of an associated cost function. Moreover, we prove the existence of optimal shapes for a minimisation problem associated with it. To achieve the well-posedness of the minimisation problem a Gagliardo regularisation is used. The considered model constitutes a generalisation of the electrical impedance tomography (EIT) problem, which can be found in [3]; see also [29] for the usage of the material derivative methods for this problem.

5.4.1 The problem setting

Also for this example, we use the notations from Assumption 5.3 of Subsection 5.2.1. We consider for $s \in (0,1)$ the cost function

$$J(\Omega) := J_1(\Omega) + \alpha J_2(\Omega) := \int_D |u(\Omega) - u_r|^2 \, dx + \alpha \hat{P}_D^s(\chi) \tag{5.52}$$

constrained by the equations

$$\begin{aligned} -\operatorname{div}(\beta_+(|\nabla u^+|^2)\nabla u^+) &= f^+ \quad \text{in} \quad \Omega^+ \\ -\operatorname{div}(\beta_-(|\nabla u^-|^2)\nabla u^-) &= f^- \quad \text{in} \quad \Omega^- \\ u &= 0 \quad \text{on } \partial D \end{aligned} \tag{5.53}$$

complemented by transmission conditions on Γ

$$[u]_\Gamma = 0 \quad \text{and} \quad \beta_+(|\nabla u^+|^2)\partial_n u^+ = \beta_-(|\nabla u^-|^2)\partial_n u^-. \tag{5.54}$$

Here, $n := n^+$ denotes the outward unit normal vector along the interface $\Gamma = \partial\Omega^+ \cap \partial\Omega^-$. We denote by $n^- := -n = -n^+$ the outward unit normal vector of Ω^-. Given a function $\varphi : D \to \mathbf{R}$, we define its restriction to Ω^i by $\varphi^i := \varphi_{|\Omega^i} : \Omega^i \to \mathbf{R}$, where $i \in \{+,-\}$. The bracket

$$[\phi]_\Gamma := \varphi^+_{|\Gamma} - \varphi^-_{|\Gamma}$$

denotes the jump of a function φ across Γ. Recall the definition of the s-perimeter in (5.52)

$$\hat{P}_D^s(\chi) = \int_D \int_D \frac{|\chi_\Omega(x) - \chi_\Omega(y)|}{|x-y|^{d+s}} \, dx \, dy.$$

For later usage it is convenient to introduce the functions $\beta_\chi : \mathbf{R} \times \mathbf{R} \to \mathbf{R}$

$$\beta_\chi(y,x) := \chi(x)\beta_+(y) + \chi^c(x)\beta_-(y),$$

where χ is a characteristic function and $\chi^c := (1-\chi)$ its complement. The derivative $\beta'_\chi : \mathbf{R} \times \mathbf{R} \to \mathbf{R}$ is defined piecewise by $\beta'_\chi(y,x) := \chi(x)\partial_y\beta_+(y) + \chi^c(x)\partial_y\beta_-(y)$. Subsequently, the characteristic function $\chi = \chi_\Omega$ is always defined by the set $\Omega = \Omega^+ \subset D$. To simplify notation, we write $\beta(|\nabla u|^2, x)$ instead of $\beta_\chi(|\nabla u|^2, x)$ and similarly $\beta'(|\nabla u|^2, x)$ for $\beta'_\chi(|\nabla u|^2, x)$. We make the following assumptions.

Assumption 5.18. *We require the functions $\beta_+, \beta_- : \mathbf{R} \to \mathbf{R}$ to satisfy the following conditions.*

1. *There exist constants $\bar{\beta}^+, \underline{\beta}^+, \bar{\beta}^-, \underline{\beta}^- > 0$ such that*

$$\bar{\beta}^+ \le \beta_+(x) \le \underline{\beta}^+, \qquad \bar{\beta}^- \le \beta_-(x) \le \underline{\beta}^- \quad \text{for all } x \in \mathbf{R}^d.$$

2. *For all $x, y \in \mathbf{R}$, we have*

$$(\beta_+(x) - \beta_+(y))(x-y) \ge 0 \text{ and } (\beta_-(x) - \beta_-(y))(x-y) \ge 0.$$

3. *The functions β_+, β_- are continuously differentiable.*

4. *There are constants $k, K > 0$ such that*

$$k|\eta|^2 \le \beta_\pm(|p|^2)|\eta|^2 + 2\beta_\pm'(|p|^2)|p\cdot\eta|^2 \le K|\eta|^2 \quad \text{for all } \eta, p \in \mathbf{R}^d.$$

Moreover, we assume that $u_r \in H^1(D)$ and $f \in C^1(\overline{D})$.

Remark 5.19. *Note that from item 4 of the previous assumption it follows by plugging $\eta = p \neq 0$ that*

$$\beta_\pm'(|\eta|^2) \le \frac{K}{2}\frac{1}{|\eta|^2} \quad \text{for all } 0 \neq \eta \in \mathbf{R}^d.$$

Thus the functions $\beta_\pm'$ are bounded and vanish at plus infinity.

The weak formulation of (5.53),(5.54) reads: find $u = u(\chi) \in H_0^1(D)$ such that

$$\int_D \beta_\chi(|\nabla u|^2, x)\nabla u \cdot \nabla\psi\, dx = \int_D f\psi\, dx \quad \text{for all } \psi \in H_0^1(D). \tag{5.55}$$

Along with the previous equation, we are going to investigate the perturbed equation: find $u^t \in H_0^1(D)$ such that

$$\int_D \beta_\chi(|B(t)\nabla u^t|^2, x)A(t)\nabla u^t \cdot \nabla\psi\, dx = \int_D \xi(t)f^t\psi\, dx \quad \text{for all } \psi \in H_0^1(D). \tag{5.56}$$

Note that for $t = 0$ both equations coincide and thus $u^0 = u$.

Convention. *When we want to make the dependence of J on the characteristic function explicit, we shall write $J(\Omega^+)$ as $\hat{J}(\chi_{\Omega^+})$.*

5.4.2 Existence of optimal shapes

We are interested in the question under which restriction on the characteristic functions a minimisation of (5.52) admits a solution. Fix $p \in (1, \infty)$ and $0 < s < 1/p$. Put $\bar{s} := ps$. We investigate the problem

$$\min \hat{J}(\chi_\Omega) \quad \text{over } \chi_\Omega \in \mathfrak{W}^{\bar{s}}(D), \tag{5.57}$$

where $\hat{J}(\chi_\Omega) := J(\Omega)$ and J is given by (5.52). In the following we use the notation $X(D)$ to indicate the set of all characteristic functions χ_Ω defined by a Lebesgue measurable set $\Omega \subset D$. For every $\bar{s} \in (0, \infty)$, we recall the definition of the space

$$\mathfrak{W}^{\bar{s}}(D) = \{\chi_\Omega : \mathbf{R} \to \mathbf{R} |\ \chi_\Omega \in X(D) \text{ and } \hat{P}_D^{\bar{s}}(\chi_\Omega) = |\chi_\Omega|_{W_p^s(D)} < \infty\},$$

which includes finite perimeter sets.

We begin with the study of the state equation (5.55) and (5.56).

Theorem 5.20. *Let $\theta \in C_c^2(D, \mathbf{R}^d)$ be a vector field and Φ_t its associated flow. Then the equation (5.56) has for each $t \in [0, \tau]$ and $\chi \in X(D)$ a unique solution in $H_0^1(D)$.*

Proof. Let $\Omega^+ \subset D$ be measurable and define the measurable set $\Omega^- := D \setminus \Omega^+$. Then by definition $D = \Omega^+ \cup \Omega^-$. Introduce the family of energy functionals

$$\begin{aligned} E(t,\varphi) := \int_D \frac{1}{2}[\chi(x)\xi(t)h_+(|B(t)\nabla\varphi(x)|^2) + (1-\chi(x))\xi(t)h_-(|B(t)\nabla\varphi(x)|^2)] \\ - \xi(t)f^t(x)\varphi(x)\,dx, \end{aligned} \tag{5.58}$$

where $h_\pm$ is the primitive of $\beta_\pm$ and given by

$$h_\pm(z) = c_\pm + \int_0^z \beta_\pm(s)\,ds,$$

for some constants $c_\pm \in \mathbf{R}$. We may choose $c_\pm = 0$. We are going to show that the energy $E(t,\varphi)$ is strictly convex with respect to φ. The first order directional derivative at $\varphi \in H_0^1(D)$ in direction $\psi \in H_0^1(D)$ reads:

$$dE(t,\varphi;\psi) = \int_D \beta(|B(t)\nabla\varphi|^2, x)A(t)\nabla\varphi\cdot\nabla\psi\,dx - \int_D \xi(t)f^t\psi\,dx.$$

Note that the equation $dE(t,u^t;\psi) = 0$ for all $\psi \in H_0^1(D)$, coincides with equation (5.56). We now prove that the second order directional derivative of $E(t,\varphi)$ exists and is strictly coercive. Note that in order to prove the existence of the second order directional derivative of $E(t,\varphi)$, it is sufficient to show that for any $u, \varphi, \psi \in H_0^1(D)$

$$s \mapsto \int_D \beta(|B(t)\nabla(u+s\varphi)|^2, x)A(t)\nabla(u+s\varphi)\cdot\nabla\psi\,dx$$

is continuously differentiable on $\mathbf{R}$. Moreover for this it is sufficient to show that

$$s \mapsto \int_{\Omega_\pm} \beta_\pm(|B(t)\nabla(u+s\varphi)|^2, x)A(t)\nabla(u+s\varphi)\cdot\nabla\psi\,dx \tag{5.59}$$

is differentiable on $\mathbf{R}$. Put $s \mapsto \alpha_s(x) := |B(t)\nabla(u+s\varphi)|^2$, then it is immediate that the function $\gamma_s^\pm(x) := \beta_\pm(\alpha_s(x))A(t)\nabla(u(x)+s\varphi(x))\cdot\nabla\psi(x)$ is differentiable for almost all $x \in \Omega_\pm$, respectively. The derivative in the respective domain Ω_+ and Ω_- (briefly $\Omega_\pm$) reads

$$\begin{aligned} \frac{d}{ds}\gamma_s^\pm(x) =& 2\beta_\pm'(|B(t)\nabla(u+s\varphi)|^2)B(t)\nabla(u+s\varphi)\cdot B(t)\nabla\varphi A(t)\nabla(u+s\varphi)\cdot\nabla\psi \\ &+ \beta_\pm(|B(t)\nabla(u+s\varphi)|^2)A(t)\nabla\varphi\cdot\nabla\psi. \end{aligned}$$

Using Assumption 5.18 item 4, we conclude that there exists a constant $K > 0$ such that

$$\frac{d}{ds}\gamma_s^\pm(x) \le K|\nabla\varphi(x)||\nabla\psi(x)|, \quad \text{for almost every } x \in \Omega_\pm \text{ for all } s \in \mathbf{R}. \tag{5.60}$$

Since $s \mapsto \frac{d}{ds}\gamma_s^\pm(x)$ is also continuous on $\mathbf{R}$, we get by the fundamental theorem of calculus

$$\begin{aligned} \frac{\gamma_s^\pm(x) - \gamma_{s+h}^\pm(x)}{h} &= \frac{1}{h}\int_s^{s+h} \frac{d}{ds}\gamma_s^\pm(x)\,ds' \\ &\overset{(5.60)}{\le} K|\nabla\varphi(x)||\nabla\psi(x)| \quad \text{for almost all } x \in \Omega_\pm. \end{aligned}$$

Note, that the constant K is independent of x and s. Thus we may apply Lebesgue's theorem of dominated convergence to show that (5.59) is indeed differentiable with derivative

$$\begin{aligned}\frac{d}{ds}\int_{\Omega_\pm} &\beta_\pm(\alpha_s(x))A(t)\nabla(u+s\varphi)\cdot\nabla\psi\,dx\\ &=\int_{\Omega_\pm} 2\beta'_\pm(\alpha_s(x))B(t)\nabla(u+s\varphi)\cdot B(t)\nabla\varphi A(t)\nabla(u+s\varphi)\cdot\nabla\psi\\ &\qquad+\beta_\pm(\alpha_s(x))A(t)\nabla\varphi\cdot\nabla\psi\,dx.\end{aligned}$$

It is immediate from the previous expression that the derivative is continuous. We conclude that $d^2E(t,\varphi;\psi,\psi)$ exists for all $\varphi,\psi\in H^1_0(D)$ and $t\in[0,\tau]$. Moreover, using Assumption 5.18 item 4, we get that there is $C>0$ such that

$$d^2_\varphi E(t,\varphi;\psi,\psi)\geq C\|\psi\|^2_{H^1(D)}\quad\text{for all }\varphi,\psi\in H^1_0(D),\quad\text{and for all }t\in[0,\tau].\tag{5.61}$$

Hence for all $t\in[0,\tau]$ the energy $\varphi\mapsto E(t,\varphi)$ is strictly convex on the Hilbert space $H^1_0(\Omega)$. Moreover, it is obvious that this functional is lower semi-continuous. Noting that $h^\pm(|z|)\geq\overline{\beta}^\pm|z|$ for all $z\in\mathbf{R}$, we get for each $t\in[0,\tau]$:

$$E(t,u)\longrightarrow+\infty\quad\text{ as }\quad\|u\|_{H^1_0(\Omega)}\longrightarrow+\infty.$$

Therefore, we may conclude from [44, Proposition 1.1, Proposition 2.1, pp. 35–37] that

$$\inf_{\varphi\in H^1_0(\Omega)}E(t,\varphi)$$

admits a unique solution, which is a solution of (5.56). Conversely, every solution of (5.56) solves the above minimisation problem. $\square$

In the next lemma, we prove the Lipschitz continuity of the mapping $X(D)\ni\chi\mapsto u(\chi)\in H^1_0(D)$, where $u(\chi)$ denotes the weak solution of (5.55) and $X(D)$ is endowed with the $L_1(D)$-norm.

Lemma 5.21. *Assume that there exist $C>0$ and $\varepsilon>0$ such that for every $\chi\in X(D)$ we have $\|u(\chi)\|_{W^{1,2+\varepsilon}(\Omega)}\leq C$, where $u=u(\chi)$ solves (5.55). Then there is a constant $C>0$ such that for all characteristic functions $\chi_1,\chi_2\in X(D)$:*

$$\|u(\chi_1)-u(\chi_2)\|_{H^1(D)}\leq C\|\chi_1-\chi_2\|_{L_1(D)},$$

where $u(\chi_1)$ and $u(\chi_2)$ are solutions of the state equation (5.55).

Proof. Let $p\in(1,\infty)$ and $0<s<1/p$. Let $u(\chi_1)=u_1$ and $u(\chi_2)=u_2$ be solutions in $H^1_0(D)$ of (5.55) associated with the functions $\chi_1,\chi_2\in X(D)$. Then by boundedness of β_{χ_1} and β_{χ_2}, we obtain

$$\begin{aligned}C_1\|u_1-u_2\|^2_{H^1(D)}&\leq\int_D\beta_{\chi_1}(|\nabla u_1|^2,x)\nabla(u_1-u_2)\cdot\nabla(u_1-u_2)\,dx\\ &=\int_D(\beta_{\chi_2}(|\nabla u_2|^2,x)-\beta_{\chi_1}(|\nabla u_1|^2,x))\nabla(u_1-u_2)\cdot\nabla u_2\,dx\end{aligned}$$

and also

$$\begin{aligned}C_2\|u_1-u_2\|^2_{H^1(D)}&\leq\int_D\beta_{\chi_2}(|\nabla u_2|^2,x)\nabla(u_1-u_2)\cdot\nabla(u_1-u_2)\,dx\\ &=\int_D(\beta_{\chi_2}(|\nabla u_2|^2,x)-\beta_{\chi_1}(|\nabla u_1|^2,x))\nabla(u_1-u_2)\cdot\nabla u_1\,dx.\end{aligned}$$

Adding both inequalities yields with $C := C_1 + C_2$

$$
\begin{aligned}
C\|u_1 - u_2\|^2_{H^1(D)} &\le \int_D (\beta_{\chi_2}(|\nabla u_2|^2, x) - \beta_{\chi_1}(|\nabla u_1|^2, x))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx \\
&= \int_D (\chi_2\beta_+(|\nabla u_2|^2) - \chi_1\beta_+(|\nabla u_1|^2))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx \\
&\quad + \int_D (\chi_2^c\beta_-(|\nabla u_2|^2) - \chi_1^c\beta_-(|\nabla u_1|^2))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx
\end{aligned}
$$

and therefore

$$
\begin{aligned}
C\|u_1 - u_2\|^2_{H^1(D)} \le &\int_D (\chi_2 - \chi_1)\beta_+(|\nabla u_2|^2))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx \\
&+ \int_D \chi_1(\beta_+(|\nabla u_2|^2) - \beta_+(|\nabla u_1|^2))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx \\
&+ \int_D (\chi_1 - \chi_2)\beta_-(|\nabla u_2|^2)\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx \\
&+ \int_D \chi_1^c(\beta_-(|\nabla u_2|^2) - \beta_-(|\nabla u_1|^2))\nabla(u_1 - u_2)\cdot\nabla(u_1 + u_2)\,dx.
\end{aligned}
\tag{5.62}
$$

Now we use the monotonicity of β_+ and β_- to conclude

$$
\begin{aligned}
&\int_D \chi_1^c(\beta_-(|\nabla u_2|^2) - \beta_-(|\nabla u_1|^2))(\nabla u_1 - \nabla u_2)\cdot(\nabla u_1 + \nabla u_2)\,dx \\
&\qquad = -\int_D (1-\chi_1)(\beta_-(|\nabla u_2|^2) - \beta_-(|\nabla u_1|^2))(|\nabla u_2|^2 - |\nabla u_1|^2)\,dx \le 0
\end{aligned}
$$

and similarly

$$
\begin{aligned}
&\int_D \chi_1(\beta_+(|\nabla u_2|^2) - \beta_+(|\nabla u_1|^2))(\nabla u_1 - \nabla u_2)\cdot(\nabla u_1 + \nabla u_2) \\
&\qquad = -\int_D \chi_1(\beta_+(|\nabla u_2|^2) - \beta_+(|\nabla u_1|^2))(|\nabla u_2|^2 - |\nabla u_1|^2) \le 0.
\end{aligned}
$$

By assumption there exist $\varepsilon > 0$ and $C > 0$ such that $\|u(\chi)\|_{W^{1,2+\varepsilon}(D)} \le C$ for all $\chi \in X(D)$. Therefore using Hölder's inequality, we deduce from (5.62)

$$
C\|u_1 - u_2\|^2_{H^1(D)} \le (\underline{\beta}^+ + \underline{\beta}^-)\|\chi_2 - \chi_1\|_{L_{2q'}(D)}\|\nabla(u_1 - u_2)\|_{L_2(D)}\|\nabla(u_1 + u_2)\|_{L_{2q}(D)},
$$

where $q = \frac{2+\varepsilon}{2}$ and $q' := \frac{q}{q-1} = \frac{2}{\varepsilon} + 1$. Finally, using Hölder's inequality and the boundedness of D it follows that there exists $C > 0$ depending on $m(D)$ such that $\|\chi_2 - \chi_1\|_{L_{2q'}(D)} \le C\|\chi_2 - \chi_1\|_{L_1(D)}$ for all $\chi_1, \chi_2 \in X(D)$. □

Corollary 5.22. *Denote by Φ_t the flow associated with $\theta \in C^1_c(D, \mathbf{R}^d)$ and put $\Omega_t := \Phi_t(\Omega)$. Let $u(\chi_\Omega) = u$ and $u(\chi_{\Omega_t}) = u_t$ be the solutions of (5.55). Then $u_t : [0,\tau] \to H^1_0(D)$ and $u^t := u_t \circ \Phi_t : [0,\tau] \to H^1_0(D)$ are right sided uniformly continuous, i.e. for any $\varepsilon > 0$ there exists a $\delta > 0$ such that for all $t \le s$, $s - t \in [0,\tau]$ with $|s-t| \le \delta$*

$$
\|u_s - u_t\|_{H^1_0(D)} \le \varepsilon, \qquad \|u^s - u^t\|_{H^1_0(D)} \le \varepsilon.
$$

In particular,

$$
\lim_{t \searrow 0}\|u_{s+t} - u_s\|_{H^1_0(D)} = 0, \qquad \lim_{t\searrow 0}\|u^{s+t} - u^s\|_{H^1_0(D)} = 0 \quad \textit{for all } s \in [0,\tau] \setminus \tau.
$$

Proof. From the previous Lemma and the change of variables $\Phi_t(x) = y$, we infer

$$\begin{aligned}\|u_s - u_t\|_{H_0^1(D)} &\le C\|\chi_{\Omega_s} - \chi_{\Omega_t}\|_{L_q(D)}\\ &= C\|\chi_\Omega \circ \Phi_s^{-1} - \chi_\Omega \circ \Phi_t^{-1}\|_{L_q(D)}\\ &= C\|\xi^{1/q}(t)(\chi_\Omega - \chi_\Omega \circ \Phi_t^{-1} \circ \Phi_s)\|_{L_q(D)}\\ &\le C\|\chi_\Omega - \chi_\Omega \circ \Phi_{s-t}\|_{L_q(D)}.\end{aligned}$$

Therefore we reduced the uniform continuity of $t \mapsto u_t$ to the continuity of $[0,\tau] \to L_q(D) : t \mapsto \chi_\Omega \circ \Phi_t$ in zero, which follows from Lemma 2.16 item (i). The continuity of $t \mapsto u^t$ now follows from item (iv) of Lemma 2.16. ☐

It is important to realise that the previous result was established under minimal assumptions on the regularity of the solutions u, u^t. We only need conditions 2,3 of Assumption 5.18.

Before we turn our attention to existence of optimal shapes, we prove the Lipschitz continuity of $t \mapsto u^t$.

Proposition 5.23. *Let us pick any measurable set $\Omega \subset D$. Let Φ_t be the flow of the vector field $\theta \in C_c^2(D, \mathbf{R}^d)$ and set $\Omega_t := \Phi_t(\Omega)$.*[1] *Then there exists $\delta > 0$ such that*

$$\|u^t - u\|_{H_0^1(D)} \le ct \quad \textit{for all } t \in [0, \delta].$$

Proof. Let $E(t,\varphi)$ be the energy defined in (5.58) and recall from the proof of Theorem 5.20 that there is $C > 0$:

$$d_\varphi^2 E(t,\varphi;\psi,\psi) \ge C\int_D |\nabla\psi|^2 dx \;\text{ for all } \psi \in H^1(D), \;\text{ for all } t \in [0,\tau].$$

Denote by u^t the unique minimum of $E(t,\cdot)$, which is characterised by

$$dE(t, u^t, \psi) = 0 \quad \text{for all } \psi \in H_0^1(D).$$

Let us first show that for all $\varphi, \psi \in H^1(D)$ the function $[0,\tau] \mapsto \mathbf{R} : t \mapsto dE(t,\varphi,\psi)$ is continuously differentiable. The only difficult part is the nonlinearity

$$t \mapsto \int_D \beta(|B(t)\nabla\varphi(x)|^2, x)A(t)\nabla\varphi \cdot \nabla\psi \, dx \tag{5.63}$$

where $\varphi, \psi \in H_0^1(D)$ are arbitrary functions. The other terms in $G(t,\varphi,\psi)$ are differentiable due to Lemma 2.16. Again it will be sufficient to show that

$$t \mapsto \int_{\Omega_\pm} \beta_\pm(|B(t)\nabla\varphi(x)|^2)A(t)\nabla\varphi \cdot \nabla\psi \, dx$$

are differentiable. We have that $t \mapsto \tilde\alpha_t^\pm(x) := \beta_\pm(|B(t)\nabla\varphi(x)|^2)A(t)\nabla\varphi(x) \cdot \nabla\psi(x)$ are differentiable for almost every $x \in \Omega^\pm$ with derivative

$$\begin{aligned}\frac{d}{dt}\tilde\alpha_t^\pm(x) = 2\beta_\pm'(|B(t)\nabla\varphi(x)|^2)B(t)\nabla\varphi(x)\cdot B'(t)\nabla\varphi\, A(t)\nabla\varphi(x)\cdot\nabla\psi(x)\\ + \beta_\pm(|B(t)\nabla\varphi(x)|^2)A'(t)\nabla\varphi(x)\cdot\nabla\psi(x).\end{aligned}$$

Since $\theta \in C_c^2(D, \mathbf{R}^d)$, we have $\tilde\alpha_t(x) \in C^1([0,\tau])$ for almost every $x \in \Omega_\pm$. Using item 4 of Assumption 5.18 and taking into account Remark 5.19, we can show that $\frac{d}{dt}\tilde\alpha_t^\pm$ is pointwise

[1] Note that $\Phi_t(\Omega)$ is Lebesgue measurable; cf. [47, Thm. 263D].

bounded by a $L_1(D)$ function. The calculation is similar to the one leading to (5.60) and omitted. Thus we may apply the Lebesgue's dominated convergence theorem to show that (5.63) is indeed differentiable and

$$\begin{aligned}\partial_t d_\varphi E(s,\varphi,\psi) = &\int_D \beta'(|B(s)\nabla\varphi|^2, x) 2(B'(s)\nabla\varphi\cdot B(s)\nabla\varphi)A(s)\nabla\varphi\cdot\nabla\psi\,dx\\ &-\int_D \xi(s)\,\operatorname{div}(\theta^s)\circ\Phi_s\, f^s\psi\,dx - \int_D \xi(s)\,B(s)\nabla f^s\cdot\theta^s\psi\,dx\\ &-\int_D \beta(|B(s)\nabla\varphi|^2,x)A'(s)\nabla\varphi\cdot\nabla\psi\,dx.\end{aligned}$$

We proceed by the observation that

$$\begin{aligned}\int_0^1 d^2_\varphi E(t,u^t_\nu;u^t-u,u^t-u)\,d\nu &= d_\varphi E(t,u^t;u^t-u) - d_\varphi E(t,u;u^t-u) &(5.64)\\ &= -(d_\varphi E(t,u;u^t-u) - d_\varphi E(0,u;u^t-u)) &(5.65)\\ &= -t\partial_t d_\varphi E(\eta_t t,u;u^t-u), &(5.66)\end{aligned}$$

where $u^t_\nu := \nu\, u^t + (1-\nu)u$. In the step from (5.65) to (5.66) we applied the mean value theorem yielding the $\eta_t\in(0,1)$. Using Hölder's inequality and item 4 of Assumption 5.18, we conclude that there is a constant $C>0$ such that

$$\partial_t d_\varphi E(s,\varphi;\psi) \le C(1+\|\varphi\|_{H^1(D)})\|\psi\|_{H^1(D)} \quad \text{for all } \varphi,\psi\in H^1(D), \quad \text{for all } s\in[0,\tau].$$

Using the previous inequality and estimating (5.64) by (5.61), we get the desired inequality

$$\|u^t-u\|_{H^1(D)} \le ct.$$

□

The considerations from the above paragraph condense in the following result.

Theorem 5.24. *Let the assumptions of Lemma 5.21 be satisfied. Let $p\in(1,\infty), 0<s<1/p$ and put $\bar{s}:=ps$. Then the optimization problem (5.57) has at least one solution $\chi=\chi_\Omega\in\mathfrak{W}^{\bar{s}}(D)$.*

Proof. We employ Theorem 2.29 to prove the statement. Let $(\chi_n)_{n\in\mathbf{N}}$ be a sequence in $X(D)$ converging in $L_2(D)$ to $\chi\in X(D)$. Due to Lemma 5.21, we obtain $u(\chi_n)\to u(\chi)$ in $H^1_0(D)$ as $n\to\infty$. Therefore $\lim_{n\to\infty}\hat{J}(\chi_n)=\hat{J}(\chi)$ and $\hat{J}: X(D)\to\mathbf{R}$ is continuous with respect to $L_2(D)$. The result follows now from Theorem 2.29. □

Remark 5.25. *The previous result remains true when we replace the penalty term in $\hat{J}$ by the perimeter $\hat{P}_D(\chi)$.*

5.4.3 Shape derivative of J_2

We show that the penalty term $J_2(\Omega)=|\chi_\Omega|^p_{W^s_p(D)}$ is shape differentiable.

Lemma 5.26. *Let $\theta\in C^2_D(\mathbf{R}^d)$. Fix $p\in(1,\infty)$ and $0<s<1/p$. Then the mapping*

$$\Omega\mapsto J_2(\Omega) := |\chi_\Omega|^p_{W^s_p(D)}$$

is shape differentiable in all open sets $\Omega^* \subset D$ satisfying $|\chi_{\Omega^*}|_{W_p^s(D)} < \infty$. The derivative is given by

$$
\begin{aligned}
dJ_2(\Omega^*)[\theta] = 2\int_\Omega \int_{D\setminus\Omega} & \frac{\operatorname{div}(\theta)(x) + \operatorname{div}(\theta)(y)}{|x-y|^{d+sp}}\,dx\,dy \\
+ c\int_\Omega \int_{D\setminus\Omega} & \frac{(x-y)}{|x-y|^{d+sp+2}} \cdot (\theta(x) - \theta(y))\,dx\,dy
\end{aligned}
$$

where $c := -2(d+ps)$. This can be written in terms of χ_Ω as

$$
\begin{aligned}
dJ_2(\Omega^*)[\theta] = & \int_D \int_D (\operatorname{div}(\theta)(x) + \operatorname{div}(\theta)(y)) \frac{|\chi_\Omega(x) - \chi_\Omega(y)|^p}{|x-y|^{d+sp}}\,dx\,dy \\
& + \frac{c}{2}\int_D \int_D \frac{|\chi_\Omega(x) - \chi_\Omega(y)|^p}{|x-y|^{d+ps+2}}(x-y)\cdot(\theta(x) - \theta(y))\,dx\,dy.
\end{aligned}
\tag{5.67}
$$

Proof: *Using the change of variables $y = \Phi_t(x)$ gives*

$$
J(\Phi_t(\Omega^*)) = 2\int_\Omega \int_{D\setminus\Omega} \frac{\xi(t)(x)\xi(t)(y)}{|\Phi_t(x) - \Phi_t(y)|^{d+ps}}\,dx\,dy
$$

and consequently using that Φ_t is injective, we obtain the desired formula by differentiating the above equation at $t = 0$.

Remark 5.27. *Note that due to the Lipschitz continuity of θ and supp$(\theta) \subset D$ the shape derivative (5.67) is well-defined.*

5.4.4 Shape derivative of J_1

We are going to prove that the cost function J_1 given by (5.52) is shape differentiable by employing the Theorem 4.2. Moreover, we derive the domain expression of the shape derivative. The main result of this subsection reads:

Theorem 5.28. *Let $D \subset \mathbf{R}^d$ be a bounded domain with Lipschitz boundary. Fix any measurable set $\Omega \subset D$. Then the shape function J_1 given by (5.52) is shape differentiable for every $\theta \in C_c^2(D, \mathbf{R}^d)$.* [2] *The domain expression reads*

$$
\begin{aligned}
dJ_1(\Omega)[\theta] = & \int_D \operatorname{div}(\theta)|u-u_r|^2\,dx - \int_D 2(u-u_r)\nabla u_r\cdot\theta\,dx - \int_D \operatorname{div}(\theta) f p\,dx \\
& - \int_D \nabla f\cdot\theta p\,dx + \int_D \beta(|\nabla u|^2, x)A'(0)\nabla u\cdot\nabla p\,dx \\
& - \int_D 2\beta'(|\nabla u|^2, x)(\partial\theta^\top\nabla u\cdot\nabla u)(\nabla u\cdot\nabla p)\,dx,
\end{aligned}
\tag{5.68}
$$

where $u \in H_0^1(D)$ satisfies (5.55) and $p \in H_0^1(D)$ solves

$$
\begin{aligned}
& \int_D 2\beta'(|\nabla u|^2, x)(\nabla u\cdot\nabla p)(\nabla u\cdot\nabla\psi)\,dx + \int_\Omega \beta(|\nabla u|^2, x)\nabla\psi\cdot\nabla p\,dx \\
& \quad = -\int_D 2(u-u_r)\psi\,dx \quad \text{for all } \psi \in H_0^1(D).
\end{aligned}
\tag{5.69}
$$

[2] We use the notation $A \Subset B$ to indicate that $A \subset B$ and $\overline{A} \subset B$ is compact.

For the first part of the theorem we let $\Omega^+ \subset D$ be any measurable set and define $\Omega^- := D \setminus \Omega^-$. We apply Theorem 4.2 to the function

$$\begin{aligned} G(t,\varphi,\psi) = &\sum_{\varsigma\in\{+,-\}} \left(\int_{\Omega^\varsigma} \xi(t)|\varphi^\varsigma - u_r^t|^2\,dx + \int_{\Omega^\varsigma} \beta_\varsigma(|B(t)\nabla\varphi^\varsigma|^2)A(t)\nabla\varphi^\varsigma\cdot\nabla\psi^\varsigma\,dx \right) \\ &- \sum_{\varsigma\in\{+,-\}} \int_{\Omega^\varsigma} \xi(t)(f^\varsigma\circ\Phi_t)\psi^\varsigma\,dx, \end{aligned}$$

with $E = H_0^1(D)$ and $F = H_0^1(D)$ to show the previous theorem. Notice that $J_1(\Omega_t) = G(t, u^t, \psi)$, where $u^t \in H_0^1(D)$ solves

$$\int_D \beta(|B(t)\nabla u^t|^2, x)A(t)\nabla u^t\cdot\nabla\psi\,dx = \int_D \xi(t)f^t\psi\,dx \quad \text{for all } \psi\in H_0^1(D). \tag{5.70}$$

Roughly speaking the function G constitutes the sum of the perturbed cost function $J(\Omega_t)$ and the weak formulation (5.70).

Let us now verify the four conditions (H0)-(H3).

(H0) Condition (iii) is satisfied by construction. As a byproduct of Theorem 5.20, we get that conditions (i) and (ii) of hypothesis (H0) are satisfied, since the Lagrangian G can be written as

$$G(t,\varphi,\psi) = \sum_{\varsigma\in\{+,-\}} \int_{\Omega_\varsigma} \xi(t)|\varphi - u_r^t|^2\,dx + dE(t,\varphi;\psi).$$

(H1) In Proposition 5.23, we proved that for all $\varphi,\psi\in H^1(D)$ the mapping $[0,\tau]\to\mathbf{R}: t\mapsto dE(t,\varphi;\psi)$ is differentiable. Therefore, the function $t\mapsto G(t,\varphi,\psi)$ is differentiable for all $\varphi,\psi\in H_0^1(D)$ with derivative

$$\begin{aligned} \partial_t G(t,\varphi,\psi) = &-\int_D 2\,\xi(t)\,(\varphi-u_r^t)B(t)\nabla u_r^t\cdot\theta^t\,dx + \int_D \xi(t)\ \mathrm{div}\,(\theta^t)\circ\Phi_t\,|\varphi-u_r^t|^2\,dx \\ &+ \int_D \beta'(|B(t)\nabla\varphi|^2,x)2(B'(t)\nabla\varphi\cdot B(t)\nabla\varphi)A(t)\nabla\varphi\cdot\nabla\psi\,dx \\ &- \int_D \xi(t)\ \mathrm{div}\,(\theta^t)\circ\Phi_t\ f^t\psi\,dx - \int_D \xi(t)\,B(t)\nabla f^t\cdot\theta^t\psi\,dx \\ &- \int_D \beta(|B(t)\nabla\varphi|^2,x)A'(t)\nabla\varphi\cdot\nabla\psi\,dx. \end{aligned}$$

(H2) Note that $E(t) = \{u^t\}$ and $Y(t,u^t,u^0) = \{p^t\}$, where $u^t\in H_0^1(D)$ is the solution of the state equation (5.70) and $p^t\in H_0^1(D)$ is the unique solution of

$$\begin{aligned} &\int_0^1\int_D 2\xi(t)\beta'(|B(t)\nabla u_t^s|^2,x)(B(t)\nabla u_t^s\cdot B(t)\nabla p^t)(B(t)\nabla u_t^s\cdot B(t)\nabla\psi)\,dx\,ds \\ &\quad+\int_0^1\int_D \beta(|B(t)\nabla u_t^s|^2,x)A(t)\nabla\psi\cdot\nabla p^t\,dx\,ds \\ &\quad= -\int_0^1\int_D \xi(t)2(u_t^s-u_r)\psi\,dx\,ds \quad \text{for all } \psi\in H_0^1(D), \end{aligned} \tag{5.71}$$

where $u_t^s := su^t + (1-s)u$. Due to condition (H0) this equation is well-defined. The existence of a solution p^t follows from the theorem of Lax-Milgram. Moreover, by Assumption 5.18, we conclude $\beta'\geq 0$ and $\beta\geq c>0$. Note that $p^0 = p\in Y(0,u^0)$ is the unique solution of the adjoint equation (5.69).

(H3) We show that for any real sequence $(t_n)_{n\in\mathbf{N}}$ such that $t_n \searrow 0$ as $n \to \infty$, there is a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $(p^{t_k})_{k\in\mathbf{N}}$, where $p^{t_k} \in Y(t_k, u^{t_k}, u^0)$ converges weakly in $H^1_0(D)$ to the solution of the adjoint equation and that $(t,\psi) \mapsto \partial_t G(t, u^0, \psi)$ is weakly continuous.

With the help of Proposition 5.23, we are able to show the following.

Lemma 5.29. *For any sequence $(t_n)_{n\in\mathbf{N}}$ of non-negative real numbers converging to zero, there is a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $(p^{t_{n_k}})_{k\in\mathbf{N}}$, where $p^{t_{n_k}}$ solves (5.71) with $t = t_{n_k}$, converges weakly in $H^1_0(D)$ to the solution p of the adjoint equation (5.69).*

Proof: *The existence of a solution of (5.71) follows from the Theorem of Lax-Milgram. Inserting $\psi = p^t$ as test function in (5.71), we see that the estimate $\|u^t\|_{H^1(D)} \le C$ implies $\|p^t\|_{H^1(D)} \le \tilde{C}$ for all sufficiently small t, where $C, \tilde{C} >$ are some constants. Now let $(t_n)_{n\in\mathbf{N}}$ be a sequence of non-negative numbers converging to zero. Then using the boundedness of $(p^{t_n})_{n\in\mathbf{N}}$, we may extract a weakly converging subsequence $(p^{t_{n_k}})_{k\in\mathbf{N}}$ converging to some $w \in H^1_0(D)$. In Proposition 5.23 we proved $u^t \to u$ in $H^1(D)$ which can be used to pass to the limit in (5.71) and obtain $p^{t_{n_k}} \rightharpoonup p$ in $H^1(D)$, for $t_{n_k} \to 0$, as $k \to \infty$, where $p \in H^1_0(D)$ solves the adjoint equation (5.69). By uniqueness of a solution of the adjoint equation, we conclude $w = p$.*

Finally note that for fixed $\varphi \in H^1_0(D)$ the mapping $(t,\psi) \mapsto \partial_t G(t,\varphi,\psi)$ is weakly continuous. This finishes the proof that condition (H3) is satisfied. Consequently, we may apply Theorem 4.2 and obtain $dJ_1(\Omega)[\theta] = \partial_t G(0, u, p)$, where $u \in H^1_0(D)$ solves the state equation (5.55) and $p \in H^1_0(D)$ is a solution of the adjoint equation (5.69). This completes the proof of Theorem 5.28.

5.4.5 Boundary integrals

It can be seen from the domain expression (5.68), that the mapping $dJ_1(\Omega) : C^\infty_c(D) \to \mathbf{R}$ is linear and continuous for the $C^1_c(D, \mathbf{R}^d)$–topology. Thus if Ω is open and $\partial\Omega$ is of class C^2, then we conclude by the structure theorem that $dJ_1(\Omega)[\theta] = g(\theta|_\Gamma \cdot n^+)$ for some distribution $g \in C^k(\Gamma)'$. It turns out that under suitable smoothness assumptions the distribution g can be indeed identified as an integral over Γ:

Theorem 5.30. *Let $\Omega := \Omega^+ \Subset D$ be a compactly contained subset of D with unitary unit normal $n := n^+$ and define $\Omega^- := D \setminus \overline{\Omega^+}$. Suppose that $\Gamma := \partial\Omega^+ \cap \partial\Omega^-$ is of class C^2. The solution u of (5.55) and the solution p of (5.73) are classical solutions by which we mean that $u^+, p^+ \in C^2(\overline{\Omega}^+)$ and $u^-, p^- \in C^2(\overline{\Omega}^-)$. Then the boundary expression is given by*

$$
\begin{aligned}
dJ_1(\Omega)[\theta] = &-\int_\Gamma \left[2\beta'(|\nabla u|^2, x)(\nabla_\Gamma u \cdot \nabla_\Gamma p + \partial_n u\, \partial_n p)\partial_n u\, \partial_n u\right]_\Gamma \theta_n ds \\
&+ \int_\Gamma \left[\beta(|\nabla u|^2, x)\nabla_\Gamma u \cdot \nabla_\Gamma p - \beta(|\nabla u|^2, x)\partial_n u\, \partial_n p\right]_\Gamma \theta_n\, ds.
\end{aligned} \tag{5.72}
$$

Proof: *By taking appropriate test functions in the weak formulation of the adjoint equation (5.69) shows that p solves*

$$
\begin{aligned}
-\operatorname{div}(\beta_+(|\nabla u^+|^2)\nabla p^+ + 2\beta_+'(|\nabla u^+|^2)(\nabla u^+ \cdot \nabla p^+)\nabla u^+) &= -2(u^+ - u_r) \quad \text{in } \Omega^+, \\
-\operatorname{div}(\beta_-(|\nabla u^-|^2)\nabla p^- + 2\beta_-'(|\nabla u^-|^2)(\nabla u^- \cdot \nabla p^-)\nabla u^-) &= -2(u^- - u_r) \quad \text{in } \Omega^-, \\
p &= 0 \quad \text{on } \partial D,
\end{aligned} \tag{5.73}
$$

complemented by transmission conditions

$$\begin{aligned}[p]_\Gamma &= 0 \quad \text{on } \Gamma,\\ \big[\beta(|\nabla u|^2,x)\,\partial_n p + 2\beta'(|\nabla u|^2,x)\,\nabla u\cdot\nabla p\,\partial_n u\big]_\Gamma &= 0 \quad \text{on } \Gamma.\end{aligned}$$

Recall the definitions $\Psi_t(f) = f\circ\Phi_t$ *and* $\Psi^t(f) = f\circ\Phi_t^{-1}$. *Using the change of variables* $\Phi_t(x) = y$, *we can rewrite the function* G *as*

$$\begin{aligned}G(t,\varphi,\psi) = &\sum_{\varsigma\in\{+,-\}}\left(\int_{\Phi_t(\Omega^\varsigma)}|\Psi^t(\varphi^\varsigma)-u_r|^2\,dx - \int_{\Phi_t(\Omega^\varsigma)} f^\varsigma\Psi^t(\psi^\varsigma)\,dx\right)\\ &+\sum_{\varsigma\in\{+,-\}}\int_{\Phi_t(\Omega^\varsigma)}\beta_\varsigma(|\nabla(\Psi^t(\varphi^\varsigma))|^2)\nabla(\Psi^t(\varphi^\varsigma))\cdot\nabla(\Psi^t(\psi^\varsigma))\,dx\end{aligned}\tag{5.74}$$

for all $\varphi,\psi\in H_0^1(D)$ *with* $\varphi^\kappa,\psi^\kappa\in C^2(\overline{\Omega}^\kappa)$, $(\kappa\in\{+,-\})$. *It is easy to verify that* $G(t,\varphi,\psi)$ *in the form of* (5.74) *is differentiable with respect to* t, *i.e.* $\partial_t G(t,\varphi,\psi)$ *exists for all* $t\in[0,\tau]$ *and* $\varphi,\psi\in H_0^1(D)$ *with* $\varphi^\kappa,\psi^\kappa\in C^2(\overline{\Omega}^\kappa)$, $\kappa\in\{+,-\}$. *To see this we extend* $\varphi^\kappa,\psi^\kappa$ *to functions* $\tilde\varphi^\kappa,\tilde\psi^\kappa$ *in* $C^2(\mathbf{R}^d)$. *This is possible by a higher order reflection technique under the assumption that* $\partial\Omega^+$ *and* $\partial\Omega^-$ *are both of class* C^2, *see e.g. [46, p.254, Theorem 1]. It is evident that the value* $G(t,\varphi,\psi)$ *does not change when we replace* $\varphi^\kappa,\psi^\kappa$ *by* $\tilde\varphi^\kappa,\tilde\psi^\kappa$ *in* (5.74). *Notice that* $\Psi_t(\varphi) = \varphi\circ\Phi_t^{-1}$ *will be independent of* t *near the boundary* ∂D *since* θ *has compact support in* D. *Therefore the regularity of* $\partial D\cap\partial\Omega^- = \partial D$ *does not enter in the above considerations, only the* C^2 *regularity for* $\partial\Omega^+\cap\partial\Omega^-$ *is needed. The assumptions of Theorem 5.30 allow us to apply the previously described extension technique to* $\varphi = u$ *and* $\psi = p$. *Thanks to Theorem 2.43 we already know that* $\frac{d}{dt}G(t,u^t,\psi) = \partial_t G(0,u,p)$ *and thus we can compute the shape derivative of* J_1 *by computing* $\partial_t G(0,u,p)$ *using formula* (5.74) *and Theorem 2.43:*

$$\begin{aligned}dJ_1(\Omega)[\theta] = &\sum_{\varsigma\in\{+,-\}}\int_{\Omega^\varsigma}2(u-u_r)\mathring{u}^\varsigma\,dx + \int_{\Omega^\varsigma}2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma\cdot\nabla\mathring{u}^\varsigma)\nabla u^\varsigma\cdot\nabla p^\varsigma\,dx\\ &+\sum_{\varsigma\in\{+,-\}}\int_{\Omega^\varsigma}\beta_\varsigma(|\nabla u^\varsigma|^2)\nabla\mathring{u}^\varsigma\cdot\nabla p^\varsigma + \beta_\varsigma(|\nabla u^\varsigma|^2)\nabla u^\varsigma\cdot\nabla\mathring{p}^\varsigma - f^\varsigma\mathring{p}^\varsigma\,dx\\ &+\int_{\partial\Omega^\varsigma}(\beta_\varsigma(|\nabla u^\varsigma|^2)\nabla u^\varsigma\cdot\nabla p^\varsigma - f^\varsigma p^\varsigma)\,\theta_{n^\varsigma}\,ds,\end{aligned}\tag{5.75}$$

where we use the notation $\mathring{u}^\varsigma = -\nabla u^\varsigma\cdot\theta$ *and* $\mathring{p}^\varsigma = -\nabla p^\varsigma\cdot\theta$. *Integrating by parts in* (5.75) *gives*

$$\begin{aligned}dJ_1(\Omega)[\theta] = &-\sum_{\varsigma\in\{+,-\}}\Bigg\{\int_{\Omega^\varsigma}\operatorname{div}\big(\beta_\varsigma(|\nabla u^\varsigma|^2)\nabla p^\varsigma + 2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma\cdot\nabla p^\varsigma)\nabla u^\varsigma\big)\,\mathring{u}^\varsigma\,dx\\ &+\int_{\Omega^\varsigma}2(u-u_r)\mathring{u}^\varsigma\,dx\Bigg\} - \sum_{\varsigma\in\{+,-\}}\int_{\Omega^\varsigma}\big(\operatorname{div}\big(\beta_\varsigma(|\nabla u^\varsigma|^2)\nabla u^\varsigma\big) + f^\varsigma\big)\,\mathring{p}^\varsigma\,dx\\ &+\sum_{\varsigma\in\{+,-\}}\int_{\partial\Omega^\varsigma}\beta_\varsigma(|\nabla u^\varsigma|^2)\mathring{u}^\varsigma\partial_{n^\varsigma}p^\varsigma + \beta_\varsigma(|\nabla u^\varsigma|^2)\mathring{p}^\varsigma\partial_{n^\varsigma}u^\varsigma\,dx\\ &+\sum_{\varsigma\in\{+,-\}}\int_{\partial\Omega^\varsigma}\beta_\varsigma(|\nabla u^\varsigma|^2)\nabla u^\varsigma\cdot\nabla p^\varsigma\,\theta_{n^\varsigma} + 2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma\cdot\nabla p^\varsigma)\partial_{n^\varsigma}u^\varsigma\mathring{u}^\varsigma ds,\end{aligned}$$

and taking into account Assumption 5.30, we see that the first two lines vanish and thus

$$
\begin{aligned}
dJ_1(\Omega)[\theta] = &\sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)(-\partial_\theta u^\varsigma)\partial_{n^\varsigma} p^\varsigma - \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_\theta p^\varsigma \partial_{n^\varsigma} u^\varsigma \, dx \\
&+ \sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\nabla u^\varsigma \cdot \nabla p^\varsigma \, \theta_{n^\varsigma} \, ds - \int_\Gamma 2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma \cdot \nabla p^\varsigma)\partial_{n^\varsigma} u^\varsigma \partial_\theta u^\varsigma ds,
\end{aligned} \tag{5.76}
$$

where $\partial_\theta u^\varsigma := \nabla u^\varsigma \cdot \theta$. According to the structure theorem the right-hand side of (5.76) depends linearly on $\theta_n = \theta \cdot n$. To see this split θ into normal and tangential part on Γ: $\theta_\Gamma := \theta|_\Gamma - \theta_n n$, where $\theta_n := \theta \cdot n$. The continuity of θ on $\overline{D}$ yields $\theta_\Gamma^+ = \theta_\Gamma^-$ and the equation $\nabla_\Gamma p^+ = \nabla_\Gamma p^-$ on Γ implies $\partial_{\theta_\Gamma} p^+ = \nabla_\Gamma p^+ \cdot \theta_\Gamma = \nabla_\Gamma p^- \cdot \theta_\Gamma = \partial_{\theta_\Gamma} p^-$. Therefore the tangential terms in (5.76) vanish:

$$
\begin{aligned}
\sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_\theta p^\varsigma \partial_{n^\varsigma} u^\varsigma \, dx = &\sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)(\partial_{n^\varsigma} p^\varsigma \partial_{n^\varsigma} u^\varsigma)\theta_{n^\varsigma} \, dx \\
&+ \underbrace{\sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_{n^\varsigma} u^\varsigma (\nabla_\Gamma p^\varsigma \cdot \theta_\Gamma^\varsigma) \, dx}_{=0,(5.54)} .
\end{aligned}
$$

Similarly one may check

$$
\begin{aligned}
&\sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_\theta u^\varsigma \partial_{n^\varsigma} p^\varsigma \, ds + \int_\Gamma \hat\beta_{\varsigma,u^\varsigma}'(\nabla u^\varsigma \cdot \nabla p^\varsigma)\partial_{n^\varsigma} u^\varsigma \partial_\theta u^\varsigma \, ds \\
&= \sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_{n^\varsigma} u^\varsigma \partial_{n^\varsigma} p^\varsigma \theta_n \, ds + \int_\Gamma 2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma \cdot \nabla p^\varsigma)\partial_{n^\varsigma} u^\varsigma \partial_{n^\varsigma} u^\varsigma \theta_n \, ds.
\end{aligned}
$$

Thus we finally obtain from (5.76) the boundary expression

$$
\begin{aligned}
dJ_1(\Omega)[\theta] = &- \sum_{\varsigma\in\{+,-\}} \int_\Gamma 2\beta_\varsigma'(|\nabla u^\varsigma|^2)(\nabla u^\varsigma \cdot \nabla p^\varsigma)(\partial_{n^\varsigma} u^\varsigma)^2 \, \theta_{n^\varsigma} ds \\
&+ \sum_{\varsigma\in\{+,-\}} \int_\Gamma \beta_\varsigma(|\nabla u^\varsigma|^2)\nabla_\Gamma u^\varsigma \cdot \nabla_\Gamma p^\varsigma \, \theta_{n^\varsigma} - \beta_\varsigma(|\nabla u^\varsigma|^2)\partial_{n^\varsigma} u^\varsigma \partial_{n^\varsigma} p^\varsigma \, \theta_{n^\varsigma} \, ds,
\end{aligned}
$$

which is equivalent to (5.72).

Remark 5.31. *Note that the functions*

$$
\mathring{p}(x) := \begin{cases} \mathring{p}^+(x), & x \in \Omega^+ \\ \mathring{p}^-(x), & x \in \Omega^- \end{cases} \qquad \mathring{u}(x) := \begin{cases} \mathring{u}^+(x), & x \in \Omega^+ \\ \mathring{u}^-(x), & x \in \Omega^- \end{cases}
$$

introduced in (5.75) are piecewise H^1-functions, but do not belong to $H_0^1(D)$. Therefore it is not allowed to insert them as test functions in the adjoint or state equation.

Remark 5.32. *If the transmission coefficients are constant in each domain, that is $\beta'(|\nabla u|^2, x) = 0$, then the formula coincides with the one in [3]. To the author's knowledge this formula also corrects the one in [29]. Using Cea's original method would lead to the wrong formula*

$$
dJ_1(\Omega)[\theta] = \int_\Gamma \left[\beta(|\nabla u|^2, x)\nabla u \cdot \nabla p\right]_\Gamma \theta_n \, ds.
$$

Chapter 6

Minimization using the volume expression

In this chapter we build the foundation for the numerical simulations presented in Chapter 7 using the volume expression of the shape derivative. As we shall see the most commonly used gradient algorithm in shape optimization can be interpreted as a discretization of gradient flows, where the flow depends on the choice of metric. For each time step the flow will belong to a certain group of diffeomorphisms. Therefore, we first review the construction of Michelletti to construct special metric groups of diffeomorphisms. In the subsequent section, this construction will be specialised to the case, where the diffeomorphisms are generated by velocity fields. This setting is appropriate for the volume expression. We use the volume expression to define gradient algorithms from two perspectives: (i) the *(classical) Eulerian point of view* in which the domain is moved in each iteration step and (ii) the *Lagrangian point of view*, where the initial domain is fixed, but the equations transform during the iterations. This latter approach allows calculations on a fixed grid and makes the method very attractive. Finally, we review representations of the shape derivative in the space of splines and recall the level set method.

6.1 A glimpse at the Michelletti construction

In the introduction of this thesis, we discussed two different ways to describe subsets of $2^{\mathbf{R}^2}$, on the one hand by means of curves and on the other by homeomorphisms in the plane. The first approach yields Riemannian manifolds and thus once a Riemannian metric is defined, we can speak of geodesics in these manifolds. The second approach yields complete metric spaces, which are not necessarily smooth manifolds. While the construction of the shape spaces as spaces of curves is naturally related to the boundary expression of the shape derivative[1], the volume expression is related to groups of homeomorphisms/diffeomorphisms constructed by Michelletti [70].

6.1.1 Michelletti space

The Michelletti space is a special case of a *diffeomorphism (sub-)group* from $\mathbf{R}^d$ into itself, which consist of perturbations of the identity. As in the introduction, we work with the

[1]Strictly speaking it is possible also to use the volume expression with the shape spaces, but it is not the natural choice.

space $\Theta := C_b^{0,1}(\mathbf{R}^d, \mathbf{R}^d)$, that is, the space of bounded Lipschitz continuous functions in $\mathbf{R}^d$.[2] We refer to Chapter 3 in [37] for other choices of Θ. Let us introduce the set

$$\mathrm{End}(\Theta) := \{f + \mathrm{id} : \ f \in \Theta\}.$$

It is shown in [37, Thm. 2.1, p. 125] and [37, Ex. 2.1–2.3., pp. 125–133] that the set

$$\mathcal{F}(\Theta) := \{\mathrm{id} + f : \ f \in \Theta, \ f + \mathrm{id} \ \text{ is bijective and } \ (f + \mathrm{id})^{-1} \in \mathrm{End}(\Theta)\}$$

is a *group of composition* with unit element $\mathrm{id}(x) := x$. It may be turned into a metric space by equipping it with the metric

$$d_{\mathcal{C}}(F, \tilde{F}) := \text{Ł}(F \circ \tilde{F}^{-1}, \mathrm{id}), \quad F, \tilde{F} \in \mathcal{F}(\Theta),$$

where the function Ł is defined for all $F \in \mathcal{F}(\Theta)$ by

$$\text{Ł}(F, \mathrm{id}) := \inf_{\substack{F = F_1 \circ \cdots \circ F_n \\ F_k \in \mathcal{F}(\Theta)}} \sum_{k=1}^{n} \|F_k - \mathrm{id}\|_\Theta + \|F_k^{-1} - \mathrm{id}\|_\Theta.$$

The function $F \mapsto \text{Ł}(F, \mathrm{id})$ may be interpreted as the length from F to id. The following result is a special case of [37, Thm. 2.6, p.134].

Theorem 6.1. *The space $(\mathcal{F}(\Theta), d_{\mathcal{C}})$ is a complete metric space.*

Notice that the continuity of $\Theta \to \mathbf{R} : \ x \mapsto f(x)$ is essential to prove the completeness stated in the previous theorem. If Θ is a Hilbert space this condition ensures the existence of a reproducing kernel, compare Section 6.2. For any closed or open crack free[3] set $\omega_0 \in \mathbf{R}^d$, we have that $\mathcal{S}_{\omega_0} := \{F \in \mathcal{F}(\Theta) : \ F(\omega_0) = \omega_0\}$ is a closed subgroup of $\mathcal{F}(\Theta)$. Therefore we can build the quotient $\mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$. Since by definition $d_{\mathcal{C}}$ is right invariant, that is, for all $F, \tilde{F}, H \in \mathcal{F}(\Theta)$

$$d_{\mathcal{C}}(F \circ H, \tilde{F} \circ H) = d_{\mathcal{C}}(F, \tilde{F}),$$

it induces a right invariant metric on the quotient space $\mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$

$$d'_{\mathcal{C}}([F], [\tilde{F}]) := \inf_{H \in \mathcal{S}_{\omega_0}} d_{\mathcal{C}}(F, \tilde{F} \circ H),$$

where $[F], [\tilde{F}] \in \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$. From [37, Thm. 2.8, p.141] we know that $(d'_{\mathcal{C}}, \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0})$ is a complete metric space. This result remains true if we choose Θ to be $C(\mathbf{R}^d, \mathbf{R}^d)$ or $C_b^k(\mathbf{R}^d, \mathbf{R}^d)$. The first space denotes the set of all continuous bounded functions and the latter one the set of k-times differentiable functions with bounded derivatives.

Each factorization $F = F_1 \circ \cdots \circ F_n = (I + \theta_0) \circ \cdots \circ (I + \theta_n) \in \mathcal{F}(\Theta)$ can be viewed as a piecewise continuous path $\Phi : [0, 1] \to \mathcal{F}(\Theta)$ by assigning for any subdivision $0 = t_0 < t_1 < \cdots < t_n = 1$ the mapping

$$\Phi(t) := \begin{cases} \mathrm{id} & \text{if } t \in [0, t_1) \\ (\mathrm{id} + \theta_0) & \text{if } t \in [t_1, t_2) \\ (\mathrm{id} + \theta_0) \circ (I + \theta_1) & \text{if } t \in [t_2, t_3) \\ \vdots & \\ (I + \theta_0) \circ (I + \theta_1) \circ \cdots \circ (I + \theta_n) & \text{if } t \in [t_{n-1}, 1] \end{cases}.$$

[2] The original construction of Michelletti was performed for the space $\Theta = C_{b,0}^k(\mathbf{R}^d, \mathbf{R}^d)$ of all k-times differentiable functions from $\mathbf{R}^d$ to $\mathbf{R}^d$ with partial derivatives vanishing at infinity. Here, $k \geq 0$ is arbitrary, but finite.

[3] An open set $\Omega \subset \mathbf{R}^d$ is *crack free* if $\mathrm{int}(\overline{\Omega}) = \Omega$.

The construction of the metric $d_{\mathcal{C}}$ can be extended to the *Fréchet spaces*[4] $C_b^\infty(\mathbf{R}^d, \mathbf{R}^d) := \cap_{k\in\mathbf{N}} C_b^k(\mathbf{R}^d, \mathbf{R}^d)$ and $C_{b,0}^\infty(\mathbf{R}^d, \mathbf{R}^d) := \cap_{k\in\mathbf{N}} C_{b,0}^k(\mathbf{R}^d, \mathbf{R}^d)$, where $C_{b,0}^k(\mathbf{R}^d, \mathbf{R}^d)$ is the space of k-times differentiable functions from $\mathbf{R}^d$ to $\mathbf{R}^d$ with vanishing partial derivatives at infinity; cf. [37].

Let a shape function $J : \Xi \subset 2^{\mathbf{R}^d} \to \mathbf{R}$ be given and assume that there is an open crack free set $\omega_0 \in \Xi$ such that $F(\omega_0) \in \Xi$ for all $F \in \mathcal{F}(\Theta)$. Then we may study the minimization problem

$$\min J_\alpha(\varphi) := J(\varphi(\omega_0)) + \alpha\, d_{\mathcal{C}}(\varphi, \mathrm{id}) \quad \text{ over } \mathcal{F}(\Theta),$$

where $\alpha > 0$ is a positive number. Notice that $d_{\mathcal{C}}(\varphi, \mathrm{id}) = \text{Ł}(\varphi, \mathrm{id})$. When J satisfies the condition $\forall H, \tilde{H}, F \in \mathcal{F}(\Theta)$ with $F(H(\omega_0)) = H(\omega_0)$, we have $J(F(H(\omega_0))) = J(F(\omega_0))$. Then we may formulate the problem on the quotient $\mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$

$$\min \bar{J}_\alpha([\varphi]) := J(\varphi(\omega_0)) + \alpha\, d'_{\mathcal{C}}([\varphi], [\mathrm{id}]) \quad \text{ over } \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0},$$

The crucial observation is that the continuity of a shape function J_α with respect to the Courant metric may be checked by the continuity of J along flows Φ_t generated by suitable vector fields θ as observed in [37, Thm. 6.1–6.3, pp. 202–207].

6.2 Groups of diffeomorphisms via velocity fields

Now we turn our attention to a special subset of $\mathcal{F}(\Theta)$ which comprises transformations generated by velocity fields. Further, we consider the constrained case, where we replace $\mathbf{R}^d$ in the definition of $\mathcal{F}(\Theta)$ by a regular domain $D \subset \mathbf{R}^d$ (cf. Definition 2.3). We denote throughout this section by $\Theta := C^{0,1}(\overline{D}, \mathbf{R}^d)$ the space of Lipschitz continuous functions in D equipped with norm

$$\|f\|_\Theta := \sup_{x\in\overline{D}} |f(x)| + \sup_{\substack{x\neq y\\ x,y\in\overline{D}}} \frac{|f(x) - f(y)|}{|x-y|}.$$

Definition 6.2. *A Banach space $\mathcal{H} \subset \Theta$ is called* admissible *if there exists a constant $C > 0$ with*

$$\forall \theta \in \mathcal{H} :\ \|\theta\|_\Theta \leq C\|\theta\|_{\mathcal{H}}. \tag{6.1}$$

Note that this last definition ensures that for any $x \in \mathcal{H}$ and $a \in \mathbf{R}^d$ the linear mapping

$$\mathcal{H} \to \mathbf{R}^d :\ v \mapsto v(x) \cdot a$$

is continuous. An admissible Hilbert space $\mathcal{H}$ is called *reproducing kernel Hilbert space* (RKHS). In each RKHS we may define a *(reproducing) kernel* as follows. For any $a \in \mathbf{R}^d$ and $x \in \overline{D}$ the mapping $v \mapsto \delta_x^a(v) := a \cdot v(x)$ is continuous, thus by Riesz representation theorem there exists $K_x^a \in \mathcal{H}$ such that $\delta_x^a(v) = (K_x^a, v)_{\mathcal{H}}$ for all $v \in \mathcal{H}$. For any $x, y \in \overline{D}$ the mapping $a \mapsto K_x^a(y)$ from belongs to $\mathcal{L}(\mathbf{R}^d, \mathbf{R}^d)$ and thus may be represented by a matrix $K(y, x) \in \mathbf{R}^{d,d}$ depending on y, x such that $K_x^a(y) = K(y, x)a$. The term 'reproducing' originates from the property

$$(K(\cdot, x)a, f)_{\mathcal{H}} = a \cdot f(x) \tag{6.2}$$

[4] A *Fréchet spaces* is a locally convex vector space which is metrizable and its topology can be induced by a translation invariant metric; [96, Def. VII.1.3].

for all $a \in \mathbf{R}^d$. So the inner product of the kernel with a function is the point evaluation. Using the reproducing property (6.2) one easily shows $K(x,y) = K^\top(y,x)$. An example of a kernel is the Gauss kernel, i.e.

$$K(x,y) = \exp\left(-\frac{|x-y|^2}{\sigma^2}\right) I,$$

where $\sigma > 0$ and I denotes the identity matrix in $\mathbf{R}^d$. These kernels can be used to obtain explicit expressions for gradients of Fréchet derivatives in image processing and diffeomorphic matching. We refer the reader to Chapter 9 of [97] for further details on reproducing kernels and how to use them for the approximation of smooth functions in the context of diffeomorphic matching.

Definition 6.3. *Let $D \subset \mathbf{R}^d$ be a k-regular domain, $k \geq 1$, with boundary $\Sigma := \partial D$. Assume that $\mathcal{H} \subset C^{0,1}(\overline{D}, \mathbf{R}^d)$ is admissible. Then we define $L_{m,0}([0,1], \mathcal{H})$, $m \in \{1,2\}$, to be the* Bochner space[5] *of all time-dependent vector fields $\theta : [0,1] \to \mathcal{H}$ satisfying the following three conditions:*

(i) For all $x \in \overline{D}$, the function $[0,1] \mapsto \mathcal{H} : \ t \mapsto \theta(t)$ is strongly Lebesgue measurable.

(ii) For almost all $t \in [0,1]$, we have $\theta(t) \in \mathcal{H}$ and

$$\|\theta\|_{L_m([0,1],\mathcal{H})} := \left(\int_0^1 \|\theta(s)\|_{\mathcal{H}}^m \, ds\right)^{\frac{1}{m}} < \infty.$$

(iii) Set $\theta(t,x) := \theta(t)(x)$. For all $x \in \Sigma$ and almost all $t \in [0,1] : \ \theta(t,x) \cdot n(x) = 0$, where n denotes the continuous unit normal vector field along Σ.

We denote by $L_m([0,1], \mathcal{H})$ the space of time-dependent vector fields satisfying (i)-(ii).

Remark 6.4. *Notice that by Pettis measurability theorem, a function $f : [0,1] \to \mathcal{H}$ is strongly Lebesgue measurable if and only if*

(a) For every continuous linear function $l \in \mathcal{H}'$ the function $t \mapsto l \circ f(t) : \ [0,1] \to \mathbf{R}$ is Lebesgue measurable.

(b) There exists a set $N \subset [0,1]$ of Lebesgue measure zero, such that $f([0,1]/N) \subset \mathcal{H}$ is separable with respect to the topology induced by the norm of $\|\cdot\|_{\mathcal{H}}$ on $\mathcal{H}$.

If $\mathcal{H}$ is a separable Banach space, then the condition (b) is automatically satisfied. We refer the reader to [7] for further details.

Recall that if $\mathcal{H} \subset \Theta = C^{0,1}(\overline{D}, \mathbf{R}^d)$ is admissible, then for $x \in D$ the mapping $\delta_x(v) := v(x)$ belongs to $\mathcal{H}'$ and thus by the previous remark $t \mapsto \delta_x \circ \theta(t) = \theta(t,x)$ is Lebesgue measurable for every $x \in D$ and $\theta \in L_m([0,1], \mathcal{H})$.

Lemma 6.5. *For $m \in \{1,2\}$ the space $L_{m,0}([0,1], \mathcal{H})$ is a Banach space.*

[5] See Definition A.5 for more details on Bochner spaces. Moreover, note that the space $L_{m,0}$ has to be understood as equivalence classes of functions as usual for L_p spaces.

Proof. Let $m \in \{1,2\}$. That $L_m([0,1],\mathcal{H})$ defined by the conditions $(i),(ii)$ is Banach space follows from the theory of Bochner spaces; cf. [7, 46]. Moreover, $L_2([0,1],\mathcal{H})$ is a Hilbert space if $\mathcal{H}$ is one. Now let $L_{m,0}([0,1],\mathcal{H})$ be defined by the conditions (i)-(iii). To check that it is Banach space let $(\theta_n)_{n\in\mathbf{N}}$ be any Cauchy sequence in $L_{m,0}([0,1],\mathcal{H})$ and $\theta_\infty \in L_m([0,1],\mathcal{H})$ its limit. By definition we have for all $n \in \mathbf{N}$, and for all $x \in \Sigma$ that $\theta_n(t,x)\cdot n(x) = 0$. Therefore for all $x \in \Sigma$ and almost all $t \in [0,1]$:

$$\begin{aligned} |\theta_\infty(t,x)\cdot n(x)| &= |\theta_\infty(t,x)\cdot n(x) - \theta_n(t,x)\cdot n(x)| \\ &\le \|n\|_{L_\infty(\Sigma)}\|\theta_n(t)-\theta_\infty(t)\|_{L_\infty(D,\mathbf{R}^d)} \\ &\le C\|n\|_{L_\infty(\Sigma)}\|\theta_n(t)-\theta_\infty(t)\|_{\mathcal{H}}, \end{aligned}$$

where we used that $\mathcal{H}$ is continuously embedded into $C^{0,1}(\overline{D},\mathbf{R}^d)$. An integration over $(0,1)$ yields

$$\int_0^1 |\theta_\infty(s,x)\cdot n(x)|^m\, ds \le C\|\theta_n - \theta_\infty\|^m_{L_m([0,1],\mathcal{H})}.$$

By definition the right hand side converges to zero as $n \to \infty$ and consequently it must hold that $\theta_\infty(t,x)\cdot n(x) = 0$ on Σ for almost all t. □

Now, we introduce for any admissible set $\mathcal{H} \subset \Theta$ the important sets

$$\begin{aligned} \mathcal{G}(\mathcal{H}) &:= \{\Phi_1^\theta :\ \theta \in L_1([0,1];\mathcal{H})\} \\ \mathcal{G}_0(\mathcal{H}) &:= \{\Phi_1^\theta :\ \theta \in L_{1,0}([0,1];\mathcal{H})\} \end{aligned}$$

of all flows defined by vector fields belonging to $L_1([0,1],\mathcal{H})$ respectively $L_{1,0}([0,1],\mathcal{H})$ and evaluated at $t = 1$.

Lemma 6.6. *Let $\mathcal{H} \subset \Theta := C^{0,1}(\overline{D},\mathbf{R}^d)$ be a Banach space with the property (6.1) and $L_1(0,1,\mathcal{H})$ be defined according to Definition 6.3. The set $\mathcal{G}_0(\mathcal{H})$ is a group, when the composition of two elements $\psi,\psi' \in \mathcal{G}_0(\mathcal{H})$ is defined by $(\psi\circ\psi')(x) := \psi(\psi'(x))$.*

Proof. Neutral element: Since $\theta = 0 \in L_{1,0}([0,1],\mathcal{H})$ it follows $\Phi_t^\theta = \mathrm{id}$ for all $t \in [0,1]$. Composition: Let $\Phi_t^{\theta_1},\Phi_t^{\theta_2}$ be given, where $\theta_1,\theta_2 \in L_{1,0}([0,1],\mathcal{H})$. We have to show that there is $\theta \in L_{1,0}([0,1],\mathcal{H})$ with $\Phi_1^{\theta_1}\circ\Phi_1^{\theta_2} = \Phi_1^\theta$. Define the vector field

$$\theta(t) := \begin{cases} \theta_2(2t) & \text{if } t \in [0,1/2) \\ 2\,\theta_1(2t-1) & \text{if } t \in [1/2,1] \end{cases}.$$

Clearly we have $\theta \in L_{1,0}([0,1],\mathcal{H})$, since $\theta = \chi_{[0,1/2)}(t)\theta_2(2t) + \chi_{[1/2,1]}(t)\theta_1(2t-1)$. Denote by Φ_t^θ the associated flow, then by uniqueness of the flow we get $\Phi_t^\theta = \Phi_t^{\theta_2}$ for all $t \in [0,1/2)$. Moreover, $t \mapsto \Phi_{2t-1}^{\theta_1}\circ\Phi_1^{\theta_2}$ solves

$$\dot{\Phi}_t^\theta = 2\,\theta_1(2t-1,\Phi_t^\theta), \quad \Phi_{1/2}^\theta = \Phi_1^{\theta_2}.$$

Therefore again by uniqueness of the flow

$$\Phi_t^\theta = \begin{cases} \Phi_t^{\theta_2} & \text{if } t \in [0,1/2) \\ \Phi_{2t-1}^{\theta_1}\circ\Phi_1^{\theta_2} & \text{if } t \in [1/2,1] \end{cases}$$

and consequently $\Phi_1^\theta = \Phi_1^{\theta_1}\circ\Phi_1^{\theta_2}$.
Inverse: Let $\theta \in L_{1,0}([0,1],\mathcal{H})$ with $\Phi_t^\theta \in \mathcal{G}_0(\mathcal{H})$. We have to find $\hat{\theta} \in L_{1,0}([0,1],\mathcal{H})$ with

$\Phi_1^{\hat{\theta}} \circ \Phi_1^{\theta} = \Phi_1^{\hat{\theta}} \circ \Phi_1^{\theta} = \mathrm{id}$. We show that $\hat{\theta}(t) := -\theta(1-t)$ is an appropriate vector field. For this note that $\Phi_t := \Phi_{1-t}^{\theta} \circ (\Phi_1^{\theta})^{-1}$ satisfies $\dot{\Phi}_t = -\theta(1-t, \Phi_t)$ on $[0,1]$ with $\Phi_0 = \mathrm{id}$ and thus $\Phi_t = \Phi_t^{\hat{\theta}}$, which entails $\Phi_1^{\hat{\theta}} \circ \Phi_1^{\theta} = \Phi_0^{\theta} \circ (\Phi_1^{\theta})^{-1} \circ \Phi_1^{\theta} = \mathrm{id}$ and $\Phi_1^{\theta} \circ \Phi_1^{\hat{\theta}} = \Phi_1^{\theta} \circ \Phi_0^{\theta} \circ (\Phi_1^{\theta})^{-1} = \mathrm{id}$. □

The previous result is important since in numerical simulations we usually deal with H^1-conformal spaces which do not allow a higher regularity. Functions from this space are usually continuous functions and satisfy (i) and (ii).

It is possible to define a distance between two elements $\psi, \psi' \in \mathcal{G}_0(\mathcal{H})$ by setting

$$d_{2,\mathcal{H}}(\psi, \psi') := \inf \left\{ \sqrt{\int_0^1 \|\theta(t)\|_{\mathcal{H}}^2 \, dt} : \theta \in L_{2,0}([0,1], \mathcal{H}) \text{ s.t. } \psi' = \psi \circ \Phi_1^{\theta} \right\},$$

and

$$d_{1,\mathcal{H}}(\psi, \psi') := \inf \left\{ \int_0^1 \|\theta(s)\|_{\mathcal{H}} \, ds : \theta \in L_{1,0}([0,1], \mathcal{H}) \text{ s.t. } \psi' = \psi \circ \Phi_1^{\theta} \right\}.$$

It is shown in [97, Thm. 8.18, p. 175] that $d_{2,\mathcal{H}}(\psi, \psi') = d_{1,\mathcal{H}}(\psi, \psi')$ for all $\psi', \psi \in \mathcal{G}_0(\mathcal{H})$, when $\mathcal{H} \subset C_c^1(D, \mathbf{R}^d)$ is admissible. Similar metrics to the above ones may be introduced on $\mathcal{G}(\mathcal{H})$. The natural energies associated with the path $t \mapsto \phi_t$ in the space $\mathcal{G}_0(\mathcal{H})$ are given by

$$\mathcal{E}^1(\phi_t) := \int_0^t \|\partial_t \phi(s, \phi^{-1}(s, \cdot))\|_{\mathcal{H}} \, ds, \quad \mathcal{E}^2(\phi_t) := \int_0^t \|\partial_t \phi(s, \phi^{-1}(s, \cdot))\|_{\mathcal{H}}^2 \, ds.$$

Note that $s \mapsto \phi_{ts}$ is a flow defined by the vector field $\theta(x,t) := t\partial_{st}\phi_{st} \circ \phi_{st}^{-1}$ and thus by definition

$$\begin{aligned} (d_{2,\mathcal{H}}(\mathrm{id}, \phi_t))^2 \leq & t \int_0^1 \|\partial_{st}\phi_{st} \circ \phi_{st}^{-1}\|_{\mathcal{H}}^2 \, ds \\ &= \int_0^t \|\partial_s \phi_s \circ \phi_s^{-1}\|_{\mathcal{H}}^2 \, ds \\ &= \mathcal{E}^2(\phi_t) \end{aligned}$$

and similarly $d_{1,\mathcal{H}}(\mathrm{id}, \phi_t) \leq \mathcal{E}^1(\phi_t)$. We have the following important theorem; cf. [97, Thm. 8.2, p.172].

Theorem 6.7. *For any admissible subset $\mathcal{H} \subset C^{0,1}(\overline{D}, \mathbf{R}^d)$ the group $(\mathcal{G}_0(\mathcal{H}), d_{2,\mathcal{H}})$ is also a complete metric space.*

The previous result is of fundamental importance for the existence of optimal shapes. In contrast to the shape spaces, the group of transformations are closed, but with Lipschitz transformations it allows still irregular shapes.

Similarly to the Michelletti construction it is natural for shape optimization problems to consider a subgroup of $\mathcal{G}_0(\mathcal{H})$ for any open subset $\omega_0 \in D$

$$\tilde{\mathcal{S}}_{\omega_0} := \{\Phi \in \mathcal{G}_0(\mathcal{H}) : \Phi(\omega_0) = \omega_0\}.$$

In complete analogy to $\mathcal{F}(\Theta)/\mathcal{S}_{\omega_0}$, we can define the quotient $\mathcal{G}_0(\mathcal{H})/\tilde{\mathcal{S}}_{\omega_0}$ and equip it with the quotient metric

$$d_{CG\mathcal{H}}([\psi], [\psi']) := \inf_{\Phi \in \tilde{\mathcal{S}}_{\omega_0}} d_{2,\mathcal{H}}(\psi, \psi' \circ \Phi).$$

Theorem 6.8. *The group $(\mathcal{G}_0(\mathcal{H})/\tilde{\mathcal{S}}_{\omega_0}, d_{CH\mathcal{H}})$ is a complete metric space.*

It is easily seen that the image set $\tilde{\mathcal{Z}}(\omega_0) := \{\Phi(\omega_0) : \Phi \in \mathcal{G}_0(\mathcal{H})\}$ is isomorphic to $\mathcal{G}_0(\mathcal{H})/\tilde{\mathcal{S}}_{\omega_0}$.

$$
\begin{tikzcd}
 & \mathcal{F}(\Theta) \arrow[r, "J_0"] \arrow[dl] \arrow[d] \arrow[dr, "\pi"] & \mathbf{R} \\
\mathbf{R} & \mathcal{Z}(\omega_0) \arrow[l, "J"'] \arrow[r] & \mathcal{F}(\Theta)/\mathcal{S}_{\omega_0} \arrow[u, "\bar{J}_0"']
\end{tikzcd}
\qquad
\begin{tikzcd}
 & \mathcal{G}_0(\mathcal{H}) \arrow[r, "J_0"] \arrow[dl] \arrow[d] \arrow[dr, "\pi"] & \mathbf{R} \\
\mathbf{R} & \tilde{\mathcal{Z}}(\omega_0) \arrow[l, "J"'] \arrow[r] & \mathcal{G}_0(\mathcal{H})/\tilde{\mathcal{S}}_{\omega_0} \arrow[u, "\bar{J}_0"']
\end{tikzcd}
$$

Figure 6.1: Relation between the shape functions J, J_0 and $\bar{J}_0$. The function π is the canonical subjection from the base space into the quotient space.

6.2.1 Minimisation over flows

Fix a set $\omega_0 \in \mathbf{R}^d$. Let $J : \Xi \to \mathbf{R}$ be a shape function defined on a $\mathcal{G}_0(\mathcal{H})$-stable set $\Xi \subset 2^{\mathbf{R}^d}$, for example $\Xi := \{F(\omega_0)| : F \in \mathcal{G}_0(\mathcal{H})\}$. Then we consider the following cost functions defined on $\mathcal{G}_0(\mathcal{H})$ and $\mathcal{G}_0(\mathcal{H})/\tilde{\mathcal{S}}_{\omega_0}$, respectively

$$J_\alpha(\phi) := J(\phi(\omega_0)) + \alpha(d_{2,\mathcal{H}}(\mathrm{id}, \phi))^2 \tag{6.3}$$

$$\bar{J}_\alpha([\phi]) := J(\phi(\omega_0)) + \alpha(d_{CG}([\mathrm{id}], [\phi]))^2. \tag{6.4}$$

For $\alpha = 0$ the minimisation over (6.4) is equivalent to

$$\min_{\Omega \in \tilde{\mathcal{Z}}(\omega_0)} J(\Omega).$$

By restricting the minimisation of $J_0(\phi)$ to the sets belonging to $\mathcal{G}_0(\mathcal{H})$ we restrict the minimisation of $J(\Omega)$ to the sets $\Omega \in \tilde{\mathcal{Z}}(\omega_0)$. If for instance ω_0 is a smooth set and $\mathcal{H} \subset C_c^1(D, \mathbf{R}^d)$ then the set $\tilde{\mathcal{Z}}(\omega_0)$ will be considerably smaller than the set of finite perimeter sets contained in D. Let $\gamma : [0,1] \to \partial\omega_0$ be a closed curve describing the boundary of ω_0. Pick any $\theta \in L_{2,0}([0,1], \mathcal{H})$. Then $\tilde{\gamma}(s) := \Phi_1^\theta(\gamma(s))$ describes the boundary of the new domain $\Omega = \Phi_1^\theta(\omega_0)$. Moreover, $\tilde{\gamma}$ is as smooth as Φ_1^θ.

The penalisation term $\alpha(d_{2,\mathcal{H}}(\mathrm{id}, \phi))^2$ forces the optimal set to be of the form $\Omega = \Phi_1^\theta(\omega_0)$ for some $\theta \in L_{2,0}([0,1], \mathcal{H})$.

The set $\omega_0 \subset \mathbf{R}^d$ is the model domain which is transformed by appropriate transformations in a desired set. By an optimal $\bar{\phi} \in \mathcal{G}_0(\mathcal{H})$ we mean

$$J_\alpha(\bar{\phi}) \le J_\alpha(\phi) \quad \text{for all } \phi \in \mathcal{G}_0(\mathcal{H}).$$

This approach does not allow topological changes of ω_0 and yields an optimal set $\bar{\varphi}(\omega_0)$ which is by definition diffeomorphic to ω_0.

6.2.2 Minimisation over vector fields

It can be shown [97, Thm. 11.2, p.254] that the minimisation of $J_\alpha(\phi)$ (defined by (6.3)) over $\mathcal{G}_0(\mathcal{H})$ is equivalent to $(\alpha > 0)$

$$\min \tilde{J}_\alpha(\theta) := J(\Phi_1^\theta(\Omega)) + \alpha \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds \quad \text{over} \quad L_{2,0}([0,1]; \mathcal{H}). \tag{6.5}$$

This reformulation has the advantage that one minimises over a Banach space $L_{2,0}([0,1]; \mathcal{H})$ and therefore standard tool from analysis, for instance, the Gateaux and Fréchet derivative are available to investigate (6.5). But the downside of this formulation is that in a minimisation algorithm we have to discretise the flow over the whole interval $[0,1]$ which is not necessary for an iterative algorithm minimizing only over J; compare Chapter 7. For $\alpha = 0$ it follows by definition

$$\min_{\theta \in L_{2,0}([0,\tau],\mathcal{H})} \tilde{J}_0(\theta) \quad \Leftrightarrow \quad \min_{\phi \in \mathcal{G}_0^2(\mathcal{H})} J_0(\phi) \quad \Leftrightarrow \min_{\Omega \in \tilde{\mathcal{Z}}(\omega_0)} J(\Omega).$$

Note that the previous three minimisation problems are not well-posed in general due to a lack of compactness. In this context let us mention the interesting work [43], where the sensitivity of the state with respect to the velocity is discussed where the state solves the Navier-Stokes equation.

We continue here the discussion of the existence of optimal shapes from Subsection 2.4.4.

Definition 6.9. *Let $k \geq 0$ and $D \subset \mathbf{R}^d$ be be regular domain. Then we say a sequence $(f_n)_{n\in\mathbf{N}}$ in $C^k(D, \mathbf{R}^d)$ converges uniformly to $f \in C^k(D, \mathbf{R}^d)$ if $\lim_{n\to\infty} \|f_n - f\|_{C^k(D,\mathbf{R}^d)} = 0$. It converges uniformly on compact subsets of D if for all compact $K \subset D$*

$$\lim_{n\to\infty} \|f_n - f\|_{C^k(K,\mathbf{R}^d)} = 0.$$

The C^k-norm is given by

$$\|u\|_{C^k(\Omega,\mathbf{R}^d)} := \sum_{i=1}^{d} \sum_{\substack{\gamma\in\mathbf{N}^d \\ |\gamma|\leq k}} \|\partial^\gamma u^i\|_{L_\infty(\Omega)},$$

where for any $\gamma = (\gamma_1, \dots, \gamma_d) \in \mathbf{N}^d$, we set $\partial^\gamma := \partial_{x_1}^{\gamma_1} \cdots \partial_{x_d}^{\gamma_d}$.

Let us introduce

$$\mathcal{G}_0^2(\mathcal{H}) := \{\Phi_1^\theta | \, \theta \in L_{2,0}([0,1], \mathcal{H})\}.$$

Theorem 6.10. *Let $\mathcal{H} \subset C_c^{k+1}(D, \mathbf{R}^d), (k \geq 0)$ be an admissible space and $\omega_0 \subset D$ contained in a ∞-regular domain $D \subset \mathbf{R}^d$ with boundary $\Sigma := \partial D$. Let $J : \Xi \subset 2^D \to \mathbf{R}$ be a shape function such that $\mathcal{G}_0^2(\mathcal{H}) \to \mathbf{R} : \varphi \mapsto J(\varphi(\omega_0))$ is bounded from below and lower semi-continuous for the uniform convergence on compact subsets of D. Put $\hat{J}(\theta) := J(\Phi_1^\theta(\omega_0)) + \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds$. Then the minimisation problem*

$$\inf_{\theta \in L_{2,0}([0,1],\mathcal{H})} \hat{J}(\theta),$$

has at least one solution.

Proof. Put $j := \inf_{\theta \in L_{2,0}([0,1],\mathcal{H})} \hat{J}(\theta)$. Now let $(\theta_n)_{n\in\mathbf{N}}$ be a minimizing sequence in the Hilbert space $L_{2,0}([0,1], \mathcal{H})$ such that $j := \lim_{n\to\infty} \hat{J}(\theta_n)$. We may subtract a weakly converging subsequence $(\theta_{n_k})_{k\in\mathbf{N}}$ with limit θ^∞. But the weak convergence of $(\theta_{n_k})_{k\in\mathbf{N}}$ to some $\theta \in L_{2,0}([0,1], \mathcal{H})$ implies that $\Phi_1^{\theta_n}$ and its derivatives converge against $\Phi_1^{\theta^\infty}$. Thus by the lower semi-continuity of J and $\theta \mapsto \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds$, we get

$$\hat{J}(\theta^\infty) \leq \lim_{k\to\infty} J(\Phi_1^{\theta_{n_k}}(\omega_0)) = \inf_{\theta \in L_{2,0}([0,1],\mathcal{H})} \hat{J}(\theta).$$

Example 6.11. *Let us consider for regular domain $D \subset \mathbf{R}^d$ the simple cost function $J(\Omega) := \int_\Omega f \, dx$ for some function $f \in C(\mathbf{R}^d)$ which is assumed to be negative on a set of positive measure, i.e. $f(x) < 0$ on some set $\Omega \subset \mathbf{R}^d$ with $m(\Omega) > 0$. Then*

$$\begin{aligned}\hat{J}(\theta) &= \int_{\Phi_1^\theta(\omega_0)} f \, dx + \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds \\ &= \int_{\omega_0} \det(\partial \Phi_1^\theta) f \circ \Phi_1^\theta \, dx + \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds.\end{aligned}$$

Clearly if $\mathcal{H} \subset C^3_c(D, \mathbf{R}^d)$ then $\varphi \mapsto J(\varphi(\omega_0))$ is continuous with respect to the uniform convergence on compact subsets of D (in $C^3_c(D, \mathbf{R}^d)$). Therefore the minimisation problem

$$\inf_{\theta \in L_{2,0}([0,1],\mathcal{H})} \hat{J}(\theta),$$

admits a solution. This solution is in general different from the global solution given by the open non-empty set $\Omega^* := f^{-1}((-\infty, 0))$.

6.3 Gradient flow and $\mathcal{H}$-gradient

Let $\mathcal{H} \subset C^{0,1}(\overline{D}, \mathbf{R}^d)$ be an admissible space, where $D \subset \mathbf{R}^d$ is a regular domain with boundary $\Sigma := \partial D$. An obvious choice for an admissible space[6] is $\mathcal{H} := H^k(D, \mathbf{R}^d) \cap H^1_0(D, \mathbf{R}^d)$ with $k \geq 1$ big enough, but also any H^1-conformal finite element space like linear or higher order Lagrange finite elements $\mathcal{H} := V_h \subset W^1_\infty(D, \mathbf{R}^d) \subset H^1(D, \mathbf{R}^d)$. Consider a shape function $J : \Xi \subset 2^D \to \mathbf{R}$ defined on a stable set $\Xi \subset 2^D$ and assume that it is shape differentiable at $\Omega \subset D$ in all directions $\theta \in C^\infty_c(D, \mathbf{R}^d)$. Moreover, assume that the shape derivative $\theta \mapsto dJ(\Omega)[\theta]$ can be extended to an element of $\mathcal{H}'$. Under these assumptions we make the following definitions.

Definition 6.12. *Let $J : \Xi \to \mathbf{R}$ be as described before and $\omega_0 \in \Xi$.*

(i) The $\mathcal{H}$-gradient of J at $\Omega \in \Xi$, denoted $\nabla^{\mathcal{H}} J(\Omega) \in \mathcal{H}$, is defined by

$$dJ(\Omega)[\zeta] = (\nabla^{\mathcal{H}} J(\Omega), \zeta)_{\mathcal{H}} \quad \text{for all } \zeta \in \mathcal{H}. \tag{6.6}$$

(ii) A function $\phi_t : [0, \infty) \to \mathcal{G}_0(\mathcal{H})$ satisfying

$$-\partial_t \phi_t = \nabla^{\mathcal{H}} J(\phi_t(\omega_0)) \circ \phi_t \quad \text{in } D \times (0, T] \tag{6.7}$$

is called gradient flow *of J in $\mathcal{G}_0(\mathcal{H})$ with respect to the metric $(\cdot,\cdot)_{\mathcal{H}}$.*

Remark 6.13. *One has to be careful with the definition of the derivative $\partial_t \phi$. Here, we define the partial derivative $\partial_t \phi(t)(x)$ pointwise in $\mathbf{R}^d$. When we only abstractly consider $\mathbf{R} \to \mathcal{G}_0(\mathcal{H}) : t \mapsto \phi(t)$ and view $\mathcal{G}_0(\mathcal{H})$ as manifold then one would expect the derivative $\partial_t \phi(t)$ to belong to the tangent space $\mathcal{H} = T_{\phi(t)} \mathcal{G}_0(\mathcal{H})$ and thus also the $\mathcal{H}$-gradient will be an element of the tangent space and thus $t \mapsto \partial_t \phi(t)$ is a vector field on $\mathcal{G}_0(\mathcal{H})$ along $t \mapsto \phi(t)$. Basically in infinite dimensions we have two different types of tangential vectors: the operational and the kinematic; cf. [64, Chap. VI]. The first one is defined as a first order differential operator on equivalence classes of smooth functions (germs) and the second one by equivalence classes of curves. For an example of a first order operator in the context of shape functions see Remarks 2.34. For the development of C^k-manifolds the view of tangent vectors as equivalence classes of curves is essential.*

[6] Note that Lipschitz functions $f \in C^{0,1}(\overline{D}, \mathbf{R}^d)$ and $W^1_\infty(D, \mathbf{R}^d)$ functions may be identified with each other by Rademacher's theorem. But in general those spaces are not equal for non-smooth boundary $\Sigma = \partial D$. Moreover, any Lipschitz function $f : D \to \mathbf{R}^d$ on an arbitrary domain D may be extended to a Lipschitz function on whole $\mathbf{R}^d$ with the same Lipschitz constant. This result is known as the Kirszbraun theorem [62].

Let $t \mapsto \phi_t$ be a gradient flow in $\mathcal{G}_0(\mathcal{H})$, $\omega_0 \in \Xi$ and suppose that $J \in C^1_D(\Xi)$. Then we infer directly from Theorem 2.10 (ii) that $\theta(z,t) := \partial_t \phi(t, \phi^{-1}(t,z))$ generates the transformation ϕ_t and thus we can compute

$$\begin{aligned}\frac{d}{dt} J(\phi_t(\omega_0)) &= dJ(\phi_t(\omega_0))[\partial_t \phi_t(\phi_t^{-1})] \\ &= (\nabla^{\mathcal{H}} J(\phi_t(\omega_0)), \partial_t \phi_t(\phi_t^{-1}))_{\mathcal{H}} \\ &= -\|\partial_t \phi_t(\phi_t^{-1})\|^2_{\mathcal{H}} \le 0.\end{aligned}$$

Therefore the cost function J decreases along the trajectory $t \mapsto \phi_t$ and $\phi_t \in \mathcal{G}_0(\mathcal{H})$ as long as $\int_0^t \|\partial_t \phi(\phi^{-1})\|^2_{\mathcal{H}}\, dt < \infty$ for $t > 0$, that is $\phi_t \in \mathcal{G}^2_0(\mathcal{H})$. Moreover, we also have a bound for how much J decreases at least since

$$J(\phi_t(\omega_0)) - J(\omega_0) = -\int_0^t \|\nabla^{\mathcal{H}} J(\phi_s(\omega_0))\|^2_{\mathcal{H}}\, ds \quad \text{for all } t \in [0, \infty].$$

Observe that in order to evaluate $\nabla^{\mathcal{H}} J(\phi_t(\omega_0))$, we have to move the domain ω_0 to $\omega_{0t} := \phi_t(\omega_0)$. As shown in [24] given a linear positive definite operator $L : \mathcal{H} \to \mathcal{H}$ allows us to define a modified flow by

$$\partial_t \phi_t = -L \nabla^{\mathcal{H}} J(\phi_t(\omega_0))(\phi_t). \tag{6.8}$$

Similar to the above calculations, we obtain

$$\begin{aligned}\frac{d}{dt} J(\phi_t(\omega_0)) &= dJ(\phi_t(\omega_0))[\partial_t \phi_t(\phi_t^{-1})] \\ &= -(\nabla^{\mathcal{H}} J(\phi_t(\omega_0)), L \nabla^{\mathcal{H}} J(\phi_t(\omega_0)))_{\mathcal{H}} \le 0.\end{aligned}$$

Depending on the problem one may choose L in such a way that J decreases faster along ϕ_t defined by (6.8) rather than (6.7).

Remark 6.14.

(i) *For certain problems the space $\mathcal{H}$ will depend on Ω and thus the metric $(\cdot,\cdot)_{\mathcal{H}(\Omega)}$ would be variable in Ω. For instance let $\mathcal{H} := H^1(\Omega, \mathbf{R}^d)$ and $J(\Omega) = \int_\Omega f\, dx$ with derivative $dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(\theta) f + \nabla f \cdot \theta\, dx$. Then $\nabla^{\mathcal{H}} J(\Omega)$ is defined by*

$$\int_\Omega \operatorname{div}(\zeta) f + \nabla f \cdot \zeta\, dx = (\nabla^{\mathcal{H}} J(\Omega), \zeta)_{H^1(\Omega)} \quad \text{for all } \zeta \in H^1(\Omega).$$

In this case the metric changes with the evolution of ϕ_t; see also Section 6.4 for more examples.

(ii) *It is worth noting that the definition of the $\mathcal{H}$-gradient in (6.6) makes sense if the shape derivative $dJ(\Omega)$ belongs to the dual of space $\mathcal{H}'$. As a result we are able to produce $\mathcal{H}$-gradients which do not generate a flow Φ_t satisfying (2.3). Nevertheless, choosing an appropriate metric and Hilbert space $\mathcal{H}$ will ensure a smooth enough $\mathcal{H}$-gradient.*

(iii) *Later we will choose Hilbert spaces $\mathcal{H}$ which do not belong to $Lip_0(D, \mathbf{R}^d)$, but to spaces containing it. When the boundaries $\Sigma = \partial D$ and $\Gamma = \partial\Omega$ are sufficiently smooth, then the numerical results show that the solutions are smooth and the flow (6.7) is well-defined, depending on the nature of the PDE constraint.*

6.4 Descent directions and the $\mathcal{H}$-gradient

Let $D \subset \mathbf{R}^d$ be an open and bounded set with smooth boundary $\Sigma := \partial D$. Let $\Xi \subset 2^D$ be a weakly flow stable. We consider a shape differentiable function $J \in C^1_D(\Xi)$ with derivative $G_\Omega := dJ(\Omega) \in \mathcal{H}'$ for all $\Omega \in \Xi$.

Definition 6.15. *We call a vector $\theta \in \mathcal{H}$ descent direction for J at $\Omega \in \Xi$ if there exists $t > 0$ such that $J(\Phi_t(\Omega)) \leq J(\Omega)$, where Φ_t denotes the flow generated by θ. In particular, any $\theta \in \mathcal{H}$ such that $dJ(\Omega)[\theta] < 0$ is a descent direction.*

We infer directly from (6.12) that $\theta := -\nabla^{\mathcal{H}} J$ is a *descent direction* for J since $dJ(\Omega)[-\nabla^{\mathcal{H}} J(\Omega)] < 0$. In this section, we give some examples of possible metrics to define the $\mathcal{H}$-gradient. According to Theorem 2.38 we know that if a shape function is of finite order, then it belongs to some Hilbert space H^{-s} with $s \geq 0$ big enough. The order also depends on the regularity of the domain, therefore s can vary during the change of the shape. Alternatively, to represent the shape derivative in a space $\mathcal{H}$ with the respective metrics it is possible to directly obtain descent directions as subsequently explained. In this section $\mathcal{H}$ will always be a Hilbert space of functions from Ω or D into $\mathbf{R}^d$, where the set D is assumed to be at least a regular domain.

6.4.1 Derivative with respect to the nodes

Before giving different examples of metrics generating $\mathcal{H}$-gradient flows, we show how to obtain descent directions on a discrete level without solving an additional partial differential equation. Essentially this idea goes back to [39], where it is used to obtain an optimal triangulation for a fixed number of nodes.

Let $D \subset \mathbf{R}^2$ be admissible and $\Xi \subset 2^D$ be weakly flow stable. We consider a shape differentiable function $J \in C^1_D(\Xi)$ with derivative $G_\Omega := dJ(\Omega) \in \mathcal{H}'$ for all $\Omega \in \Xi$. Suppose $V_h \subset \mathcal{H}$ is a finite element space of dimension $2N \in \mathbf{N}$ and $\{\phi_1, \ldots, \phi_{2N}\}$ is a basis of V_h. Let Ω_h be a triangulation $\tau_h(x_1, \ldots, x_n)$ with nodes $\{x_1, \ldots, x_n\}$. Assume that the shape derivative $dJ(\Omega_h)[\theta]$ exists for all vector fields $\theta \in \mathcal{H}$. We make the ansatz

$$\theta_h(x) = \sum_{i=1}^{2N} a_i\, \phi_i(x), \quad (a_i \in \mathbf{R})$$

then $dJ(\Omega_h)[\theta_h] = \sum_{i=1}^{2N} a_i\, dJ(\Omega)[\phi_i]$, and thus setting $a_i := -dJ(\Omega_h)[\phi_i]$ implies that $dJ(\Omega)[\theta_h] \leq 0$. Note that the corresponding $\mathcal{H}$-gradient is the solution of: find $x \in \mathbf{R}^{2N}$ such that $Ix = a$, $(a := (a_1^\top, \ldots, a_N^\top)^\top)$. Here, I is the identity matrix in $\mathbf{R}^{2N,2N}$ and it can be interpreted as a metric on the discrete finite element space. Other choices for I to favor certain movements of the vectors a_i are possible.

Let now $D \subset \mathbf{R}^2$, $\mathcal{H} := H^1_0(D)$ and assume that $\{\psi_1, \ldots, \psi_N\} \subset H^1_0(D)$ are *Lagrange finite elements* which satsify $\psi_i(x_j) = \delta_{ij}$. Note that in this particular case $n = N$. We construct a basis of V_h by

$$\phi_i := e_1\, \psi_i \quad \text{and} \quad \phi_{n+i} = e_2\, \psi_i \quad \text{for } i = 1, \ldots N,$$

where e_1 and e_2 denote the canonical unit normal vectors in $\mathbf{R}^2$. Then the shape derivative in the direction ϕ_i coincides with the derivative of the function $J(\Omega_h)$ with respect to the x^1 or x^2 component of the i-th node $x_i = (x_i^1\ x_i^2)^\top$; cf. [39]. To be more precise denote by $(\mathbf{R}^2)^N \to 2^{\mathbf{R}^2}$ $(x_1, \ldots, x_N) \mapsto \Omega_h(x_1, \ldots, x_N)$ assigning to any N points $x_1, \cdots, x_N \in \mathbf{R}^2$

the corresponding discrete set Ω_h. Now, if we put $\hat{J}(x_1,\dots,x_N) := J(\Omega_h(x_1,\dots,x_N))$ then

$$\begin{aligned} dJ(\Omega_h)[\phi_i] &= \partial_{x_i^1}\hat{J}(x_1,\dots,x_N) \quad \text{for } i=1,\dots,N \\ dJ(\Omega_h)[\phi_i] &= \partial_{x_i^2}\hat{J}(x_1,\dots,x_N) \quad \text{for } i=N+1,\dots,2N. \end{aligned}$$

That $dJ(\Omega_h)[\phi_i] \neq 0$ in general, even if $\theta(x)\cdot n(x) = 0$ on $\partial\Omega_h$, is due to the fact that $\Phi_t(\Omega_h(x_1,\dots,x_N)) \neq \Omega_h(x_1,\dots,x_N)$ for all $t \in (0,\tau]$, which is only true in the discrete case. Note that this relation is not true for the boundary expression of the shape derivative in general since the required regularity for second order PDEs is H^2 and the regularity of linear finite elements cannot be improved. Nevertheless using H^2 conformal elements this representation remains true.

6.4.2 Flows generated by metrics of $H^1(\operatorname{div})$ and H^k

Subsequently let $D \subset \mathbf{R}^d$, $d = 2,3$, be a regular domain with boundary $\Sigma := \partial D$. Moreover, denote by $\Omega \subset D$ any open subset with boundary $\Gamma := \partial\Omega$ such that for some $\varepsilon > 0$ we have $d_\Omega(x) > \varepsilon$ for all $x \in \Sigma$. We will denote by n the unit normal vector along Γ.

Example 6.16 (H^1 *flow - boundary shape gradient*). *Let Γ and Σ be of class C^k, where $k \geq 3$. Assume $J(\Omega)$ admits a shape derivative in a boundary form as in (2.17):*

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} g\,\theta\cdot n\,ds \tag{6.9}$$

where $g \in H^{k-3/2}(\partial\Omega)$. Take $\mathcal{H} = H^1(\Omega,\mathbf{R}^d)$ with inner product $(v,w)_{\mathcal{H}} = (v,w)_{H^1(\Omega,\mathbf{R}^d)}$. The $\mathcal{H}$-gradient $\theta := \nabla^{\mathcal{H}}J(\Omega)$ is solution of the variational problem

$$\int_\Omega \partial\theta : \partial\zeta + \theta\cdot\zeta\,dx = \int_\Gamma g\,\zeta\cdot n\,ds \quad \text{for all } \zeta \in H^1(\Omega,\mathbf{R}^d).$$

The strong form of this problem reads:

$$\begin{aligned} -\Delta\theta + \theta &= 0 \quad \text{in } \Omega \\ -\partial_n\theta &= g \quad \text{on } \Gamma. \end{aligned}$$

Example 6.17 (*Transmission problem - boundary expression*). *Assume that Γ is of class C^k, where $k \geq 3$. Set $\Omega^+ := \Omega$ and $\Omega^- := D\setminus\overline{\Omega}$ such that $D = \Omega^+\cup\Omega^-\cup\Gamma$. Assume that the shape derivative of $J(\Omega^+)$ has the form (2.17), i.e.*

$$dJ(\Omega^+)[\theta] = \int_\Gamma g\,\theta\cdot n\,ds$$

where $g \in H^{k-3/2}(\Gamma)$. Take $\mathcal{H} = H^1_0(D,\mathbf{R}^d)$ with inner product $(v,w)_{\mathcal{H}} := (v,w)_{H^1(D,\mathbf{R}^d)}$. The $\mathcal{H}$-gradient $\theta := \nabla^{\mathcal{H}}J(\Omega^+) \in \mathcal{H}$ solves the transmission problem

$$\int_D \partial\theta : \partial\zeta + \theta\cdot\zeta\,dx = \int_\Gamma g\,\zeta\cdot n\,ds \quad \text{for all } \xi \in \mathcal{H},$$

which has the following strong form

$$\begin{aligned} -\Delta\theta^+ + \theta^+ &= 0 \quad \text{in } \Omega^+ \\ -\Delta\theta^- + \theta^- &= 0 \quad \text{in } \Omega^- \\ \theta &= 0, \quad \text{on } \Sigma, \\ [\theta] = 0, \quad [\partial_n\theta] &= -g\,n \quad \text{on } \Gamma \end{aligned}$$

where $\theta = \theta^+\chi_{\Omega^+} + \theta^-\chi_{\Omega^-}$ and $[\partial_n\theta] := \partial_n\theta^+ - \partial_n\theta^-$.

Example 6.18 (H^1 *flow - volume expression*). *Let* Γ *and* Σ *be both of class* C^3 *and assume that* J *has a shape derivative of the form*

$$dJ(\Omega)[\theta] = \int_\Omega F_\Omega[\theta]\,dx, \tag{6.10}$$

where $F_\Omega : C_c^k(D,\mathbf{R}^d) \to H^1(\Omega,\mathbf{R})$, $k \geq 1$ *is linear in* θ. *Let* $\mathcal{H} = H^1(\Omega,\mathbf{R}^d)$ *and* $(v,w)_{\mathcal{H}} := (v,w)_{\mathcal{H}}$. *Assume that* F_Ω *can be extended to a function* $F_\Omega : H^1(D,\mathbf{R}^d) \to H^1(\Omega,\mathbf{R})$. *The* $\mathcal{H}$*-gradient* $\nabla^{\mathcal{H}} J(\Omega) := \theta \in H^1(\Omega,\mathbf{R}^d)$ *satisfies by definition*

$$\int_\Omega \partial\theta : \partial\zeta + \theta\cdot\zeta\,dx = \int_\Omega F_\Omega[\zeta]\,dx \quad \textit{for all } \zeta \in H^1(\Omega,\mathbf{R}^d).$$

Choosing $\mathcal{H} = H_0^1(D,\mathbf{R}^d)$ *instead of* $H^1(\Omega,\mathbf{R}^d)$ *yields the transmission problem: find* $\theta \in H_0^1(D,\mathbf{R}^d)$ *such that*

$$\int_D \partial\theta : \partial\zeta + \theta\cdot\zeta\,dx = \int_\Omega F_\Omega[\zeta]\,dx \quad \textit{for all } \zeta \in H_0^1(D,\mathbf{R}^d).$$

With such a choice we build an extension of θ *to* $\overline{D}$.

Example 6.19 (H^k *flow - volume expression*). *Assume that* Σ *is* C^1. *Consider the space* $\mathcal{H}^k = H^k(D,\mathbf{R}^d) \cap H_0^1(D,\mathbf{R}^d)$ *for* $k \geq 1$ *and the inner product* $(\theta,\zeta)_{\mathcal{H}} := (\theta,\zeta)_{H^k(D,\mathbf{R}^d)}$. *Assume* J *has a shape derivative* $dJ(\Omega)[\theta]$ *which belongs to the dual of* $\mathcal{H}^k$. *By the Riesz representation theorem the following equation admits a unique solution* $\theta \in \mathcal{H}^k$:

$$(\theta,\zeta)_{\mathcal{H}^k} = dJ(\Omega)[\zeta] \quad \textit{for all } \zeta \in \mathcal{H}^k.$$

By Sobolev embeddings, the vector field θ *can be made arbitrary smooth choosing* $k \geq 1$ *large enough.*

Example 6.20 ($H_0^1(\operatorname{div})$ *flow*). *Let* Γ *be smooth. In this example, we consider vector fields in*

$$\mathcal{H} := H_0^1(\operatorname{div})(D) := \{\boldsymbol{v} \in L_2(D,\mathbf{R}^d) :\ \operatorname{div}(\boldsymbol{v}) \in L_2(D,\mathbf{R}^d),\ v\cdot n = 0 \textit{ on } \Sigma\}.$$

This space becomes a Hilbert space when equipped with the metric

$$(\theta,\zeta)_{H_0^1(\operatorname{div})(D)} := \int_D \operatorname{div}(\theta)\operatorname{div}(\zeta) + \theta\cdot\zeta\,dx.$$

The associated $\mathcal{H}$*-gradient* $\theta =: \nabla^{\mathcal{H}} J$ *is defined as the solution of*

$$dJ(\Omega)[\zeta] = (\theta,\zeta)_{H_0^1(\operatorname{div})(D)} \quad \textit{for all } \zeta \in H_0^1(\operatorname{div})(D). \tag{6.11}$$

Assume that the shape derivative of J *has a boundary expression with regular* $g \in C^1(\overline{\Omega})$:

$$dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(g\,\theta)\,dx = \int_\Omega \nabla g\cdot\theta + g\operatorname{div}(\theta)\,dx.$$

Then we see that $dJ(\Omega) \in (H_0^1(\operatorname{div})(D))'$ *and thus* (6.11) *is well defined. Note that a solution* θ *is actually not regular enough to define a differentiable flow* Φ_t^θ. *Nevertheless, the solution will be more regularity if we assume higher regularity for the boundary* Σ.

Example 6.21 ($H^1_0(\operatorname{div}) \cap H^1(\operatorname{rot})$ ***flow***). *Assume $D \subset \mathbf{R}^d$, $(d = 2, 3)$, is a $C^{1,1}$-domain or convex. Let $\mathcal{H} := H^1_0(D, \mathbf{R}^d)$ be endowed with the scalar product*

$$(v, w)_{\mathcal{H}} := (\operatorname{div}(v), \operatorname{div}(w))_{L_2(D)} + (\operatorname{rot} v, \operatorname{rot} w)_{L_2(D,\mathbf{R}^d)} + (v, w)_{L_2(D,\mathbf{R}^d)}.$$

Let $\Omega \subset D \subset \mathbf{R}^d$ be a smooth set. The associated $\mathcal{H}$-gradient is defined as the solution of

$$dJ(\Omega)[\zeta] = (\theta, \zeta)_{\mathcal{H}} \text{ for all } \zeta \in H^1_0(D, \mathbf{R}^d).$$

This equation admits a unique solution; cf. [11].

Example 6.22 (*boundary versus domain representation*). *Consider the simple example $J(\Omega) = \int_{\mathbf{R}^d} \chi_\Omega \, dx$ of the volume of a domain Ω. When Γ is of class C^1, the normal vector n is $C(\partial\Omega)$ and*

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} \theta \cdot n \, ds. \tag{6.12}$$

In this case, we are in the framework of Example 6.17 and we can use $\mathcal{H} := H^1_0(D, \mathbf{R}^d)$ to get enough regularity for θ.

When Ω is only bounded and measurable, the integral representation (6.12) does not exist, but we can still compute the domain representation

$$dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(\theta) \, dx.$$

In this case, the required regularity $\theta \in W^{1,\infty}(D, \mathbf{R}^d)$ can be obtained by using $\mathcal{H} := H^k(D, \mathbf{R}^d) \cap H^1_0(D, \mathbf{R}^d)$ with k large enough as in Example 6.19. Using $\mathcal{H} := H^1_0(D, \mathbf{R}^d)$ in this case would not provide enough regularity for θ, but the finite element approximation would.

Using a bilinear form in Ω or D we obtain a vector field θ which is defined on the domain Ω or D and not only on the interface Γ. This is often a desired property for numerical applications. For instance in the level set method, the common practice is to obtain a vector field on the interface Γ and to extend it on the entire domain D by solving a parabolic equation. Moreover, this allows to use the volume expression (6.10) as in Example 6.18 instead of the boundary shape gradient (6.9) as in Examples 6.16 and 6.17. The volume expression (6.10) is easier to handle compared to the boundary expression (6.9) from a numerical point of view as it does not require to determine quantities on the interface such as the normal vector or the curvature which require interpolation and therefore lead to additional approximation errors.

Remark 6.23. *Note that the discrete finite element solution of the previous equations will be in $W^{1,\infty}$ and therefore after discretisation the flow will be well-defined.*

6.5 Lagrangian vs. Eulerian point of view

We begin with a definition which formalises the transformation behavior of the shape derivative under a change of variables.

Definition 6.24. *Let $(\phi_t)_{t\geq 0} : \mathbf{R}^d \to \mathbf{R}^d$ be a family of transformation and $D \subset \mathbf{R}^d$ be open and bounded. Assume that the shape function $J : \Xi \subset 2^D \to \mathbf{R}$ is shape differentiable in $\phi_t(\Omega) \subset \mathbf{R}^d$ for all $t \geq 0$. We say that the shape derivative $dJ(\phi_t(\Omega))$ admits a* fixed domain representation *if there is linear function $d\mathcal{J}^{\phi_t}(\Omega)[\cdot]$ depending on ϕ_t such that*

$$dJ(\phi_t(\Omega))[\theta] = d\mathcal{J}^{\phi_t}(\Omega)[\theta \circ \phi_t] \text{ for all } t \in [0, \tau], \text{ for all } \theta \in \mathcal{H}.$$

Example 6.25. *Let us again consider the shape function $J(\Omega) = \int_\Omega f\,dx$ with shape derivative $dJ(\Omega)[\theta] = \int_\Omega f \operatorname{div}(\theta) + \nabla f \cdot \theta\,dx$. Then*

$$d\mathcal{J}^{\phi_t}(\Omega)[\theta^t] = \int_\Omega \xi(t)\, f^t\, tr(\partial\theta^t B^\top(t)) + \xi(t)B(t)\nabla f^t \cdot \theta^t\,dx,$$

where $\xi(t) = \det(\partial\phi_t)$, $f^t = f \circ \phi_t$ and $B(t) = \partial\phi_t^{-\top}$.

Assume now that we have chosen a Hilbert space $\mathcal{H}$ of functions $f : D \subset \mathbf{R}^d \to \mathbf{R}^d$ with inner product $(\cdot,\cdot)_\mathcal{H}$. Given an isomorphism $\mathcal{K}(\phi_t) : \mathcal{H} \to \mathcal{H} : f \mapsto \mathcal{K}(\phi_t)(f)$ such that for some $C, c > 0$

$$c\|v\|_\mathcal{H} \le \|\mathcal{K}(\phi_t)(v)\|_\mathcal{H} \le C\|v\|_\mathcal{H} \quad \text{for all } v \in \mathcal{H},\ \text{for all } t \in [0,\infty)$$

we may introduce a new inner product on $\mathcal{H}$ by setting

$$(v,w)^{\phi_t}_\mathcal{H} := (\mathcal{K}(\phi_t)(v), \mathcal{K}(\phi_t)(w))_\mathcal{H}.$$

For the special (family of) isomorphisms $\mathcal{K}(\phi_t)(v) := v \circ \phi_t^{-1}$ it follows that solving

$$(\theta_t, \zeta)_\mathcal{H} = dJ(\phi_t(\Omega))[\zeta] \quad \text{for all } \zeta \in \mathcal{H} \tag{6.13}$$

where $\theta_t =: \nabla^\mathcal{H} J(\phi_t(\Omega))$ is equivalent to

$$(\theta^t, \tilde\zeta)^{\phi_t}_\mathcal{H} = d\mathcal{J}^{\phi_t}(\Omega)[\tilde\zeta] \quad \text{for all } \tilde\zeta \in \mathcal{H} \tag{6.14}$$

where $\theta^t(x) = \nabla^\mathcal{H} J(\phi_t(\Omega))\circ\phi_t(x)$ and in particular $\theta^t = \theta_t \circ \phi_t$. Now, the crucial observation is that we do not need to move the domain Ω in order to calculate θ^t, which makes it not necessary to move the domain to compute ϕ_t.

Example 6.26 ($H^1_0(D,\mathbf{R}^d)$). *Let J be as in Example 6.25. Equip $\mathcal{H} := H^1_0(D,\mathbf{R}^d)$ with inner product*

$$(v,w)_{H^1_0(D,\mathbf{R}^d)} := \int_D \partial v : \partial w + v \cdot w\,dx$$

and define the family of isomorphisms by

$$\mathcal{K}(\phi_t) : H^1_0(D,\mathbf{R}^d) \to H^1_0(D,\mathbf{R}^d) : v \mapsto v \circ \phi_t^{-1}.$$

Then after the change of variables $\phi_t(x) = y$ the new product $(v,w)^{\phi_t}_{H^1_0(D,\mathbf{R}^d)}$ on $H^1_0(D,\mathbf{R}^d)$ takes the form

$$(v,w)^{\phi_t}_{H^1_0(D,\mathbf{R}^d)} = \int_D A(t)\partial v : \partial w + \xi(t) v \cdot w\,dx.$$

Finally (6.14) reads

$$\int_D A(t)\partial\theta^t : \partial v + \xi(t)\theta^t \cdot v\,dx = \int_\Omega \xi(t)\, f^t\, tr(\partial v B^\top(t)) + \xi(t)B(t)\nabla f^t \cdot v\,dx$$

for all $v \in H^1_0(D,\mathbf{R}^d)$.

Example 6.27 ($H^1_0(\operatorname{div}, D)$). *Let J be as in Example 6.25. Equip $\mathcal{H} := H^1_0(\operatorname{div}, D)$ with the inner product*

$$(v,w)_{H^1_0(\operatorname{div},D)} := \int_D \operatorname{div}(v)\operatorname{div}(w) + v \cdot w\,dx$$

and define the isomorphism called Piola-Kirchoff transformation *(cf. [17, 43])* $\mathcal{K}(\phi_t) : H_0^1(\operatorname{div}, D) \to H_0^1(\operatorname{div}, D) : v \mapsto ((\det(\partial\phi_t))^{-1}\partial\phi_t\, v) \circ \phi_t^{-1}$. *Recalling the identity*

$$\operatorname{div}(v) \circ \phi_t = \xi^{-1}(t)\ \operatorname{div}(\xi(t)\,\partial\phi_t^{-1}\,(v \circ \phi_t))$$

the change of variables $\phi_t(x) = y$ *shows that the new product* $(v, w)^{\phi_t}_{H_0^1(\operatorname{div}, D)}$ *on* $H_0^1(\operatorname{div}, D)$ *takes the form*

$$(v, w)^{\phi_t}_{H_0^1(\operatorname{div}, D)} = \int_D \xi^{-1}(t)\,(\operatorname{div}(v)\ \operatorname{div}(w) + \partial\phi_t\, v \cdot \partial\phi_t\, w)\, dx.$$

Finally (6.14) *reads*

$$\begin{aligned}\int_D \xi^{-1}(t)\,(\operatorname{div}(v)\ \operatorname{div}(w) + \partial\phi_t\, v \cdot \partial\phi_t\, w)\, dx \\ = \int_\Omega f^t\ \operatorname{div}(v) + B(t)\nabla f^t \cdot \partial\phi_t\, v\, dx\end{aligned}$$

for all $v \in H_0^1(\operatorname{div}, D)$. *Notice that also* $(v, w)^{\phi_t}_{H_0^1(\operatorname{div}, D)}$ *is an inner product on* $H_0^1(\operatorname{div}, D)$ *and that the induced norm* $\|v\|_{H_0^1(\operatorname{div}, D), \phi_t} = \sqrt{(v, v)^{\phi_t}_{H_0^1(\operatorname{div}, D)}}$ *is equivalent to the norm* $\|\cdot\|_{H_0^1(\operatorname{div}, D)}$.

Definition 6.28. *When the gradient flow or $\mathcal{H}$-gradient is expressed on the* fixed domain Ω *such as in* (6.14) *we speak of the* Lagrangian point of view. *When the gradient flow or $\mathcal{H}$-gradient is expressed on the* moved domain $\phi_t(\Omega)$ *such as in* (6.13) *we speak of the* Eulerian point of view.

6.5.1 A simple transmission problem

Let us apply the Lagrangian point to a simple transmission problem with a domain cost function. We refer the reader to Subsection 7.2 for numerical results for the subsequent equations and to Section 5.4 for a non-linear variant of this model. We use the same notations as in Assumption 5.3 of Subsection 5.2.1. The governing equations describing the transmission problem read

$$\boxed{\begin{aligned} -\operatorname{div}(\beta_+\nabla u^+) = f &\quad \text{in } \Omega^+ \\ -\operatorname{div}(\beta_-\nabla u^-) = f &\quad \text{in } \Omega^- \\ u = 0 &\quad \text{on } \Sigma \end{aligned}} \tag{6.15}$$

supplemented by the transmission conditions

$$\boxed{\beta_+\partial_n u^+ = \beta_-\partial_n u^- \quad \text{and} \quad u^+ = u^- \quad \text{on } \Gamma.} \tag{6.16}$$

Here, we suppose that $f : \overline{D} \to \mathbf{R}$ is of class C^1 and $\beta^+, \beta^- > 0$ are positive numbers. We seek weak solutions of the equations (6.15)-(6.16) in $H_0^1(D)$, which takes into account the transmission conditions (6.16): Find $u \in H_0^1(D)$ such that

$$\int_D \beta_\chi \nabla u \cdot \nabla\psi\, dx = \int_D f\psi\, dx \quad \text{for all } \psi \in H_0^1(D), \tag{6.17}$$

where $\beta_\chi := \beta_+\chi + \beta_-(1-\chi)$. Given the target function $u_r \in C_b^1(\overline{D})$ the optimal design problem can be stated as:

$$\min J(\Omega) = \int_D |u(\chi_\Omega) - u_r|^2\, dx \quad \text{over } \chi_\Omega \in X(D), \tag{6.18}$$

where $u = u(\chi_\Omega) \in H_0^1(D)$ solves the state equation. Recall that $X(D)$ denotes the set of characteristic functions χ defined by measurable sets $\Omega \subset D$. Note that in general the minimisation problem (6.18) will be ill-posed and may lead in the limit to functions χ with values between 0 and 1; cf. [76]. The reason for this phenomenon is that $X(D)$ is not closed for the weak convergence in $L_p(D)$. This can be avoided by adding a perimeter term in J or by a Gagliardo penalisation as outlined in Section 2.4; cf. Sections 5.2-5.4. As discussed above, another way which is more adapted to the shape derivative, is the minimisation problem

$$\min \tilde{J}(\phi_1(\omega_0)) := J(\phi_1(\omega_0)) + (d_{2,\mathcal{H}}(\mathrm{id}, \phi_1))^2 \quad \text{over } \mathcal{G}_0(\mathcal{H}), \tag{6.19}$$

where $\omega_0 \subset D$ is some given set. By [97, Lem. 11.3, p. 254] the minimisation problem (6.19) is equivalent to

$$\min \hat{J}(\theta) := J(\Phi_1^\theta(\omega_0)) + \int_0^1 \|\theta(s)\|_{\mathcal{H}}^2 \, ds \quad \text{over } L_{2,0}([0,1], \mathcal{H}).$$

The penalisation term $(d_{2,\mathcal{H}}(\mathrm{id}, \phi_1))^2$ measures the energy it takes to deform the set ω_0 into the set $\phi_t(\omega_0)$ by means of the L_1 norm of the minimal vector field generating the flow connecting id and ϕ_1; cf. Section 6.2. Compared with the perimeter and Gagliardo penalisation the optimal set will be smoother. The existence can be easily established by an adaption of Theorem 6.10. A drawback of this minimisation problem is that we introduce a penalisation term.

The Lagrangian point of view of the transmission problem

The cost function J defined in (6.18) is known to be shape differentiable; cf. [82] and [3]. A non-linear generalisation of this model will be treated in Section 5.4. Let $\omega_0 \subset D$. Note that the cost function J defined above transforms under the change of variables ϕ_t as

$$J(\phi_t(\omega_0)) = \int_D \xi(t)|u_t \circ \phi^t - u_r \circ \phi_t|^2 \, dx, \tag{6.20}$$

where $\xi(t) := \det(\partial\phi_t)$. Setting $A(t) := \xi(t)\partial\Phi_t^{-1}\partial\Phi_t^{-\top}$ it can be seen by a change of variables that $u^t := u_t \circ \phi_t$ solves

$$\int_D \beta_\chi A(t)\nabla u^t \cdot \nabla\varphi \, dx = \int_D \xi(t) f^t \varphi \, dx \quad \text{for all } \varphi \in H_0^1(D). \tag{6.21}$$

Here, u_t solves the transmission problem (6.17) with the characteristic function $\chi = \chi_{\phi_t(\omega_0)}$. Let us introduce the associated Lagrangian of (6.20),(6.21):

$$G(t, \varphi, \psi) := \int_D \xi(t)|\varphi - u_r \circ \phi_t|^2 \, dx + \int_D \beta_\chi A(t)\nabla\varphi \cdot \nabla\psi \, dx - \int_D \xi(t) f^t \psi \, dx$$

From Lemma 2.14, we infer that $t \mapsto G(t, \varphi, \psi)$ is differentiable for all $\varphi, \psi \in H_0^1(D)$. Thus using the material from Chapter 4 it is readily seen that

$$\frac{d}{dt} J(\phi_t(\omega_0)) = \partial_t G(t, u^t, p^t),$$

where the perturbed adjoint state p^t solves

$$\int_D \beta_\chi A(t)\nabla\psi \cdot \nabla p^t \, dx = -\int_D 2\xi(t)(u^t - u_r^t)\psi \, dx \quad \text{for all } \psi \in H_0^1(D).$$

Therefore the shape derivative at the point $\phi_t(\omega_0)$ in direction $w\circ\phi_t^{-1}$ is given by

$$\begin{aligned} dJ(\phi_t(\omega_0))[w\circ\phi_t^{-1}] = &\int_D \xi(t)(\mathrm{tr}(\partial w\, B^\top(t))|u^t-u_r^t|^2\,dx - 2(u^t-u_r^t)B(t)\nabla u_r^t\cdot w)\,dx\\ &-\int_D \xi(t)(\mathrm{tr}(\partial w\, B^\top(t))f^tp^t + B(t)\nabla f^t\cdot w\,p^t)\,dx\\ &+\int_D \beta_\chi \mathcal{A}(t,w)\nabla u^t\cdot\nabla p^t\,dx, \end{aligned}$$

where we introduced $\mathcal{A}(t,w):=\mathrm{tr}(\partial w B^\top(t))A(t)-\mathrm{sym}(B^\top(t)\partial w A(t))$ and $B(t):=\partial\phi_t^{-\top}$. Therefore according to Definition 6.24, we have $d\mathcal{J}^{\phi_t}(\omega_0)[\theta]=dJ(\phi_t(\omega_0))[\theta\circ\phi_t^{-1}]$. Moreover, we have for all $v,w\in H^1(D,\mathbf{R}^d)$

$$(v,w)^{\phi_t}_{H^1(D,\mathbf{R}^d)} = \int_D A(t)\partial v:\partial w+\xi(t)v\cdot w\,dx.$$

Note that this is a scalar product since A is coercive and ξ bounded away from zero and from above. Moreover, the induced norm $\|v\|_{H^1(D),\phi_t}:=\sqrt{(v,v)^{\phi_t}_{H^1(D,\mathbf{R}^d)}}$ constitutes an equivalent norm to $\|\cdot\|_{H^1(D,\mathbf{R}^d)}$ on $H^1(D,\mathbf{R}^d)$; cf. Example 6.26. Now we assemble all equations to list the complete system determining the gradient flow ϕ_t:

$$\partial_t\phi_t(x) = -\nabla^{\mathcal{H}}J(\phi_t(\omega_0))\circ\phi_t(x)$$

where the $\mathcal{H}$-gradient $\theta^t:=\nabla^{\mathcal{H}}J(\phi_t(\omega_0))\circ\phi_t(x)$ solves

$$(\theta^t,w)^{\phi_t}_{H^1(D,\mathbf{R}^d)} = d\mathcal{J}^{\phi_t}(\omega_0)[w]\quad \text{for all } w\in H^1_0(D,\mathbf{R}^d).$$

The mapping $t\mapsto\phi_t$ is a priori no path in $\mathcal{G}_0(\mathcal{H})$. But the discretisation will lead to a path in $\mathcal{F}(W^1_\infty(D))$, since it is a mapping $t\mapsto\phi_t:[0,\infty)\to V_h\subset W^1_\infty(D,\mathbf{R}^d)$, where V_h is a finite element space.

The Eulerian point of view of the transmission problem

In the *Eulerian* approach of shape optimization all computations are performed on the moving domain. Instead of solving the equation (6.7), we consider the equivalent version

$$\partial_t\phi_t(\phi_t^{-1}(z)) = -\nabla^{\mathcal{H}}J(\phi_t(\omega_0))(z)\quad \text{for } z\in\phi_t(D)=D. \tag{6.22}$$

For our transmission problem we want to solve (6.22) and compute $\nabla^{\mathcal{H}}J(\phi_t(\omega_0))(z):=\theta_t$ by

$$(\theta_t,w)_{H^1(D,\mathbf{R}^d)} = dJ(\phi_t(\omega_0))[w]\quad \text{for all } w\in H^1_0(D,\mathbf{R}^d)$$

where

$$\begin{aligned} dJ(\phi_t(\omega_0))[w] = &\int_D \beta_{\chi_{\phi_t(\omega_0)}}\mathcal{A}(0,w)\nabla u_t\cdot\nabla p_t\;dx - \int_D \mathrm{div}\,(w)fp_t+\nabla f\cdot\theta_t\,p_t\,dx\\ &+\int_D \mathrm{div}\,(w)|u_t-u_r|^2\;dx - \int_D 2(u_t-u_r)\nabla u_r\cdot w\,dx, \end{aligned}$$

and the state u_t and adjoint state p_t solve

$$\begin{aligned} \int_D \beta_{\chi_{\phi_t(\omega_0)}}\nabla u_t\cdot\nabla\varphi\,dx &= \int_D f\,\varphi\,dx \quad \text{for all } \varphi\in H^1_0(D)\\ \int_D \beta_{\chi_{\phi_t(\omega_0)}}\nabla\psi\cdot\nabla p_t\,dx &= -\int_D 2(u-u_r)\psi\,dx \quad \text{for all } \psi\in H^1_0(D). \end{aligned}$$

Using once more that $\theta(t,z) := \partial_t\phi_t(\phi_t^{-1}(z)) = \partial_t\phi(t,\phi^{-1}(t,z))$ generates the flow ϕ_t, we get for small $h>0$

$$\phi_{t+h}(\phi_t^{-1}(z)) - \phi_t(\phi_t^{-1}(z)) \approx h\,\theta(t,z) = -h\,\nabla^{\mathcal{H}} J(\phi_t(\omega_0))(z),$$

which gives an approximation of the function ϕ_{t+h} since $\phi_{t+h}(\phi_t^{-1}(z)) \approx z - h\nabla^{\mathcal{H}} J(\phi_t(\omega_0))(z)$. Note that the function ϕ_{t+h} is not explicitly given on the domain ω_0 but only through ϕ_t^{-1} on $\phi_t(\omega_0)$, which makes it difficult to determine ϕ_{t+h}, numerically. But we may easily obtain an approximation of the moved domain $\Omega_{t+h} := \phi_{t+h}(\omega_0)$ by $\Omega_{t+h} = \phi_{t+h}(\phi_t^{-1}(\omega_0)) = (I - h\nabla^{\mathcal{H}} J(\phi_t(\omega_0)))(\omega_0)$. Of course due to the structure Theorem 2.38, we can consider (6.22) only on the boundary $\partial\phi_t(\omega_0) = \phi_t(\partial\omega_0)$ in order to obtain the new domain Ω_{t+h}. Indeed letting $\mathcal{H} = L_2(\partial\omega_0)$ and $dJ(\omega_0)[\theta] = \int_\Gamma g\theta\cdot n\,ds$ we get $\nabla^{\mathcal{H}} J(\phi_t(\omega_0))(z) = g\theta\cdot n$ and thus

$$\partial\Omega_{t+h} = \phi_{t+h}(\phi_t^{-1}(\partial\omega_0)) = (\mathrm{id} - gn)(\partial\phi_t(\omega_0)).$$

Remark 6.29. *We see that with this approach a movement of the domain ω_0 is necessary in order to evaluate the gradient $\nabla^{\mathcal{H}} J(\phi_t(\omega_0)))$. Therefore in a numerical algorithm only a few remeshings of the domain are needed.*

6.5.2 Discretisation of the gradient flow

In the recent works [57, 81] it has been shown numerically and theoretically that using a fixed discretisation for the shape derivative the volume expression is always approximated more accurately, at least using finite elements.

Let a shape function $J : \Xi \subset 2^D \to \mathbf{R}$ be given. Assume that $G_{\omega_0} := dJ(\omega_0) \in \mathcal{H}'$ for all $\omega_0 \in \Xi$ and that J admits a fixed domain representation $d\mathcal{J}^{\phi_t}(\omega_0)[\partial_t\phi_t] = dJ(\phi_t(\omega_0))[\partial_t\phi_t(\phi_t^{-1})]$. We aim to discretise the following equations

$$\begin{aligned}(\theta^t,\zeta)^{\phi_t}_{H^1(D,\mathbf{R}^d)} &= d\mathcal{J}^{\phi_t}(\omega_0)[\zeta] \quad \text{for all } \zeta\in\mathcal{H} &(6.23)\\ \theta^t &=: \nabla^{\mathcal{H}} J(\phi_t(\omega_0))\circ\phi_t \\ \partial_t\phi_t(x) &= -\nabla^{\mathcal{H}} J(\phi_t(\omega_0))\circ\phi_t(x) \quad \text{in } [0,T]\times\overline{D}, &(6.24)\end{aligned}$$

or equivalently

$$\begin{aligned}(\theta_t,\hat\zeta)_{H^1(D,\mathbf{R}^d)} &= dJ(\phi_t(\omega_0))[\hat\zeta] \quad \text{for all } \hat\zeta\in\mathcal{H}\\ \theta_t &=: \nabla^{\mathcal{H}} J(\phi_t(\omega_0))\\ \partial_t\phi_t(\phi_t^{-1}(z)) &= -\nabla^{\mathcal{H}} J(\phi_t(\omega_0))(z) \quad \text{in } [0,T]\times\overline{D},\end{aligned}$$

where by definition $\theta^t = \theta_t\circ\phi_t$. Suppose $V_h \subset H^1_0(D,\mathbf{R}^d)$ is a finite element space of dimension $N\in\mathbf{N}$ and $\{\phi_1,\dots,\phi_N\}$ is a basis of V_h. For simplicity assume that D and ω_0 have a polygonal boundary $\Sigma, \partial\omega_0$, respectively. Usually, V_h will consist of continuous and piecewise polynomial functions $f:\overline{D}\to\mathbf{R}^d$. We discretise (6.24)-(6.23) with an explicit Euler method in time and with the described FE approximation V_h of $\mathcal{H}$ and obtain the fully discrete system

$$\begin{aligned}\phi_{t+h}(x) - \phi_t(x) &= -h\nabla^{V_h} J(\phi_t(\omega_0))\circ\phi_t \quad \text{in } \overline{D}\\ (\nabla^{V_h} J(\phi_t(\omega_0))\circ\phi_t,\zeta)_{\mathcal{H}} &= d\mathcal{J}^{\phi_t}(\phi_t(\omega_0))[\zeta] \quad \text{for all } \zeta\in V_h &(6.25)\end{aligned}$$

or equivalently

$$\begin{aligned}\phi_{t+h}(\phi_t^{-1}(z)) - z &= -h\nabla^{V_h} J(\phi_t(\omega_0)) \quad \text{in } \overline{D}\\ (\nabla^{V_h} J(\phi_t(\omega_0)),\zeta)_{\mathcal{H}} &= dJ(\phi_t(\omega_0))[\zeta] \quad \text{for all } \zeta\in V_h. &(6.26)\end{aligned}$$

Let us sketch a basic gradient algorithm.

Algorithm 1: Gradient flow algorithm in Lagrangian coordinates

Data: Let $n = 0$, $\gamma > 0$ and $N \in \mathbf{N}$ be given. Initialise domain $\omega_0 \subset D$, time $t_n = 0$ and $n_{\text{iter}} = 0$. Initialise $\phi_{t_n} = \text{id}$.

initialisation;

while $n \le N$ **do**

1.) solve (6.25) with $t = t_n$ to obtain $\theta^{t_n} = \nabla^{V_h} J(\phi_{t_n}(\omega_0))(\phi_{t_n}(x)) \in V_h \subset \mathcal{H}$;

2.) choose $\Delta t_n > 0$ such that $J((\phi_{t_n} - \Delta t_n \theta^{t_n})(\omega_0)) \le J(\phi_{t_n}(\omega_0))$;

3.) set $t_{n+1} = t_n + \Delta t_n$ and $\phi_{t_{n+1}}(x) := \phi_{t_n}(x) - \Delta t_n \theta^{t_n}(x)$;

if $J(\phi_{t_n}(\omega_0)) - J(\phi_{t_{n+1}}(\omega_0)) \ge \gamma(J(\omega_0) - J(\phi_{t_1}(\omega_0)))$ **then**

step accepted, continue program

else

exit program, no sufficient decrease ;

increase $n \to n + 1$;

Remark 6.30. *The previous algorithm has some nice features. Observe that we only choose once the initial domain Ω_0 on which all calculations are performed.*

Alternatively, we propose the following algorithm to determine a sequence of domains Ω_{t_n} such that $J(\Omega_{t_{n+1}}) \le J(\Omega_{t_n})$ instead of the transformation ϕ_t.

Algorithm 2: Gradient algorithm in Eulerian coordinates

Data: Let $n = 0$, $\gamma > 0$ and $N \in \mathbf{N}$ be given. Initialise domain $\Omega_0 \subset D$, time $t_n = 0$ and $n_{\text{iter}} = 0$.

initialisation;

while $n \le N$ **do**

1.) solve (6.26) with $t = t_n$ to obtain $\theta_{t_n} = \nabla^{V_h} J(\Omega_n)(x) \in V_h \subset \mathcal{H}$;

2.) choose $\Delta t_n > 0$ such that $J((I - \Delta t_n \theta_{t_n})(\Omega_{t_n})) - J(\Omega_{t_n}) \le 0$;

3.) set $t_{n+1} = t_n + \Delta t_n$ and $\Omega_{t_{n+1}} := (I - \Delta t_n \theta_{t_n})(\Omega_{t_n})$;

if $J(\Omega_n) - J(\Omega_{n+1}) \ge \gamma(J(\Omega_0) - J(\Omega_1))$ **then**

step accepted, continue program

else

exit program, no sufficient decrease ;

increase $n \to n + 1$;

Remark 6.31. *Saving the solutions $\tilde{\phi}_{t_n}(x) := (x - \Delta t_n \theta_{t_n}(x))$ from the previous algorithm in each iterations step, we may build a diffeomorphism $\tilde{\phi}_t^{final} : D \to \mathbf{R}^d$:*

$$\tilde{\phi}^{final}(x) := \tilde{\phi}_{t_N} \circ \tilde{\phi}_{t_{N-1}} \cdots \circ \tilde{\phi}_{t_0}(x).$$

This transformation maps the initial domain Ω_0 onto the optimal $\widetilde{\Omega} := \tilde{\phi}^{final}(\Omega_0)$. It is the very same diffeomorphism we obtain from Algorithm 1:

$$\phi^{final}(x) := \phi_{t_0}(x) + \phi_{t_1}(x) + \cdots + \phi_{t_N}(x).$$

Observe the different decomposition of the functions $\tilde{\phi}^{final}$ and ϕ^{final}: in the Lagrangian algorithm it is addition and in the Eulerian the function composition, which is the group operation on $\mathcal{G}_0(\mathcal{H})$. We have

$$\tilde{\phi}^{final}(\Omega_0) \approx \phi^{final}(\omega_0).$$

After discretisation, the two sets are not exactly equal anymore, but close to each other. This is due to the numerical error of the $\mathcal{H}$-gradient.

6.6 Translations and rotations

In some problems the shape of an object may be known but the location and orientation may be unknown. It is then meaningful to use translations and rotations to move the shape, which considerably reduces the amount of unknowns. As mentioned earlier in this section, until now descent directions have been mostly determined directly by using the boundary form of the shape derivative (2.17) by taking $\theta \cdot n = -g$ and $\theta_\Gamma \equiv 0$. This approach produces a vector field θ which is normal to the boundary. Such a choice of θ cannot produce a translation, although this would be the natural transformation in some applications where the shape is known but not the location.

In order to produce a transformation which is locally a translation, one needs to take a non-zero tangential component θ_Γ and an appropriate normal component $\theta \cdot n$. In $\mathbf{R}^d$ a transformation combining translation and rotation is a mapping $\Phi : \mathbf{R}^d \to \mathbf{R}^d$ which is locally of the form

$$\Phi(x) := \mathcal{A}x + b,$$

where $b \in \mathbf{R}^d$ and $\mathcal{A} \in \mathbf{R}^{d,d}$ is an orthogonal matrix, i.e. $\mathcal{A}\mathcal{A}^\top = \mathcal{A}^\top\mathcal{A} = I$. Therefore we can define a translation by the formula $\partial\Phi(\partial\Phi)^\top = I$. For small t the flow Φ_t of the vector field $\theta \in C_c^\infty(\mathbf{R}^d, \mathbf{R}^d)$ has the form

$$\Phi_t(x) = x + t\theta(x).$$

To obtain a translation one may assume $\partial\theta(\partial\theta)^\top = I$. For a combination of translations and rotations in $\mathbf{R}^2$ we choose a vector field θ which satisfies locally

$$\theta(x) = \mathcal{A}x + b, \quad \mathcal{A} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}, \quad \beta = (\beta_1\ \beta_2)^\top \in \mathbf{R}^2,\ \alpha \in \mathbf{R}.$$

The shape derivative is then determined by three parameters α and β_1, β_2. Note that in this case the vector field θ is not normal to the boundary of Ω. Assume the shape derivative has the form (2.17)

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} g\, \theta \cdot n\, ds.$$

Then plugging in $\theta(x) = \mathcal{A}x + \beta$ with $x = (x_1 x_2)^\top$ one obtains

$$\begin{aligned} dJ(\Omega)[\theta] = &\cos(\alpha) \int_{\partial\Omega} g(n_1x_1 + n_2x_2)\, ds + \sin(\alpha) \int_{\partial\Omega} g(-n_1x_2 + n_2x_1)\, ds \\ &+ \beta_1 \int_{\partial\Omega} n_1 g\, ds + \beta_2 \int_{\partial\Omega} n_2 g\, ds. \end{aligned}$$

In view of this formula, one may choose the parameters

$$\alpha = -\arctan \frac{\int_{\partial\Omega} g(n_1x_1 + n_2x_2)}{\int_{\partial\Omega} g(-n_1x_2 + n_2x_1)}\, ds, \qquad \beta_1 = -\int_{\partial\Omega} n_1 g\, ds, \qquad \beta_2 = -\int_{\partial\Omega} n_2 g\, ds$$

to get a descent direction θ which is a translation and a rotation. Note that using the boundary form (2.17) one may consider a transformation θ which is only locally a transformation and a rotation. This is often more meaningful for applications since we consider shapes contained in D which is fixed, which implies that θ must vanish on the boundary of D, in which case we cannot take θ as a translation everywhere.

Using the volume expression (2.16), the determination of the parameters α and β is not as straightforward for this reason. One may choose θ as a piecewise linear function so that

θ is a translation on the interface Γ and vanishes on Σ. Assume the shape derivative has the form

$$dJ(\Omega)[\theta] = \int_\Omega F_1[\theta_1] + F_2[\theta_2]\, dx,$$

where $F_1[\theta_1]$ and $F_2[\theta_2]$ are linear with respect to θ_1 and θ_2 with $\theta = (\theta_1, \theta_2)$. In order to obtain a transformation which is locally a translation, one may choose the following class of vector fields

$$\theta = \eta \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix},$$

where η is a smooth function equal to one in a neighborhood Ω^* of Ω, equal to zero on Σ. The choice of η depends on Ω and D and we have

$$dJ(\Omega)[\theta] = \beta_1 \int_\Omega F_1[\eta]\, dx + \beta_2 \int_\Omega F_2[\eta]\, dx.$$

Therefore a descent direction is easily found as

$$\beta_1 = -\int_\Omega F_1[\eta]\, dx, \quad \beta_2 = -\int_\Omega F_2[\eta]\, dx.$$

6.7 Splines and the $\mathcal{H}$-gradient

In the previous sections, we have seen how it is possible to use the volume expression of the shape derivative to obtain descent directions. This requires, at least theoretically, no discretisation of the domain. Nevertheless, as it is traditionally done, it is possible to discretise first the boundary of the domain by splines and then determine in a similar fashion as for the volume expression a descent direction using the boundary expression of the shape derivative.

6.7.1 Definition of B-Splines and basic properties

Let $k, N \in \mathbf{N}$ be fixed integers, define $p := k-1$ and $m := p + N + 1 = N + k$. We define recursively the basis functions $N_k^i : [t_0, t_m] \to \mathbf{R}$ by

$$N_i^0(t) := \begin{cases} 1 & \text{if } t_i < t_{i+1} \text{ and } t_i \le t \le t_{i+1} \\ 0 & \text{else} \end{cases},$$

and

$$N_i^r(t) = \frac{t - t_i}{t_{i+r-1} - t_i} N_i^{r-1}(t) + \frac{t_{i+r} - t}{t_{i+r} - t_{i+1}} N_{i+1}^{r-1}(t),$$

where $i = 0, 1, \dots, N$ and $r \in \mathbf{N}$. Here the numbers $t_0, \dots, l_{m+1} \in \mathbf{R}$ are called knots and assembled in the knot vector $(t_0, t_1, \dots, t_{N+k-1}, t_{N+k}) \in \mathbf{R}^{m+1}$. The functions $\{N_0^r(t), N_1^r(t), \dots, N_{N-1}^r(t), N_N^r(t)\}$ are called *basis function* of order r. They constitute polynomials of degree r.

Definition 6.32. *Let $N+1$ vectors $U_0, \dots, U_N \in \mathbf{R}^2$, called* control points*, be given. A* basis spline curve *(short B-Spline) $\gamma : [t_0, t_m] \to \mathbf{R}^2$ of* order *k is defined by*

$$\gamma(t) = \sum_{i=0}^{N} N_i^k(t) U_i. \tag{6.27}$$

Note that since $N_i^k(t) = 0$ for $t \in \mathbf{R} \setminus [t_i, t_{i+k}]$ the curve is local in the sense that if we move the point U_i it affects maximal k curve segments, which makes those curves attractive for shape optimization problems.

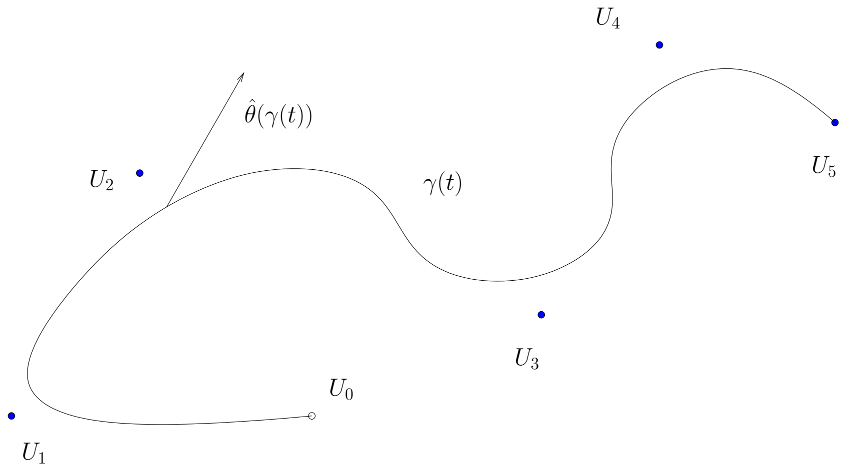

Figure 6.2: B-Spline γ defined by points $U_0, \ldots, U_5$.

6.7.2 Clamped and closed B-Splines

Let $\Omega \subset \mathbf{R}^2$ be a bounded domain with smooth boundary. Let $\Gamma \subset \partial\Omega$ be a simply connected part of the boundary . When Γ is not the whole boundary we describe it by a *clamped B-Spline curve* and in the other case by a *closed B-Spline curve.*

Definition 6.33. *A B-Spline curve $\gamma : [0,1] \to \mathbf{R}^2$ defined by (6.27) is called*

(i) clamped *at a, b if $\gamma(0) = U_0, \gamma(1) = U_N$*

(ii) closed *if $\gamma(0) = \gamma(1)$.*

(iii) open *if $\gamma(0) \neq U_0, \gamma(1) \neq U_N$*

For a given set of control points $\{U_0, \ldots, U_N\}$, we define a clamped B-Spline by

$$\gamma(t) = \sum_{i=0}^{N} N_i^k(c\,t)U_i,$$

with the choice $c := n - k + 2$ and

$$t_j = \begin{cases} 0 & \text{if } j < k, \\ j - k + 1 & \text{if } k \leq j \leq N, \\ N - k + 2 & \text{if } j > N, \end{cases} .$$

A closed B-Spline curve on $[0,1]$ is given by the formula

$$\gamma(t) = \sum_{i=k-1}^{N-k} N_i^k(ct)U_i + \sum_{i=N-k}^{N} (N_{i-(N-k)}^k(ct) + N_i^k(ct))U_i,$$

where $c := t_{m-k}$. Here we define the basis N_i^k by uniform knot vectors satisfying $t_{j+1} - t_j = 1/m$ by $t_j := j/m$ for $j = 0, 1, \ldots, m$. Additionally, we have to overlap k control points as follows $U_i = U_{N-(k-1)+i}$ for $i = 0, 1, \ldots, k-1$. For a clamped respectively closed B-Spline, we introduce the vector field $\theta : \Gamma \to \mathbf{R}^2$

$$\theta_{\text{cla}}(x) := c \sum_{i=0}^{N} c_i N_i^k(\gamma^{-1}(x))\tilde{U}_i, \tag{6.28}$$

respectively

$$\theta_{\text{clo}}(x) := \sum_{i=k-1}^{N-k} N_i^k(\gamma^{-1}(x))\hat{U}_i + \sum_{i=N-k}^{N} (N_{i-(N-k)}^k(\gamma^{-1}(x)) + N_i^k(\gamma^{-1}(x)))\hat{U}_i, \tag{6.29}$$

where $1/c_i = \int_\Gamma N_i^k(\gamma^{-1}(x))\,dx = \int_\Gamma |\gamma'(s)|\,N_i^k(s)\;ds > 0$ and $c = \sum_{i=1}^N c_i$ and the control points $\tilde{U}_i$ respectively $\hat{U}_i$ are to be determined. The scaling in (6.28) is necessary to achieve that the perimeter minimisation is exact in the sense that if we start with a quarter circle the quarter circle is shrinking to a point. Without the scaling this would lead to strange effects of the behavior of control points near U_0 and U_N as was observed in [92]. We denote by $\hat{\theta}(t) := \theta(\gamma(t)) : [0,1] \to \mathbf{R}^2$ the reduced vector field. Suppose we are given a shape function J which is shape differentiable in $\Omega \subset \mathbf{R}^2$. According to Theorem 2.38 if $g \in L_1(\Gamma)$ it has the following form

$$dJ(\Omega)[\theta] = \int_\Gamma g\,\theta \cdot n\;ds. \tag{6.30}$$

Inserting (6.28) respectively (6.29) into (6.30) leads to

$$dJ(\Omega)[\theta_{\text{cla}}] = \sum_{i=0}^{N} d\hat{J}_i \cdot \hat{U}_i, \qquad dJ(\Omega)[\theta_{\text{clo}}] = \sum_{i=k-1}^{N-k} d\tilde{J}_i \cdot \tilde{U}_i + \sum_{i=N-k}^{N} d\tilde{J}_i \cdot \tilde{U}_i$$

where $\Gamma := \partial\Omega$. The planar vectors $d\hat{J}_i$ and $d\tilde{J}_i$ are defined by

$$\begin{aligned}
d\hat{J}_i &:= c\int_0^1 c_i\,g(\gamma(s))\,N_i^k(s)\,J\dot{\gamma}(s)\;ds \qquad (i = 0,\dots,N-k)\\
d\tilde{J}_i &:= \int_0^1 g(\gamma(s))\,N_i^k(s)\,J\dot{\gamma}(s)\;ds \qquad (i = k-1,\dots,N-k)\\
d\tilde{J}_i &:= \int_0^1 g(\gamma(s))(N_i^k(s) + N_{i-(N-k)}^k(s))J\dot{\gamma}(s))\;ds \qquad (i = N-k+1,\dots,N).
\end{aligned}$$

Here, we have defined the normal vector along γ by $n(s) := J\dot{\gamma}(s)/|J\dot{\gamma}(s)| = J\dot{\gamma}(s)/|\dot{\gamma}(s)|$. Obvious descent directions may be defined by

$$\begin{aligned}
\hat{U}_i &= -c\int_0^1 c_i\,g(\gamma(s))\,N_i^k(s)\,J\dot{\gamma}(s)\;ds, \qquad (i = 0,\dots,N) \qquad (6.31)\\
\tilde{U}_i &= -\int_\Gamma g(\gamma(s))N_i^k(s)J\dot{\gamma}(s)\;ds, \qquad (i = k-1,\dots,N-k)\\
\tilde{U}_i &= -\int_\Gamma g(\gamma(s))(N_i^k(s) + N_{i-(N-k)}^k(s))J\dot{\gamma}(s))\;ds, \qquad (i = N-k+1,\dots,N).
\end{aligned}$$

The $\mathcal{H}$-gradient in the space of basis splines of order k and N control points $B(N,k)$ equipped with the metric I is given by $\nabla^{B(N,k)}J(\Omega) = -\theta_{\text{cla}}$ and $\nabla^{B(N,k)}J(\Omega) = -\theta_{\text{clo}}$. Note that we have the following relation between the moved curve and the moved control points, here exemplary for the clamped B-Spline,

$$\Gamma_t = (\gamma + \alpha\,\theta \circ \gamma)([0,1]), \quad \gamma(t) + \alpha\,\theta(\gamma(t)) = \sum_{i=0}^{N} N_i^k(t)(U_i + \alpha\,c\,c_i\tilde{U}_i), \quad (\alpha > 0).$$

For an application of the clamped basis splines we refer the reader to Section 7.4 and also [66], where Bézier splines (special basis splines) are used.

6.8 The level set method

The *level set method*, introduced in [80] is a general framework for tracking evolving surfaces. The key idea of the method is to describe a domain implicitly by the level set of a scalar function $\phi : \mathbf{R}^d \to \mathbf{R}$. With the level set function it is then possible to recover the boundary of the domain. We point out that in general level sets of smooth functions can be arbitrarily irregular as can be seen by the Whitney theorem or by simply considering the Lipschitz continuous distance function $\phi(x) := d_\Omega(x)$ associated with an arbitrary set Ω. Still in numerical practice the level sets define smooth domains.

Assume that for each $t \in [0, \tau]$ the domain $\Omega_t = \Phi_t(\Omega)$ and its boundary $\partial\Omega_t$ can be described by a C^1-function $\phi : D \times [0, \tau] \to \mathbf{R}$, that is

$$\Omega_t = \{x \in D : \phi(x,t) < 0\}, \quad \partial\Omega_t = \{x \in D : \phi(x,t) = 0\}.$$

We call the function ϕ level set function. Differentiating the equation $\phi(\Phi_t(x), t) = 0$ with respect to t leads to the *Hamilton-Jacobi* equation

$$\partial_t\phi(t,x) + \theta(x) \cdot \nabla\phi(t,x) = 0 \quad \text{in } \partial\Omega_t \times [0, \tau]. \tag{6.32}$$

Note that the level set equation (6.32) is only defined on the unknown boundary $\partial\Omega_t$. To get rid of this we can extend the equation onto a domain D containing all Ω_t, $(t \geq 0)$. Initially, the level set method was designed to track smooth interfaces moving along the normal direction to the boundary. Theoretically, if the domain Ω_t and $L_2(\Gamma)$ representation of $dJ(\Omega)[\theta]$ are smooth enough then we have $dJ(\Omega_t)[\theta] = \int_{\Gamma_t} g_t\, \theta \cdot n_t\, ds$. Therefore we may take as normal perturbation field $\theta := -g_t\, n_t$, where $n_t := \nabla\phi/|\nabla\phi|$ is the unit normal vector field expressed by the level set function ϕ. One obtains from (6.32) the level set equation

$$\partial_t\phi + \theta_n|\nabla\phi| = 0 \quad \text{in } D \times [0, \tau]. \tag{6.33}$$

Observe that in order to make sense of the previous equation, we need to extend θ to D or at least to a neighborhood of Γ, which requires an extension of g_t to D. In the case were the shape derivative is only available in the form of Theorem 2.38 (ii), as a domain integral, then ϕ is not governed by (6.33) but rather by the Hamilton-Jacobi equation (6.32). It turns out that (6.32) is actually easier to handle numerically. Therefore it is more natural to use (6.32) with a θ which is already defined in the domain as is the case with the volume expression of the shape derivative used in this paper, providing a natural extension to the entire domain. In addition θ_n is computed on the boundary $\partial\Omega_t$ which usually does not match the grid nodes where ϕ and the solutions of the possible partial differential equations are defined in the numerical application. Therefore the computation of θ_n requires to determine the boundary $\partial\Omega_t$ explicitly and to interpolate on $\partial\Omega_t$ quantities defined on the grid, which makes the numerical implementation more complicated and introduces an additional interpolation error. This is an issue in particular for interface problems where θ_n is usually the jump of a function across the interfaces which requires multiple interpolations and is error-prone. In our framework we never need to resolve the interface $\partial\Omega_t$ explicitly during the optimization, and θ only needs to be defined at the grid nodes.

Initial data and boundary conditions have to be imposed together with the Hamilton-Jacobi equation (6.32). The initial data $\phi(0, x) = \phi_0(x)$ is chosen as the signed distance function b_{Ω_0} to the initial boundary $\partial\Omega_0 = \partial\Omega$. Dirichlet boundary conditions also have to be imposed on the part of the boundary $\Sigma = \partial D$ of D which is fixed.

6.8.1 Discretisation and reinitialisation of the level set equation

In the usual level set method, the level set equation (6.33) is discretised using an explicit upwind scheme proposed by Osher and Sethian; [79],[80],[88]. The level set equation (6.32) is solved in a special way described later.

Let D be the unit square $D = (0,1) \times (0,1)$ to fix ideas. For the discretisation of the Hamilton-Jacobi equation (6.32), we first define the mesh grid of U. We introduce the nodes P_{ij} whose coordinates are given by $(i\Delta x, j\Delta y)$ where Δx and Δy are the steps discretisation in the x and y directions respectively. Let us also note $t^k = k\Delta t$ the discrete time for $k \in \mathbb{N}$, where Δt is the time step. We then seek an approximation $\phi_{ij}^k \simeq \phi(P_{ij}, t^k)$.

For numerical accuracy, the solution of the level set equation (6.32) should not be too flat or too steep. This is fulfilled for instance if ϕ is the distance function i.e. $|\nabla\phi| = 1$. Unfortunately, even if we start with a (signed) distance function for the initial data ϕ_0, the solution ϕ of the level set equation (6.32) does not generally remain close to a distance function. We can perform a reinitialisation of ϕ at time t by solving the solution $\varphi = \varphi(\tau, x)$ of the following equation, up to the stationary state (see [83])

$$\begin{aligned} \varphi_\tau + S(\phi)(|\nabla\varphi| - 1) &= 0 \text{ in } \mathbb{R}^+ \times U, \\ \varphi(0,x) &= \phi(t,x), \; x \in U. \end{aligned}$$

Here, S is an approximation of the sign function, for instance, $S(d) = d/\sqrt{d^2 + |\nabla d|^2\varepsilon^2}$ with $\varepsilon = \min(\Delta x, \Delta y)$ where Δx and Δy stand for the space steps discretisation in the x and y direction (see below). Other choices are possible for the approximate sign function. We refer to [83] for details.

Remark 6.34. *This technique allows to compute and update the level set only on a narrow band around the interface. In this way the complexity of the problem is only $N\log(N)$ instead of N^2.*

Chapter 7

Numerical simulations

This last chapter is devoted to the numerical treatment of some shape optimization problems employing the material from Chapter 6. We provide a numerical validation that the volume expression allows very accurate approximations and can even reconstruct domains with corners. We begin with numerical results for simple unconstrained domain integrals. Subsequently, we present numerics for the transmission problems from Section 5.2, Subsection 6.5.1 and the EIT problem of Section 5.3. Except for the example from Section 5.2, where we use the boundary expression and basis splines, all computations use the domain expression. We discretise the arising partial differential equations by means of the finite element method. All implementations in this chapter have been done either using the WIAS toolbox PDELib or the FENICS finite element toolbox. The author acknowledges here the implementation of the example from Section 7.2 by Martin Eigel and the level set method of Section 7.3 by Antoine Laurain.

7.1 Unconstrained volume integrals: gradient methods

Let $f \in W^{1,1}_{loc}(\mathbf{R}^2)$ be a given function. Denote by $\Xi \subset 2^{\mathbf{R}^2}$ the set of all open and bounded domains $\Omega \subset \mathbf{R}^2$. We consider the problem

$$\min J(\Omega) := \int_\Omega f(x)\, dx \quad \text{ over } \Omega \in \Xi \tag{7.1}$$

and solve it by finding zeros of $\Omega \mapsto dJ(\Omega)$. As we have seen before, the volume expression of J exists in all directions $\theta \in C^1_c(D, \mathbf{R}^d)$ and for all measurable domains $\Omega \subset D$

$$dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(\theta) f + \nabla f \cdot \theta\, dx.$$

By density, we may extend $dJ(\Omega)$ to $H^1(\Omega, \mathbf{R}^d)$. In order to solve (7.1), we make use of the general framework of Chapter 6 and use Algorithm 2. We compute a descent direction θ as the negative gradient of the cost J with respect to the space $\mathcal{H} := H^1(\Omega; \mathbf{R}^d)$:

$$(\theta, \zeta)_{H^1(\Omega;\mathbf{R}^2)} = -dJ(\Omega)[\zeta] \ \text{ for all } \zeta \in H^1(\Omega; \mathbf{R}^2), \tag{7.2}$$

This equation is discretised using the finite element method as outlined in Section 6.5.2. We run the Algorithm 2 and take two different choices for f:

(i) $f(x, y) = \frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 \in C^\infty(\mathbf{R}^2)$,

(ii) $f(x, y) = |x| + |y| - 1 \in W^{1,\infty}_{loc}(\mathbf{R}^2)$.

The optimal shape is an ellipse in case (i) and a square in case (ii). In Figure 7.1 an example for case (i) with the choices $a = 1.5$ and $b = 3$ is given. The initial shape (heart-shaped) is not convex, whereas the final shape (an ellipse) is convex and smooth. Case (ii) is illustrated in Figure 7.2. One observes that the method is able to create the corners of the square starting from a smooth boundary. For these two examples, we solved (7.2) using a grid consisting of 8121 elements and first order elements.

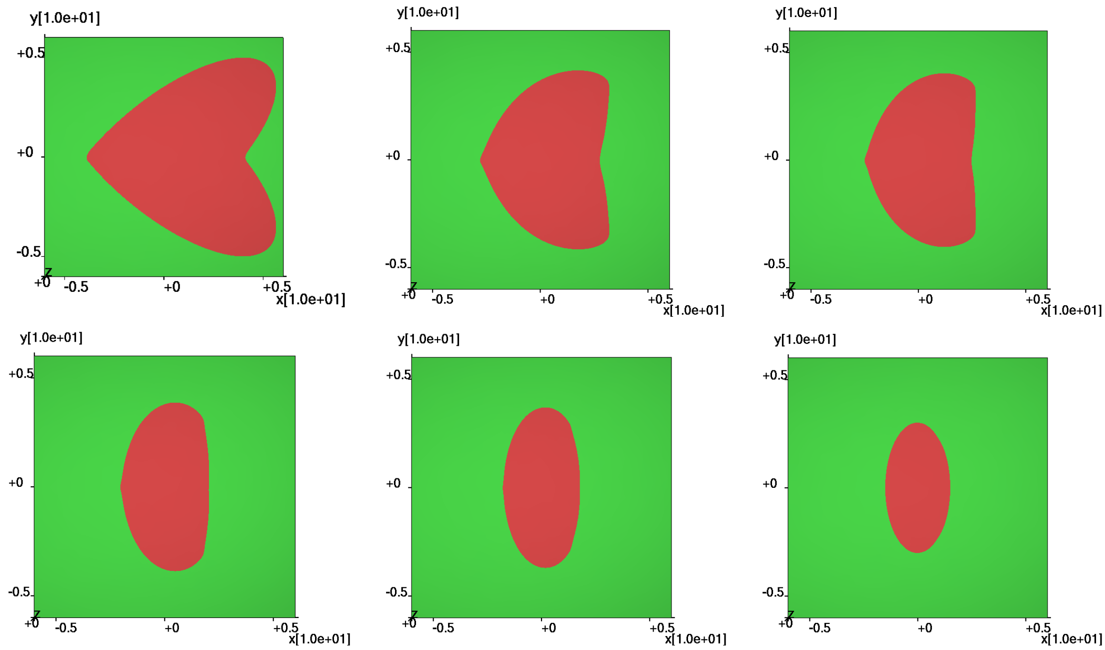

Figure 7.1: From left to right and top to bottom: iterations $0, 2, 3, 6, 10, 100$

7.2 A transmission problem: gradient method and volume expression

We consider the problem from Subsection 6.5.1. Put $\mathcal{H} := H_0^1(D; \mathbf{R}^2)$ and choose a P2 finite element space $V_h \subset \mathcal{H}$. Then the discreted optimization problems reads

$$\min J(\Omega) = \int_D |u_h - u_r|^2 \, dx \quad \text{subject to } u_h \text{ solves} \tag{7.3}$$

$$\int_D \beta_\chi \nabla u_h \cdot \nabla \psi \, dx = \int_D f \psi \, dx \quad \text{for all } \psi \in V_h. \tag{7.4}$$

The function u_r is the target function, which is defined as the solution of (7.4) with right hand side $f := 1$ and χ chosen according to the orange rightmost domain in Figure 7.3. The problem (7.3) is solved by finding zeros of the shape derivative: Find $\Omega \subset D$ such that

$$dJ(\Omega)[\theta] = 0 \quad \text{for all } \theta \in C_c^1(D, \mathbf{R}^d).$$

To produce Figure 7.3, we used the Euler algorithm (Algorithm 2). In this picture the initial, optimal and desired domains are depicted. One observes that the irregular, non-convex optimal shape is quite accurate reconstructed. In Figure 7.4, we used the Lagrange algorithm (Algorithm 1). We remeshed four times.

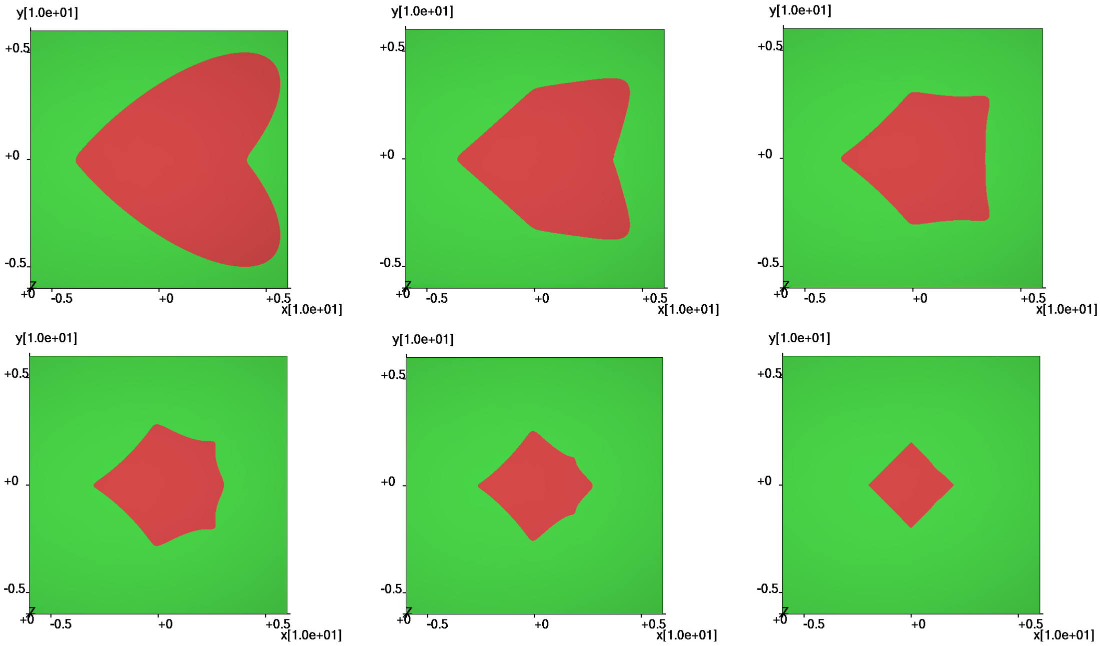

Figure 7.2: From left to right and top to bottom: iterations $0, 2, 4, 7, 12, 100$

Figure 7.3: From left to right: initial domain, optimal domain, reference domain

7.3 The EIT problem: level set method and volume expression

In this section we give numerical results for the problem of electrical impedance tomography presented in Section 5.3.1. Using the notations of Section 5.3.1 we take $\Omega = (0,1) \times (0,1)$ and $\Gamma_D = \emptyset$, i.e. we have measurements on the entire boundary Γ. For for sake of implementation, we consider a slightly different problem than the one in Section 5.3.1. Denote Γ_t, Γ_b, Γ_l and Γ_r the four sides of the square, where the indices t, b, l, r stands for top, bottom, left and right, respectively. We consider the following problems: find $u_N \in H^1_{tb}(\Omega)$ and $u_D \in H^1_{lr}(\Omega)$ such that

$$\int_D \sigma \nabla u_N \cdot \nabla \varphi = \int_D f\varphi + \int_{\Gamma_l \cup \Gamma_r} g\varphi \quad \text{for all} \quad \varphi \in H^1_{0,tb}(\Omega) \tag{7.5}$$

$$\int_D \sigma \nabla u_D \cdot \nabla \varphi = \int_D f\varphi + \int_{\Gamma_t \cup \Gamma_b} g\varphi \quad \text{for all} \quad \varphi \in H^1_{0,lr}(\Omega) \tag{7.6}$$

Figure 7.4: From left to right: initial domain, optimal domain, reference domain

where

$$\begin{aligned} H^1_{tb}(D) &:= \{v \in H^1(D) \mid \ v = h \text{ on } \Gamma_t \cup \Gamma_b\}, \\ H^1_{lr}(D) &:= \{v \in H^1(D) \mid \ v = h \text{ on } \Gamma_l \cup \Gamma_r\}, \\ H^1_{0,tb}(D) &:= \{v \in H^1(D) \mid \ v = 0 \text{ on } \Gamma_t \cup \Gamma_b\}, \\ H^1_{0,lr}(D) &:= \{v \in H^1(D) \mid \ v = 0 \text{ on } \Gamma_l \cup \Gamma_r\}. \end{aligned}$$

The results of Section 5.3.1 can be straightforwardly extended to equations (7.5), (7.6) and using shape function (5.37) leads to the same optimization problem.

We use the software package FEniCS for the implementation; see [68]. The domain Ω is meshed using a uniform grid of 128×128 elements. The conductivity values are set to $\sigma_0 = 1$ and $\sigma_1 = 10$. We compute the $\mathcal{H} := H^1_0(D; \mathbf{R}^d)$ gradient with respect to the metric $(v, w)_{\mathcal{H}} = \int_D \partial v : \partial w \, dx$. We obtain measurements h_k corresponding to fluxes g_k, $k = 1, .., K$, by taking the trace on Γ of the solution of a Neumann problem where the fluxes are equal to g_k. To simulate real noisy EIT data, the measurements h_k are corrupted by adding a normal Gaussian noise with mean zero and standard deviation $\delta * |h_k|_\infty$, where δ is a parameter. The noise level is computed as

$$noise = \frac{\sum_{k=1}^K \|h_k - \tilde{h}_k\|_{L^2(\Gamma)}}{\sum_{k=1}^K \|h_k\|_{L^2(\Gamma)}},$$

where $\tilde{h}_k$ is the noisy measurement and h_k the synthetic measurement without noise on Γ.

We use the shape function (5.37), that is, $J(\Omega^+) = \frac{1}{2} \int_D \sum_{k=1}^K |u_{D,k}(\Omega^+) - u_{N,k}(\Omega^+)|^2 \, dx$, where $u_{D,k}$ and $u_{N,k}$ correspond to the different fluxes g_k.

Since we use a gradient-based method we implement an Armijo line search to adjust the time-stepping. The algorithm is stopped when the decrease of the shape function becomes insignificant, practically when the following stopping criterion is repeatedly satisfied:

$$J(\Omega^+_n) - J(\Omega^+_{n+1}) < \gamma(J(\Omega^+_0) - J(\Omega^+_1))$$

where Ω^+_n denotes the n-th iterate of Ω^+. We take $\gamma = 5.10^{-5}$ in our tests.

In Figure 7.5 we compare the reconstruction for different noise levels computed using 7.3. We take in this example $K = 3$, i.e. we use three fluxes g_k, $k = 1, 2, 3$, defined as follows:

$$\begin{aligned} g_1 &= 1 \text{ on } \Gamma_l \cup \Gamma_r \text{ and } g_1 = -1 \text{ on } \Gamma_t \cup \Gamma_b, \\ g_2 &= 1 \text{ on } \Gamma_l \cup \Gamma_t \text{ and } g_2 = -1 \text{ on } \Gamma_r \cup \Gamma_b, \\ g_3 &= 1 \text{ on } \Gamma_l \cup \Gamma_b \text{ and } g_3 = -1 \text{ on } \Gamma_r \cup \Gamma_t. \end{aligned}$$

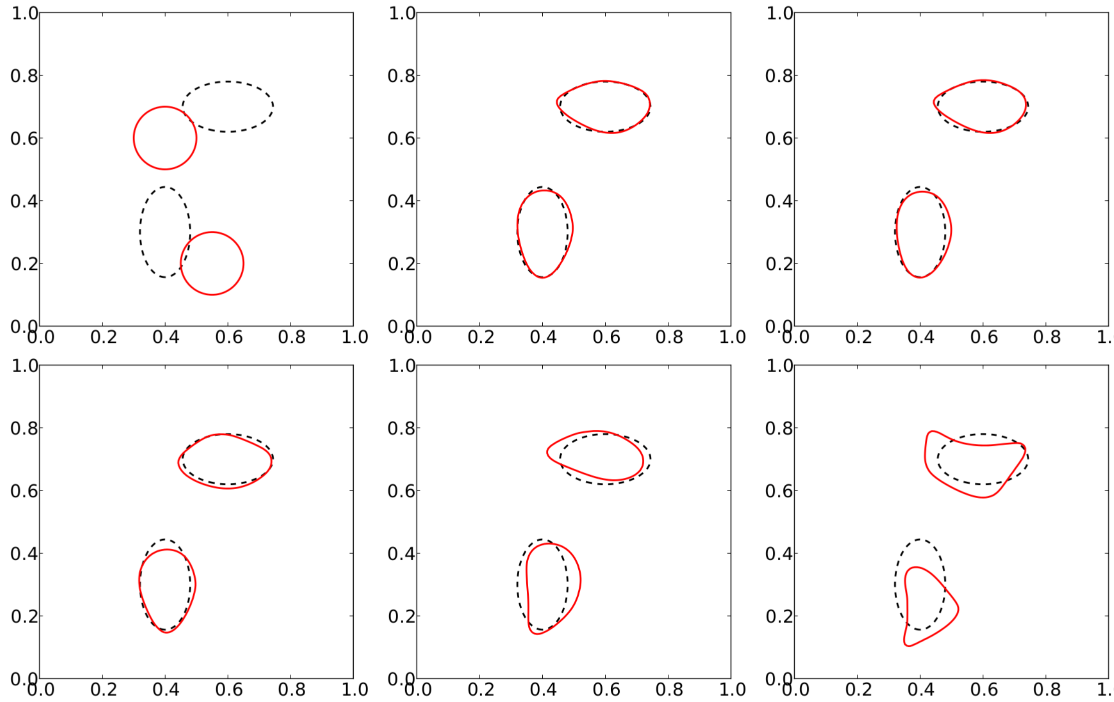

Figure 7.5: Reconstruction (continuous contours) of two ellipses (dashed contours) with different noise levels and using three measurements. From left to right and top to bottom: initialisation (continuous contours - top left), 0% noise (367 iterations), 0.43% noise (338 iterations), 1.44% noise (334 iterations), 2.83% noise (310 iterations), 7% noise (356 iterations).

Without noise, the reconstruction is very close to the true object and degrades as the measurements become increasingly noisy, as is it usually the case in EIT. However, the reconstruction is quite robust with respect to noise considering that the problem is severely ill-posed. We reconstruct two ellipses and initialise with two balls placed at the wrong location. The average number of iterations until convergence is around 340 iterations.

In Figure 7.6 we reconstruct three inclusions this time using $K = 7$ different measurements, with 1.55% noise. The reconstruction is close to the true inclusion and is a bit degraded due to the noise.

7.4 Distortion compensation via optimal shape design using basis splines

In this section we show numerical results for the transmission problem from Section 5.2. Let $D \subset \mathbf{R}^2$ be open and bounded with smooth boundary ∂D. We consider the problem

$$\min J(\Omega) = \int_\Sigma \|\mathbf{u}(\chi_\Omega) - \mathbf{u}_r\|^2 \, ds \quad \text{over all smooth subsets } \Omega \subset D,$$

where $\mathbf{u}(\chi_\Omega)$ is a solution of (5.17) and $\mathbf{u}_r$ is a smooth target which is specified below. Although the previous minimisation problem has in general no solution without the perimeter penalisation, in practice it turns out that it is not needed. An explanation for this phenomenon is that we approximate the boundary $\partial\Omega$ by a basis spline, which yields a

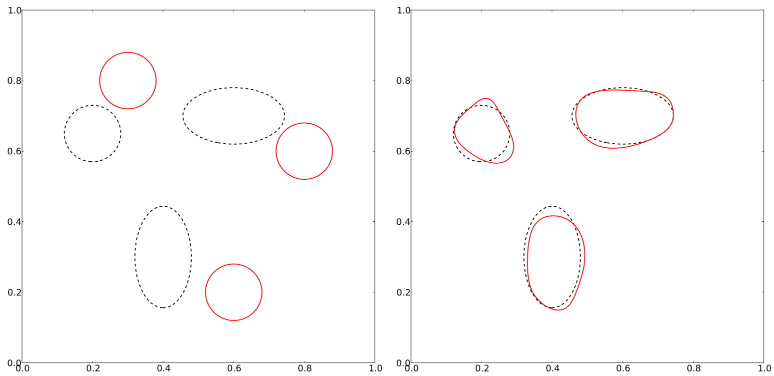

Figure 7.6: Initialisation (continuous contours - left) and reconstruction (continuous contours - right) of two ellipses and a ball (dashed contours) with 1.55% noise (371 iterations) and using seven measurements.

regularisation of the problem itself. More precisely, we described the boundary $\partial\Omega$ by a closed B-Spline curve of degree $k = 3$ as described in Section 6.7. Recall the formula (6.28) for a basis spline:

$$\gamma(t) = \sum_{i=1}^{n} N_i^3(t) U_i. \tag{7.7}$$

We proceed by calculating the control points $\tilde{U}_i$ using the Formula 6.31. As a result the vector field θ defined in by (6.29) constitutes a descent direction. Finally, we move the old control points U_i by adding the control points $\tilde{U}_i$, i.e. we put $U_i^{new} := U_i + \alpha\tilde{U}_i$, where $\alpha > 0$ is scalar such that we have a sufficient decrease. The boundary of the new domain is then $\partial\Omega_{new} := \gamma([0,1])$, where γ is defined by (7.7) but U_i replaced by U_i^{new}.

7.4.1 Numerical results

In this section, we provide the numerical results obtained by our algorithm for two different test examples. In our numerics we use cubic B-Spline curves to model the interface, i.e. we choose $k = 4$. Moreover we have $A_2 = A_1 = A$, $\beta_2 = 0$ and $\beta_1 = (1+\nu)\alpha\frac{1}{2}$, where ν is the shear contraction number and $\alpha = \frac{\varrho_1}{\varrho_2} - 1$, i.e. $\sigma_\chi = \lambda \operatorname{div}(\mathbf{u})I + 2\mu\varepsilon(\mathbf{u}) - (1+\nu)\alpha\frac{1}{2}\chi I$. By this choice no stresses occur whenever there is only one phase present, i.e. if $\Omega = \emptyset$. Then $\chi = 0$ a.e. on D and thus $\sigma_\chi = 0$. The state and adjoint state are discretised by the finite element method with linear (and globally continuous) elements as implemented in the FE/FV toolbox PDELib. The material data correspond to plain carbon steel; see Table 7.1.

Spherification of an ellipse

In the first example we consider a work piece, whose reference configuration is a quarter ellipsoid with periodic boundary conditions, i.e. we set $u_y := 0$ on the x-axes and $u_x := 0$ on the y-axes. The x-axis is 15.3 and y-axis is 15.0 units long. On the curved part of the boundary we impose homogeneous Neumann boundary conditions. Our goal is to modify the ellipse to a quarter circle. For this purpose we take the following cost function into consideration: $J(\Omega) := \int_{\tilde{\Sigma}} (|\mathbf{u}(x) + x| - R)^2\, dx$, where $R = 15.4$ denotes the desired radius of the circle, $\mathbf{u}(x) + x$ is the actual deformation of the material point $x \in D$ and $\tilde{\Sigma}$ denotes

Algorithm 3: Gradient flow algorithm

Data: Set $k = 0$. Choose initial domain $\Omega_k \subset \mathbf{R}^2$ with initial control points $U_1^k, \ldots, U_n^k$ such that $\gamma([0,1]) \approx \partial\Omega_k$.

initialisation;

while $n \leq N$ **do**

1.) Calculate $\tilde{U}_1, \ldots, \tilde{U}_n$ using equation (6.31). ;

2.) Associate with $\alpha > 0$ a new B-Spline curve

$$\gamma^\alpha(t) = \sum_{i=1}^{n} N_i^3(t)(U_i^n + \alpha\tilde{U}_i^n),$$

and a domain Ω_k^α with boundary $\gamma^\alpha([0,1]) =: \partial\Omega^\alpha$. Choose $\alpha > 0$ such that $J(\Omega^\alpha) \leq J(\Omega_n)$;

3.) set $t_{n+1} = t_n + \Delta t_n$ and $\Omega^{n+1} := \Omega_\alpha$ and $U_i^{n+1} := U_i^n + \alpha\tilde{U}_i^n$;

if $J(\Omega_n) - J(\Omega_{n+1}) \geq \gamma(J(\Omega_0) - J(\Omega_1))$ **then**

step accepted, continue program

else

exit program, no sufficient decrease ;

increase $n \to n + 1$,;

ϱ_1	ϱ_2	λ	μ
7850 kg	7770 kg	$1.5 \cdot 10^{11}$ Pa	$7.5 \cdot 10^{11}$ Pa

Table 7.1: Material data for a plain carbon steel.

the curved part of the boundary. Unfortunately, since the densities in different steel phases only differ by less than 1%, the ellipticity is hardly visible. The major axis is in the $x-$ and the minor axis in the $y-$ direction. Figure 7.7 shows the $y-$ component of the adjoint p for several iterations of the optimization algorithm. Since the derivative of the cost function acts as a force in the adjoint equation and the $y-$ component of the ellipse has to be pushed upwards to obtain a circle, this quantity is especially relevant. We discretised the state and adjoint state on a triangular grid with 96607 nodes using Lagrange linear finite elements.

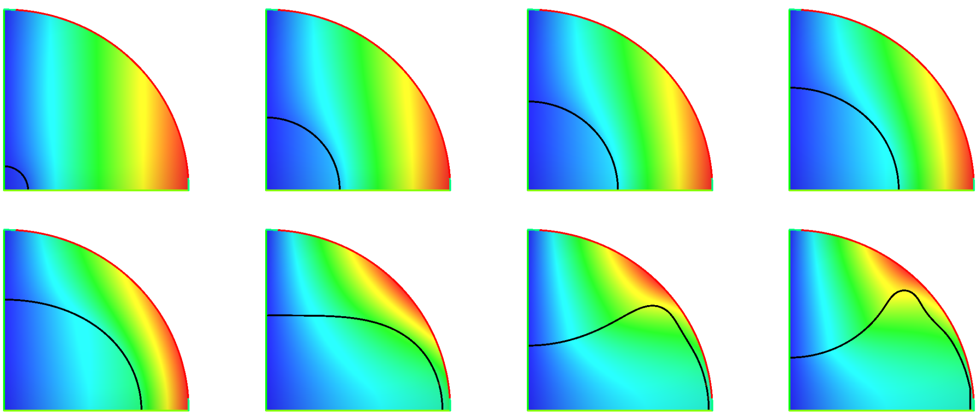

Figure 7.7: Several iterations for p_x with $\boldsymbol{p} = (p_x, p_y)$.

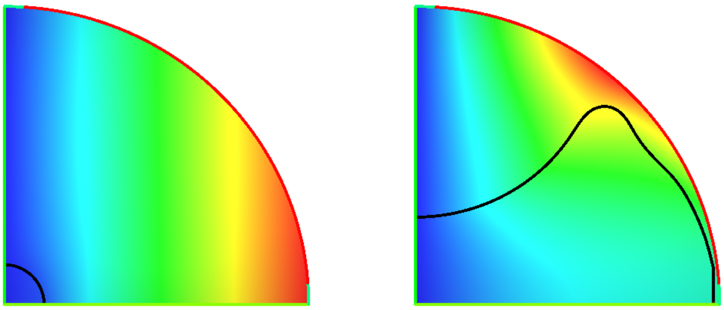

Figure 7.8: Initial and optimal shape.

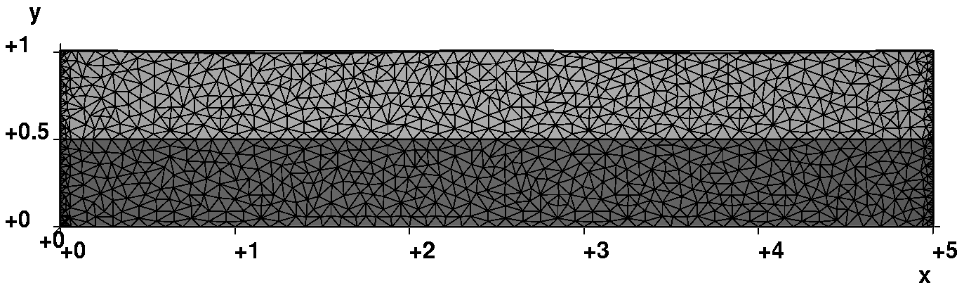

Figure 7.9: Triangulation of the wavy block.

Straightening of a wavy block

As the second example we consider a rectangular domain D with a wavy upper surface. We assume Dirichlet boundary conditions on the bottom and Neumann conditions on the top and on the sides and use the cost shape function $J(\Omega) = \int_{\tilde{\Sigma}} |u_y - R|^2 ds$ with $R = 1.0195$.

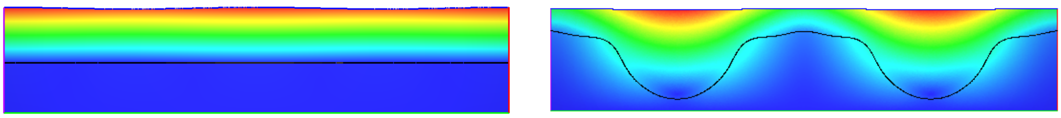

Figure 7.10: Initial (left) and optimal shape (right). Shading: $\|\mathbf{u}\|$ over D.

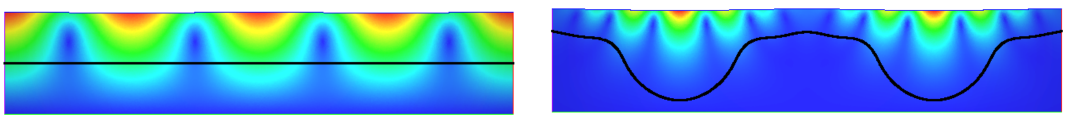

Figure 7.12: Distortion compensation: norm $\|\boldsymbol{p}\|$ of the adjoint over D

The goal is to straighten the upper surface. The initial and final block shape are depicted in Figure 7.10. Unfortunately, since the densities in different steel phases only differ by less than 1%, the waviness of the upper surface is hardly visible. Figure 7.11 shows the magnified shape of the upper boundary for several iterations of the optimization algorithm. One can indeed observe how the surface gradually straightens over the iterations. As discretisation

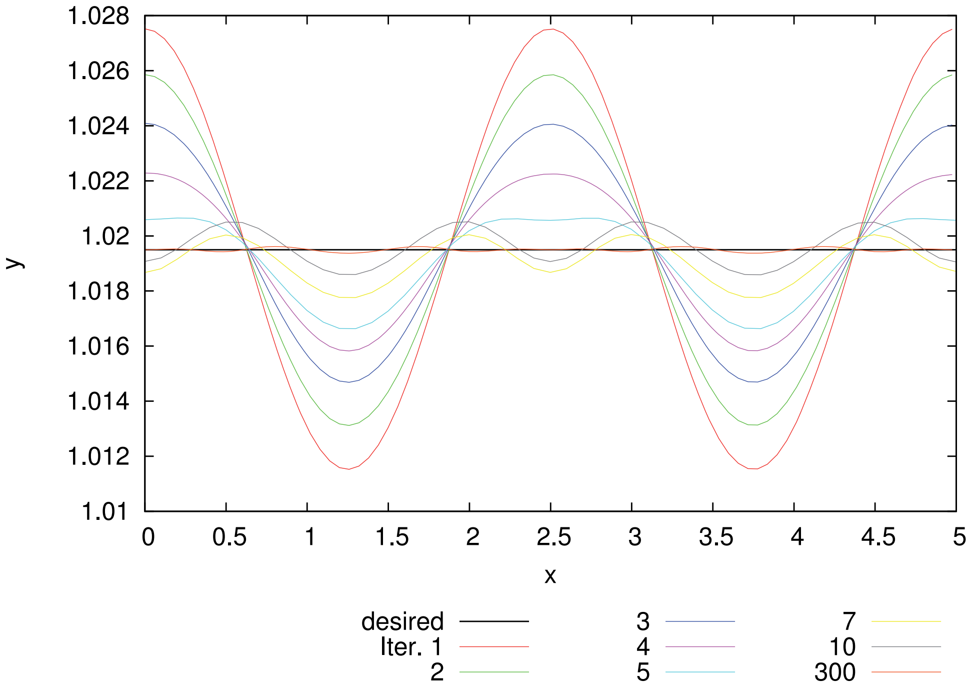

Figure 7.11: Surface shape of the wavy block for different iteration steps.

of the state and adjoint state, we chose 82724 nodes on a triangular grid and Lagrange linear finite elements.

Finally, Figure 7.13 shows several iterations of the y-component of the adjoint variable, where the gradient acts as a force term on the upper boundary.

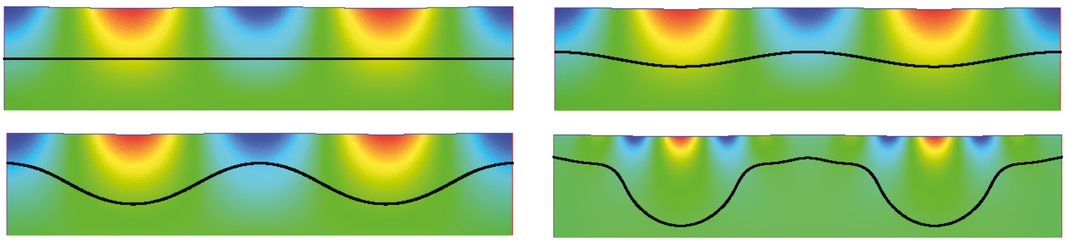

Figure 7.13: Several iterations of p_y with $\boldsymbol{p} = (p_x, p_y)$.

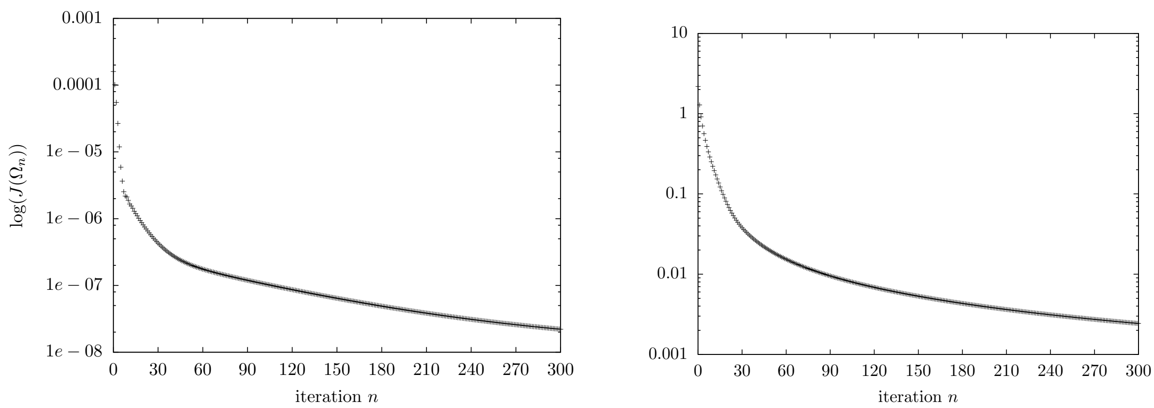

Figure 7.14: Convergence history for the wavy block and ellipse, respectively.

Conclusion

What have we done in this thesis?

This thesis contributed in several ways to the mathematical understanding of shape optimization problems as detailed here.

In Chapter 3, we have reviewed available methods to prove the shape differentiability of shape functions which depend implicitly on the solution of a semi-linear partial differential equation. Among these methods two are of particular interest, namely the material derivative method and the minimax method. In some situations the differentiability of the minimax can be justified by the theorem of Correa-Seeger. It was an open question whether Theorem 3.9 may be extended to situations, where the associated Lagrangian has no saddle points. In this situation, only the material derivative method or the rearrangement method can be applied.

In Chapter 4, Theorem 3.9 has been extended and a novel approach to the differentiability of a minimax function has been presented. The novelity is the introduction of a special averaged adjoint equation. This approach is designed for the special class of Lagrangian functions, that is, a cost function plus a equality penalisation namely the state equation. In concrete examples the required regularity of the cost function and the state equation with respect to the unknown is lower than previous results and only a certain continuity of the averaged adjoint equation is required. Moreover, we discussed how the assumptions of the new theorem can be applied under various assumptions.

In Chapter 5 it was shown that the new approach (Theorem 4.2) is also applicable when the classical material derivative method cannot be applied. This can be seen in the quasi-linear example from Section 5.4. The new result is particularly easy to apply to linear problems as shown in the elasticity example from Section 5.2. Furthermore, with Theorem 4.5 a version of Theorem 4.2 was presented that allows to compute shape derivative for coupled systems and also for second order shape derivatives. We applied this latter result to an EIT problem with coupling in the cost function.

In Chapter 6, constructions to build groups of diffeomorphisms from spaces $\mathcal{H} \subset C^{0,1}(D, \mathbf{R}^d)$ have recalled and it has been shown how the groups are linked with shape functions and the volume expression. Moreover, it has shown that the volume expression of the shape derivative is the natural form of the shape derivative in this context. By choosing appropriate scalar products on $\mathcal{H}$, we could demonstrate that a gradient flow in the space of diffeomorphisms is nothing but a usual gradient algorithms frequently used in applications. With the gradient flow interpretation it is now possible to define algorithms which do not change the underlying grid of the discretised domain, instead the state and adjoint equation are transformed in each step. This approach, also called Lagrangian view, has for small variations of the shape advantages over the usual Eulerian view. Nevertheless, the Eulerian approach in combination with the domain expression yields also very smooth deformations of the grid. Therefore, even when the grid is moved in each step a remesh has to be done only after several steps.

In Chapter 7, we have shown that the developed tools from Chapter 6 have an impact on the numerical treatment of shape optimization problems as well. We could successfully use the domain expression to reconstruct optimal shapes for simple unconstrained shape functions. We were also able to treat an ill-posed EIT problem and a simple transmission problem. Compared to the $L_2(\Gamma)$ gradient which is frequently used in applications, we have shown that better results can be obtained with less implementation effort.

Which questions remain open for further research?

The investigations of the previous chapters leave space for further investigations towards several directions.

Theorem 4.2 was applied to a quasi-linear problem, where an application of the implicit function theorem is not possible without further investigations of the solution of the PDE. Now the next step is to apply the new theorem or possibly an extension of it to more complicated problems. For instance it should be possible to apply Theorem 4.2 to the p-Laplacian or more complicated quasi-linear problems. The difficulty arises when the averaged equation for this problem has only solutions in a weighted Sobolev space. Therefore, the general version of the theorem we gave has to be adapted to these situations. To be more precise the space

$$Y(t,x^t,x^0) := \left\{ q \in F |\ \int_0^1 d_x G(t, sx^t + (1-s)x^0, q; \hat{\varphi})\, ds = 0 \quad \text{for all } \hat{\varphi} \in E \right\}.$$

should be replaced by something like

$$\mathfrak{Y}(t,x^t,x^0) := \left\{ q \in \tilde{F}^t |\ \int_0^1 d_x G(t, sx^t + (1-s)x^0, q; \hat{\varphi})\, ds = 0 \quad \text{for all } \hat{\varphi} \in \tilde{F}^t \right\},$$

where $\tilde{F}^t$ will be weighted space depending on x^t and x^0. In general we will satisfy neither $\tilde{F}(x^t,x^0) \subset F$ nor $F \subset \tilde{F}(x^t,x^0)$. One can already suspect that to check the conditions of Theorem 4.2 for $\mathfrak{Y}(t,x^t,x^0)$ will be more difficult than for $Y(t,x^t,x^0)$.

Another point is that we did not present an example where the set $X(t)$ and/or $Y(t,x^t,x^0)$ ($x^t \in X(t)$, $x^0 \in X(0)$) are truly multi-valued. So we have to reformulate Theorem 4.2 for this particular case. The conditions should be similar to the ones used in Theorem 3.9, where the sets $X(t)$ and $Y(t)$ were introduced. These have to be replaced by $X(t)$ and $Y(t,x^t,x^0)$. This is a challenging task which needs to be done in further studies.

In [97] (see also references therein) the author used reproducing kernel Hilbert spaces $\mathcal{H} \subset C^1_c(D,\mathbf{R}^d)$ to approximate Gradients of functionals $f \in \mathcal{H}'$. This is connected to our setting by $f = dJ(\Omega)$ and for instance $\mathcal{H} = H^k(D,\mathbf{R}^d)$, $(k \geq 1)$. The idea of reproducing kernel Hilbert spaces goes back to developments of Nachman Aronszajn[1] and Stefan Bergman[2] in 1950. By definition each reproducing kernel Hilbert space has a reproducing kernel $K(x,y)$ with which it is possible to obtain concrete expressions for gradients of Fréchet derivatives. In this case it would be interesting to study the feasibility of the Eulerian approach for image processing problems with for instance the H^1-metrics; cf. Section 6.5.1 and Algorithm 2. Also we did not consider other metrics than H^1 numerically. For instance in order to approximate the H^2 metric it is thinkable to use discontinuous Galerkin methods.

[1]Nachman Aronszajn (26 July 1907 – 5 February 1980) was a Polish American mathematician.

[2]Stefan Bergman (5 May 1895 – 6 June 1977) was a Polish-born American mathematician.

Chapter 8

Appendix

In the appendix, we collect the basic definitions. Most of them are standard but we gather them here for the convenience of the reader.

A Measure spaces

Definition A.1. *Let X be a set. A σ-algebra is collection of subsets $\mathcal{A} \in 2^X$ such that*

(i) $\Omega \in \mathcal{A}$.

(ii) For all $\Omega \in \mathcal{A} \Longrightarrow \Omega^c := X/\Omega \in \mathcal{A}$.

(iii) For all $\Omega_0, \Omega_1, \ldots \in \mathcal{A} \Longrightarrow \cup_{n\in\mathbf{N}} \Omega_n \in \mathcal{A}$

The Borel algebra on a topological space X is the smallest σ-algebra containing all open sets

Definition A.2. *Let X be a set. An outer measure on X is a function $\mu : 2^X \to [0, \infty]$ such that*

(i) $\mu(\emptyset) = 0$

(ii) For any two subsets $\Omega, \omega \in 2^X$

$$\omega \subset \Omega \Longrightarrow \mu(\omega) \leq \mu(\Omega).$$

(iii) For all $\Omega_0, \Omega_1, \ldots \in \mathcal{A}$:

$$\mu\left(\bigcup_{n\in\mathbf{N}} \Omega_n\right) \leq \sum_{n=0}^{\infty} \mu(\Omega_n).$$

Definition A.3. *Let X be a set and $\mathcal{A}$ an σ-algebra over X. A measure on X is a function $\mu : \mathcal{A} \to [0, \infty]$ such that*

(i) $\mu(\emptyset) = 0$

(ii) For all countable pairwise disjoint collections of sets $\Omega_0, \Omega_1, \ldots \in \mathcal{A}$

$$\mu\left(\bigcup_{n\in\mathbf{N}} \Omega_n\right) = \sum_{n=0}^{\infty} \mu(\Omega_n).$$

Note that the properties (ii),(iii) of Definition A.2 are automatically satisfied for a measure. A triplet $(X, \mathcal{A}, \mu)$ is called measure space *if X is a set $\mathcal{A}$ a σ-algebra over X and $\mu : \mathcal{A} \to \mathbf{R}$ a measure.*

DEFINITION A.4. *Let $\mathcal{A} \subset 2^{\mathbf{R}^d}$ the Borel σ-algebra on $\mathbf{R}^d$. We call μ*

(i) inner regular if for all $A \in \mathcal{A}$:

$$\mu(A) = \sup\{\mu(K) \mid \text{compact } K \subseteq A\}.$$

(ii) locally finite if for every point $p \in X$, there is an open neighbourhood N_p of p such that the $\mu(N_p) < \infty$.

(iii) A Radon measure *if it is inner regular and locally finite.*

DEFINITION A.5.

In the following let $(X, \mathcal{A}, \mu)$ be a measure space.

LEMMA A.6 (Fatou). *Let $(f_n)_{n\in\mathbf{N}} : X \to \mathbf{R}$ be a squence of non-negative μ-measurable functions. Define pointwise for all $x \in \mathbf{R}^d$ the function $f(x) := \liminf_{n\to\infty} f_n(x)$. Then*

$$\int_X f(x)\, dx \le \liminf_{n\to\infty} \int_X f_n(x)\, dx.$$

If the sequence $(f_n)_{n\in\mathbf{N}}$ converges pointwise almost everywhere in $\mathbf{R}^d$ to a μ-measurable function f, then the previous inequality is still valid.

THEOREM A.7 (Lebesgue dominated convergence). *Assume that $(f_n)_{n\in\mathbf{N}}$ is a sequence of functions in $L_1(X, \mu)$ and $f \in L_1(X, \mu)$ such that*

$$f_n(x) \to f(x) \text{ for a.e. } x \in X \quad \text{and } |f_n(x)| \le g(x) \text{ for a.e. } \quad x \in X,$$

for some function $g \in L_1(X, \mu)$. Then:

$$\lim_{n\to\infty} \int_X f_n\, d\mu = \int_X f\, d\mu.$$

B Bochner integral

Let $(X, \mathcal{A}, \mu)$ be a σ-finite, complete measure space and $(E, \|\cdot\|)$ a Banach space.

DEFINITION B.1. *A simple function function $f : \Omega \to E$ is a function of the form*

$$f(x) = \sum_{k=0}^{n} \alpha_i\, \chi_{U_i},$$

where $n \in \mathbf{N}, \alpha_i \in E$ and $U_i \in \mathcal{A}$. The set of simple functions is denoted by $\mathcal{EF}(X, \mu, E)$. The integral $\int : E \to \mathbf{R}$ of a simple function is defined by

$$\int_E f(x)\, dx := \sum_{i=0}^{n} \alpha_i \mu(U_i).$$

For any $A \in \mathcal{A}$, we set

$$\int_A f(x)\, dx := \int_E \chi_A f\, dx.$$

We denote the induced norm on $\mathcal{EF}(X, \mu, E)$ by $\|f\|_1 := \int_X |f|\, d\mu$ and call a Cauchy sequence in this space also $\mathcal{L}_1$ Cauchy sequence.

Definition B.2. *A function $f : \Omega \to E$ is called μ-measurable or strongly measurable if there exists a sequence of simple functions $(\chi_n)_{n\in\mathbf{N}}, \chi_n \in \mathcal{EF}(X,\mu,E)$ such that we have $\lim_{n\to\infty}\chi_n(x) = f(x)$ for μ-almost every $x \in X$. A function $f \in E^X$ is called μ-integrable if there exists a $\mathcal{L}_1$ Cauchy sequence in $(\chi_n)_{n\in\mathbf{N}} \in \mathcal{EF}(X,\mu,E)$ converging μ-almost everywhere to f. The space of μ-integrable function is denoted by $L_1(X,\mu,E)$. When μ is the Lebesgue measure, then we write $L_1(X,E)$.*

Theorem B.3. *A $f : X \to E$ is μ-measurable if and only if*

(i) For any continuous functional $\phi \in E'$ the function $\phi \circ f : X \to \mathbf{R}$ is μ-measurable.

(ii) There exists a set of μ-measure zero $N \subset \mathcal{A}$ such that $f(X/N) \subset E$ is separabel with respect to the norm topology.

One can show that for a $\mathcal{L}_1$ Cauchy sequence in $(\chi_n)_{n\in\mathbf{N}} \in \mathcal{EF}(X,\mu,E)$ converging μ-almost everywhere to f the sequence $\left(\int_X \chi_n\mu\right)_{n\in\mathbf{N}}$ is also a Cauchy sequence.

Definition B.4. *The integral of f over X is defined by*

$$\int_X f\,d\mu := \lim_{n\to\infty}\left(\int_X \chi_n\,d\mu\right)_{n\in\mathbf{N}}.$$

Lemma B.5. *A strongly measurable function $f : X \to E$ is integrable if and only if*

$$\int_X \|f\|_E\,d\mu < \infty.$$

C Sobolev spaces

In this Section we recall the some important theorems from analysis which are used throughout this thesis.

In order to define Sobolev spaces we recall the notion of weak derivative:

Definition C.1. *We say that $g \in L_p(\Omega)$ is the γ-th weak derivative of $f \in L_p(\Omega)$, where $\gamma = (\gamma_1,\dots,\gamma_n) \in \mathbf{N}^n$ with $|\gamma| = \sum_{i=1}^n \gamma_i$, if there is a function such that*

$$\int_\Omega g\varphi\,dx = (-1)^{|\gamma|}\int_\Omega fD_\gamma\varphi\,dx \quad \forall\varphi \in C_c^\infty(\Omega).$$

$$W_p^k(\Omega) := \{f \in L_p(\Omega) :\ D_\gamma f \in L_p(\Omega)\ \forall\gamma \in \mathbf{N}^n \text{ with } |\gamma| \le k\} \quad (1 \le k \le \infty,\ 1 \le p \le \infty)$$
$$W_p^s(\Omega) := \{f \in W_p^{\lfloor s\rfloor}(\Omega)|\ \sup_{|\gamma|=\lfloor s\rfloor}|\partial_\gamma f|_{W_\eta^p(\Omega)} < \infty\} \quad (\eta := s - \lfloor s\rfloor \in (0,1),\ s > 0)$$

Let us continue with the important Sobolev embedding theorems for Sobolev spaces.

Theorem C.2 (Sobolev embedding theorem). *Let $\Omega \subset \mathbf{R}^d$ be open and bounded with Lipschitz boundary. Moreover, let two integers $m_1 \ge 0, m_2 \ge 0$ as well as $1 \le p_1 < \infty$ and $1 \le p_2 < \infty$ be given. Then it holds*

(i) If $m_1 - d/p_1 \ge m_2 - d/p_2$ and $m_1 \ge m_2$, then there exists a continous embedding

$$id : W_{p_1}^{m_1}(\Omega) \to W_{p_2}^{m_2}(\Omega).$$

More precisely for each $u \in W_{p_1}^{m_1}(\Omega)$ there is a constant $C > 0$ depending on $n, \Omega, m_1, m_2, p_1, p_2$ such that

$$\|u\|_{W_{p_2}^{m_2}(\Omega} \le C\|u\|_{W_{p_1}^{m_1}(\Omega)}.$$

(ii) *If $m_1 - d/p_1 > m_2 - d/p_2$ and $m_1 > m_2$, then there exists a continous and compact embedding*

$$id : W_{p_1}^{m_1}(\Omega) \to W_{p_2}^{m_2}(\Omega).$$

Under certain conditions the Sobolev spaces embed into Hölder spaces as is stated in the following

THEOREM C.3. *Let $\Omega \subset \mathbf{R}^d$ be open and bounded with Lipschitz boundary. Moreover, let an integer $m \geq 1$ as well as $1 \leq p < \infty$, an integer $k \geq 0$ and $0 \leq \alpha \leq 1$ be given. Then it holds*

(i) *If $m - d/p = k + \alpha$ and $0 < \alpha < 1$, then there exists a continous embedding*

$$id : W_p^m(\Omega) \to C^{k,\alpha}(\overline{\Omega}).$$

More precisely for each $u \in W_p^m(\Omega)$ there is a constant $C > 0$ depending on the constants $n, \Omega, m, p, \alpha, k$ such that

$$\|u\|_{W_p^m(\Omega)} \leq C\|u\|_{C^{k,\alpha}(\overline{\Omega})}$$

(ii) *If $m_1 - d/p_1 > m_2 - d/p_2$ and $m_1 > m_2$, then there exists a continous and compact embedding*

$$id : W_{p_1}^{m_1}(\Omega) \to W_{p_2}^{m_2}(\Omega).$$

Since functions $f \in W_p^k(\Omega)$, where $1 < p < \infty$, $k \geq 1$, are only defined up to a set of measure zero it is delicate to define a trace, that is, $f_{|\partial\Omega}$.

THEOREM C.4. *Assume that Ω has Lipschitz boundary, then there exists a linear operator $\gamma : W_p^k(\Omega) \to W_p^{k-1/p}(\Omega)$ such that*

(i) $\gamma(f) = f|_{\partial\Omega}$ *for* $f \in C(\overline{\Omega}) \cap W_p^k(\Omega)$

(ii) $\|\gamma(f)\|_{W_p^k(\Omega)} \leq C\|f\|_{W_p^{k-1/p}(\Omega)}$.

Instead of $\gamma(f)$ we simply write $f|_{\partial\Omega}$.

With this definition it is possible to introduce for $k \geq 1$ the following subspace

$$\mathring{W}_p^k(\Omega) := \{f \in W_p^k(\Omega) : \ f|_{\partial\Omega} = 0\}.$$

For space dimension $d \geq 1$ it is convenient to introduce for a number $p \in \mathbf{R}^+$ its conjugate p^* by

$$p^* \stackrel{\text{def}}{=} \begin{cases} \frac{dp}{d-p}, & \text{if } p < 1 \\ \infty, & \text{if } p = d \end{cases},$$

We will frequently make use of (one of) the Poincaré inequality.

THEOREM C.5. *Let $1 \leq p \leq \infty$. There exists a constant $C_{\Omega,p}$ dependent on Ω and p such that*

$$\|f - (f)\|_{W_p^1(\Omega)} \leq C_{\Omega,p}\|f\|_{L_p(\Omega)} \quad \textit{for all } f \in \breve{W}_p^1(\Omega),$$

with $(f) := \frac{1}{|\Omega|}\int_\Omega f dx$.

Vector valued function spaces will be denoted by $W_p^s(\Omega;\mathbf{R}^d)$, $C^k(\Omega,\mathbf{R}^d)$, $C_c^k(\Omega,\mathbf{R}^d)$ and so forth. The norms of those spaces are given in the natural way. For instance if $\mathbf{u}=(u_1,\dots,u_n)$ we set $\|\mathbf{u}\|_{W_p^s(\Omega;\mathbf{R}^d)} := \sum_{i=1}^n \|u_i\|_{W_p^s(\Omega)}$. Let $\Gamma\subset\partial\Omega$ be a subset with positive Hausdorff measure. We introduce the vector valued space

$$W_{\Gamma,p}^1(\Omega;\mathbf{R}^d) := \{\mathbf{u}\in W_p^1(\Omega;\mathbf{R}^d) |\ \mathbf{u}=0 \text{ on } \Gamma\}.$$

Similar to the Poincaré inequality in the scalar case is the Korn equality vector valued case.

Theorem C.6. *There exists a constant K_Ω depending on the domain Ω, such that*

$$\|\boldsymbol{\varphi}\|^2_{W_1^2(\Omega;\mathbf{R}^d)} \le K_\Omega \int_\Omega \varepsilon(\boldsymbol{\varphi}):\varepsilon(\boldsymbol{\varphi})dx \quad \forall \boldsymbol{\varphi}\in W_{\Gamma,2}^1(\Omega;\mathbf{R}^d).$$

Theorem C.7 (Carathéodory). *Let $\tau>0$ and $f:[0,\tau]\times\mathbf{R}^d\to\mathbf{R}^d$ satisfy the following conditions*

$$\begin{aligned} &f(\cdot,\zeta) \ \ \textit{is measurable for all } \zeta\in\mathbf{R}^d\\ &f(t,\cdot) \ \ \textit{is continuous for almost all } t\in[0,\tau]\end{aligned}$$

and there exists $\gamma\in L_1((0,\tau))$ and $C>0$ such that

$$\forall z\in\mathbf{R}^d,\ \forall t\in[0,\tau]:\ |f(t,z)|\le\gamma(t)+C|z|.$$

Then

(i) The initial-value problem

$$\dot z(t) = f(t,z(t)) \textit{ for almost all } t\in[0,\tau],\quad z(0)=z_0\in\mathbf{R}^d$$

has a unique solution $z\in W_1^1([0,\tau],\mathbf{R}^d)$.

(ii) If f is Lipschitz continuous with repect to ζ, then the solution is unique.

D Groups and metrics

We collect some basic definitions from group theory and differential geometry.

Definition D.1. *A* group *is a set G with an operation $\circ: G\times G\to G$ such that*

Neutral element: *There exists $e\in G$ such that for all $a\in G:\ e\circ a = a\circ e = a$.*
Inverse element: *For every $a\in G$ there exists $a^{-1}\in G$ such that $a\circ a^{-1} = a^{-1}\circ a = e$*
Associative law: *For all $a,b,c\in G:\ (a\circ b)\circ c = a\circ(c\circ b)$.*

If G is also a topological space such that the inversion $a\mapsto a^{-1}$ and group composition $(a,b)\mapsto a\circ b$ are continuous continuous, then G is called topological group*.*

Definition D.2. *A* metric space *is a pair (M,d) consisting of a set M and a* distance *$d: M\times M\to\mathbf{R}$, i.e., for all $x,y,z\in M$*

$$\begin{aligned} &1.\ d(x,y)=0 \Leftrightarrow x=y\\ &2.\ d(x,y)=d(y,x)\\ &3.\ d(x,z)\le d(x,y)+d(y,z)\end{aligned}$$

If M is also a group, we call M a metric group*. The metric is called* right-invariant *if for all $x,y,z\in M$*

$$d(x\circ z, y\circ z) = d(x,y).$$

Definition D.3 (Lie derivative). *Let $\mathcal{M}$ be a finite dimensional manifold and $X : \mathcal{M} \to T\mathcal{M}$ a smooth vector field with (global) flow $\Phi : [0, \tau] \times \mathcal{M} \to \mathcal{M}$. One way to define the Lie derivative of a smooth function $f \in C^\infty(\mathcal{M})$ is by $\mathcal{L}_\theta(f) := \lim_{t \searrow 0}(f(\Phi_t(x)) - f(x))/t$.*

List of Figures

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