Shape derivative techniques in optimal design

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Zagreb, 2020

Sveučilište u Zagrebu

PRIRODOSLOVNO - MATEMATIČKI FAKULTET
MATEMATIČKI ODSJEK

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Tehnike derivacije oblika u optimalnom dizajnu

DOKTORSKI RAD

Mentor:
Izv. prof. dr. sc. Marko Vrdoljak

Zagreb, 2020.

Acknowledgements

Zahvaljujem mentoru, izv. prof. dr. sc. Marku Vrdoljaku na prenošenju znanja i iskustava te nesebičnoj pomoći i trudu na mom znanstvenom putu. Također mu zahvaljujem na strpljenju, podršci, ohrabrenju i motivaciji.

Zahvaljujem prof. dr. sc. Nenadu Antoniću na podršci i korisnim savjetima.

Hvala svim kolegama, profesorima, znanstvenicima i prijateljima. Hvala Ani.

Na kraju, zahvaljujem svojoj obitelji na njihovoj ljubavi, podršci i strpljenju.

Summary

Optimal design theory, also known as shape optimization is quite indispensable in many fields like aeronautics, architecture, medicine, computer science. Applications vary from classical, as construction of an aircraft wing, to more recent as in inverse problems of electrical impedance tomography (non-invasive method of medical scanning), picture segmentation or in 3D printing. From the engineering point of view the main aspect of design process is improving a current design. In such optimal design problems the shape sensitivity analysis plays a central role in finding a solution and creation of numerical methods.

In this thesis we consider optimal design problems for stationary diffusion equation, seeking for an arrangement of two isotropic materials, with prescribed amounts, which maximizes a given functional. The optimality of a distribution is measured by an objective function, which is usually an integral functional depending on the distribution of materials and the state function, obtained as a solution of the associated boundary value problem for the corresponding partial differential equation. Commonly, optimal design problems do not have solutions (if they exist, such solutions are usually called *classical*). Therefore, one can consider a proper relaxation of the original problem by the homogenization method which consists of using generalized composite materials.

By enlarging the admissible set of the relaxed problem we can consider an artificial optimal design problem which can be rewritten as a saddle point problem. We further show that it is equivalent to a simpler relaxation problem given only in terms of the local proportion of the original materials for which necessary and sufficient conditions of optimality are obtained. Since every classical solution of the considered artificial optimal design problem is also a (classical) solution of the original problem it can be used to construct a family of classical solutions.

The aim of the first chapter of the thesis is to present some classes of optimal design problems on an annulus with classical solutions. The first class is a single state equation problem with a constant right-hand side and homogeneous Dirichlet boundary condition. By analysing the optimality conditions, we are able to show that there exists a unique (classical) solution. We prove that, depending on the amounts of given materials, only two optimal configurations in both two- and three-dimensional case are possible. The second class of problems deals with a two-state optimal design problem.

In the second chapter shape derivative results for the considered problem are presented.

Assuming that the interface between phases is regular, for the optimal design problem the first and the second order shape derivative are calculated using different techniques e.g. the chain rule approach and the averaged adjoint approach. The presented results are later used in construction of numerical methods.

Shape derivatives can be written in a form of domain integral or as an integral over the interface. The domain expression or distributed shape derivative seems more appropriate for numerical implementation since boundary representations include jumps of a discontinuous functions over the interface.

The third chapter is devoted to numerical methods for the optimal design problem presented in the first section. Descent methods based on distributed first and second order shape derivatives are implemented and tested. We observe a stable convergence of both descent methods with a novel Newton-like method converging in half as many steps.

Keywords: optimal design, homogenization, optimality conditions, shape derivative, shape optimization, Newton method, gradient method

Sažetak

Teorija optimalnog dizajna, poznata i kao teorija optimizacije oblika je izuzetno važna zbog svog teorijskog i praktičnog aspekta. Postoje mnoge njene primjene u različitim interdisciplinarnim područjima poput mehanike, arhitekture, medicine i računarstva. Primjene su široke od klasičnih problema poput konstrukcije krila aviona pa sve do aktualnih kao što su inverzni problem električne impedancijske tomografije (neinvazivne metode medicinskog snimanja), problem segmentacije slike ili 3D printanje.

U ovom radu promatra se problem optimalnog dizajna u kojem je cilj odrediti raspored jednog ili više materijala u danom univerzalnom skupu. Optimalnost rasporeda (distribucije) materijala mjeri se funkcionalom energije koji ovisi o rješenju jednog ili više rubnih problema. U pripadnoj parcijalnoj diferencijalnoj jednadžbi koeficijenti ovise o rasporedu materijala. Zadaća optimalnog dizajna najčešće nema rješenje (tzv. *klasična rješenja*). Upravo zato je potrebno gledati pogodnu relaksaciju originalnog problema.

U prvom poglavlju disertacije proučava se relaksirana zadaća koju uz proširenje dopustivog dizajna dopušta primjenu teorije sedlaste točke. Nova, proširena zadaća optimalnog dizajna može se zapisati koristeći samo lokalni omjer količina originalnih materijala. Problem se dodatno može zapisati kao konveksni problem minimizacije što daje mogućnost proučavanja nužnih i dovoljnih uvjeta optimalnosti. S obzirom da je svako klasično rješenje novog problema ujedno i rješenje originalnog problema dobivamo mogućnost konstrukcije klasičnih rješenja.

Cilj ove disertacije je proučiti probleme na prstenu u kojima se javljaju klasična rješenja. Konkretno, za stacionarnu jednadžbu difuzije s konstantnom desnom stranom pokazana je egzistencija i jedinstvenost rješenja. Ovisno o danoj količini materijala za prostor dimenzije 2 i 3 postoje samo dvije moguće strukture za optimalni dizajn. Promatra se i zadaća optimalnog dizajna, s dva rubna problema, u kojoj postoji klasično rješenje.

Drugo poglavlje disertacije posvećeno je analizi derivacije oblika. Uz dodatnu regularnost granice između materijala analizira se osjetljivost oblika zadaće transmisije. Konkretno, koriste se dvije tehnike derivacije oblika: lančano pravilo i usrednjena adjungirana metoda. Obje tehnike su uspješno iskorištene čime je dobivena derivacija oblika prvog i drugog reda.

Prema strukturnom teoremu, derivacije oblika dopuštaju zapis preko volumnih integrala ili preko integrala po rubu. Pokazuje se da je volumna forma prikladnija numeričkom rješavanju kod zadaća transmisije. Naime, pripadnu graničnu formu derivacije oblika je numerički teže tretirati u kontekstu derivacije oblika zbog prekida podintegralne funkcije na rubu.

Treće poglavlje disertacije posvećeno je numeričkim metodoma za probleme optimalnog dizajna iz prvog poglavlja. Metode silaska koje koriste prvu i drugu derivaciju oblika su implementirane te testirane na zadaćama optimalnog dizajna za koje imamo klasična rješenja. Opažena je stabilna konvergencija prema optimalnom rješenju za obje metode s time da aproksimativna Newtnonova metoda ima dvostruku veću brzinu konvergencije. Obje metode konvergiraju neovisno o početnoj aproksimaciji.

Ključne riječi: optimalni dizajn, homogenizacija, uvjeti optimalnosti, derivacija oblika, optimizacija oblika, Newtonova metoda, gradijentna metoda

Contents

Introduction

Shape optimization

Optimizing the shape of an object to make it the most efficient with a respect to a one or several different criteria is rather an old task. There are a lot of applications in many interdisciplinary areas like mechanics, physics, medicine, architecture and computer science. Classical applications come from industries like aeronautics where design of an airfoil can improve the performance and running costs of an aircraft, medicine where non-invasive methods of scanning (electrical impedance tomography) determine an inverse problems, or computer science where image segmentation is used to track moving interfaces.

Usually, shape optimization problems seek for an extremum of a given functional over a set of admissible domains:

$$\min_{\omega \in \mathcal{O}} J(\omega). \tag{1}$$

The elements of $\mathcal{O}$ are called *admissible shapes* which are usually a class of subsets of $\mathbb{R}^d$ and J is called a *shape functional*. We are particularly interested in optimization problems where admissible domains satisfy non linear constraint $A(\omega, u(\omega)) = 0$. The map $\omega \mapsto A(\omega, \cdot)$ is defined by a a boundary value problem which consists of a partial differential equation or a system of partial differential equations whose operators depends on ω and $u(\omega)$ represents a state solution of this boundary value problem. Shape optimization can be therefore regarded as a part of optimal control theory, were domains act as controls.

The question of existence of an optimal shape $\omega_0 \in \mathcal{O}$ such that

$$J(\omega_0) \leq J(\omega), \quad \omega \in \mathcal{O},$$

is non trivial to answer and for many problems which comes from applications it remains an open problem. Indeed, if we wish the family of admissible domains to be compact, then we should choose a topology as coarse as possible. On the other hand if we want the functional that we minimize to be continuous we should impose a fine topology. The other difficulty arises because of the absence of a vector space structure on the family of admissible domains which a priori prevents us from using the classical theory to obtain necessary conditions of optimality. In fact this offers us the possibility to study and apply several different frameworks: from the homogenization theory to the theory of shape analysis.

In this thesis we consider an optimal design problem for stationary diffusion equation. Let Ω be an open bounded subset of $\mathbb{R}^d$. It consists of two isotropic phases: a better conductor with conductivity β and worse with conductivity α, with the prescribed volume of the phase α. Denoting by χ the characteristic function of the worse conductor, the overall conductivity is written by $\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$ and state functions $u_1, ..., u_m \in \mathrm{H}_0^1(\Omega)$ are uniquely determined by a boundary value problem:

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u_i) = f_i \\ u_i \in \mathrm{H}_0^1(\Omega) \end{cases} \quad i = 1, 2, ...m. \tag{2}$$

where the right-hand sides $f_1, ..., f_m \in \mathrm{H}^{-1}(\Omega)$. The aim is to find an optimal configuration of phases α and β such that a conic sum of energies obtained for each state problem is maximized.

There are conceptually, two different directions on how we can solve this optimal design problem. The first direction considers enlarging the space of admissible designs to domains which fail to be "regular", i.e. to the point where we are dealing with mixtures of phases (v. [5],[40],[41]). The second direction restricts admissible designs, e.g. the region occupied by the phase α may admit Lipschitz boundary or be connected. Other possible constraints could be a given length of the perimeter, number of connected components, or higher regularity of the interface (v. [10],[30],[21]).

Relaxation by homogenization

A relaxation by the homogenization theory consists in introducing generalized materials, which are the mixtures of the original materials on the micro-scale. Perhaps standard way to relax characteristic functions is by the closure in L^∞ weak $*$ topology. On one hand for the conductivity L^∞ weak $*$ topology ensures compactness of conductivities, but on the other it disables the continuity of the energy functional. For that reason H-topology is introduced giving rise to a proper relaxed problem.

Historically, these questions were introduced in [47] through the concept of G-topology for stationary diffusion equation. The notion of H-topology was also originally introduced for the stationary diffusion equation in [40]. It differs from the concept of G-topology, as it treats the convergence of coefficients appearing in the equation, instead of the convergence of corresponding solution operators. However, for symmetric coefficients these two notions are equivalent.

Through the homogenization method one can show that the relaxed problem always admits a "generalized solution". Unfortunately, "generalized solutions" of optimal design problems are rarely *classical solutions*, i.e. the solution of original, non-relaxed problems. In the literature there are very few examples of optimal design problems with *classical solutions*, and all of them are given on a ball ([41],Remark 40): in the case of energy maximization with one state equation on a ball and a constant right-hand side the better conductor should be placed inside a smaller (concentric) ball, whose radius can easily be calculated from the constraint on given amounts of materials. For multiple state optimal design problems on a ball see [55]. This problem has interesting applications, e.g. in elasticity it models the maximization of the torsional rigidity of a cylindrical rod with uniform cross section made of two given materials. Another application is the problem of arrangement of two viscous fluids in the Poiseuille flow through the pipe with uniform cross-section that maximizes the flow rate. It is well known that classical solutions on a simply connected domain can appear only in the case of a ball (see [41],[14]). Therefore, in this thesis we shall address the analogous problem on an annulus. Although both domains are rather simple (spherically symmetric), it is important to stress that problem on a ball is much easier to solve as optimality conditions are given in terms of the known flux, while for the annulus one obtains a whole family of possible fluxes (dependent on an integration constant).

Shape derivative

In order to solve the above optimal design problem one considers an additional constraint on the admissible designs: the region occupied by the phase α denoted with Ω_α is a Lipschitz domain. Then the solution (2) satisfies transmission conditions, i.e. continuity of state functions and fluxes on the interface. We are interested in the behaviour of a shape functional with respect to small perturbations of the domain. A classical way to introduce this perturbations of domains is by constructing a family of homeomorphisms. There are several different notion on how this can be done, most notably by the method of perturbation of identity and by the speed method (v. [30],[54],[44],[46]). Perturbation of identity takes a small θ in a normed space such as $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ or $C_b^k(\mathbb{R}^d;\mathbb{R}^d)$ and creates a homeomorphism from $\mathbb{R}^d$ onto $\mathbb{R}^d$ by the map $\mathrm{Id}+\theta$. Particularly, one is interested in Eularian semi-derivative:

$$J'(\Omega_\alpha;\theta) := \lim_{t\searrow 0} \frac{J((\mathrm{Id}+t\theta)\Omega_\alpha) - J(\Omega_\alpha)}{t} \tag{3}$$

also called shape derivative of the functional J at Ω_α in the direction θ whenever the map $\theta \mapsto J'(\Omega_\alpha;\theta)$ is linear and continuous. This concept was originally developed by Hadamard in his study of elastic plates in his pioneering paper in 1908 [28]. For more about history and further development of the theory one can find in [30] and [46].

Calculations of (3) is tedious and error prone task, especially for the transmission problem, where we are also dealing with the lack of regularity of state functions due to discontinuity of coefficients along the interface. This was recognized in [43],[7] meaning that formal Cea's method [15] which introduces the Lagrange functional to formally calculated shape derivative becomes rather complex.

For that reason two fundamentally different techniques of calculating the shape derivative were chosen:

1. a standard approach via the so called chain rule (v. [39],[38],[44]),

2. an averaged adjoint method (v. [50],[35]).

"Chain rule" is rather classical approach in the literature which uses the inverse function theorem to show differentiability of the state function composed by the map $\mathrm{Id} + \theta$, thus giving directional derivative also known as *material derivative*. This material derivative can then be directly used to calculate the shape derivative or to define a *local derivative*. While technically more tedious it offers more substantial information with stronger notion of differentiability, e.g. Fréchet derivative. The averaged adjoint method is straightforward approach similar to formal Cea's method where to the shape functional is added a weak formulation (linear penalization) of the state equation. The usual adjoint state function is then replaced with a limit of an "averaged' family of adjoint functions and rigorously justified.

By the Hadamard structure theorem the shape derivative depends only on the normal component of the variation θ on the interface Γ. The first, chain rule approach, gives shape derivative exactly in this boundary form. The second approach by an averaged adjoint method gives the same shape derivative in the distributional (volume) form. This difference will be useful later for calculations of the second order shape derivative in both representational forms.

The study of the second order shape derivative was initiated in the paper [45] by J. Simon. The idea behind this notion is rather simple, because we would like to have a second order Taylor expansion of the shape functional

$$J((\mathrm{Id} + t\theta)\Omega_\alpha) = J(\Omega_\alpha) + tJ'(\Omega_\alpha;\theta) + \frac{t^2}{2}J''(\Omega_\alpha;\theta,\theta) + o(t^2).$$

Here the very definition of the second order shape derivative is crucial because

$$J''(\Omega_\alpha;\theta,\psi) \neq (J'(\Omega_\alpha;\theta))'(\Omega_\alpha;\psi)$$

meaning that second order derivative cannot be obtained simply as a variation of the first order shape derivative. It is also important to note that the Hadamard structure theorem highly depends on the choice of family of homeomorphism (see [54]).

The objective of this thesis

The main results of this thesis are:

1. Construction of classical solutions for optimal design problems on annulus with qualitative analysis of some examples.

2. Application and comparison of several techniques for calculations of the first and the second order shape derivative.

3. Numerical implementation of several gradient methods and Newton-like methods using distributional (volume) shape derivative. To the best of our knowledge this is the first such kind of implementation of Newton method to a shape functional with PDE constraints.

The structure of this thesis

Now we turn to a brief overview of the thesis.

Chapter 1: Classical optimal designs for energy maximization

The first chapter starts with introductory overview of the homogenization theory and H-topology introduced by Murat and Tartar. Important results as characterization of $\mathcal{K}(\theta)$, a set of all effective conductivities obtained by mixing original phases with local fraction θ, or the fact that H-topology is metrizable are given. A proper relaxation of the original optimal design problem is given with an admissible set $\mathcal{A}$ of relaxed designs. The set $\mathcal{A}$ is artificially enlarged to a convex set $\mathcal{B}$ which offers a reinterpretation of a new optimal design problem as a minimax problem and consequently can be viewed as a simpler relaxation problem only in terms of local fraction. From there necessary and sufficient conditions of optimality are obtained, which is utilized to create a classical solution of the original optimal design problem.

As the first example a single state problem with a constant right-hand side f is studied. We are able to show that in the case of annulus, the solution of the relaxed problem is unique, classical and radial. Depending on the amounts of given materials, we find two possible optimal configurations. If the volume of the first phase is less than some critical value, then the better conductor should be placed in an outer annulus. Otherwise, the optimal configuration consists of an annulus made of the better conductor, surrounded by two annuli of the worse conductor. The choice for right hand sides when creating classical solutions is delicate. Although, it is easy to prove the existence of unique solution by a simple criteria, the analysis of possible optimal designs could become tedious. Therefore, an example of multiple state problem is presented for which determining possible configuration of the optimal solution is straightforward. Once the configuration is known radii between phases are computed by solving a system of nonlinear equations (numerically).

Chapter 2: Calculations of shape derivative

In the second chapter we focus on calculation of the first and the second order shape derivative.

Section 2.1 deals with a definition of Lipschitz domains and their characterization. It is rather well known that the image of Lipschitz domain under a bi-Lipschitz map from $\mathbb{R}^d$ onto $\mathbb{R}^d$ is not necessarily a Lipschitz domain. A simple sufficient condition which ensures that perturbation of identity of the form $\mathrm{Id} + \theta$ for $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$, maps a Lipschitz domain onto a Lipschitz domain is demonstrated. We show that state equation of the original optimal design problem with assumption that the region occupied by phase α, denoted with Ω_α, is a Lipschitz domain is equivalent to a transmission system. This play a key role in understanding the shape differentiability of the state function and consequently of the energy functional.

In Section 2.2 material derivative of a transmission model is calculated through the use of the implicit function theorem. Particularly, the map $\theta \mapsto u(\theta) \circ (\mathrm{Id} + \theta)$ is well defined and Fréchet differentiable in a zero-neighbourhood of $\mathrm{W}^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ to $\mathrm{H}_0^1(\Omega)$. In case of higher regularity of the interface Γ between phases and of the right hand-side in the state equation one can demonstrate Fréchet differentiability in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ to $\mathrm{H}_0^1(\Omega) \cap \mathrm{H}^k(\Omega_\alpha \cap \Omega_\beta)$. As a consequence a local derivative is well defined and it satisfies a generalized transmission problem with jump conditions on the interface. Several techniques were used to calculate a shape derivative of the energy functional: a direct chain rule approach for material derivative, an indirect approach via local derivative, and an averaged adjoint method which due to linearity simplifies to the standard adjoint method. We present the shape derivative both in boundary and distributed (volume) representation.

In Section 2.3 the second order shape derivative is derived by two different techniques already mentioned for the first order shape derivative. It seems that an averaged adjoint method is well suited to calculate distributional form of the second order shape derivative and in this case with non-linear averaged adjoint equation. The calculations although more complex are then analogously done as in the previous section.

Chapter 3: Numerical approximation

The final third chapter deals with numerical implementations of the first and the second order shape derivative.

In Section 3.1 an algorithm overview of gradient methods and a novel Newton-like method is done with focus on different possible implementations. Classical tools in shape modelling as level set function, distance function and advection equations are explained and used in numerical implementations. The most important part is description of Newton-like method for several reasons. Firstly, it is based on the distributional form of the shape derivative, meaning that an ascent vector is created on the whole domain Ω (although, its support can be properly reduced). Secondly, it is faster (it achieves convergence in less then half iterations of the gradient method).

Section 3.2 is dedicated to numerical testing and results. For gradient method we have observed stable convergence. To demonstrate that the gradient method based on shape derivative converges to the optimal solution we make an extensive test and find that discrepancy between radius of numerical and exact radii of the interface between phases is due to numerical error.

Chapter 1

Classical optimal designs for energy maximization

1.1 Existence of solutions and relaxation

1.1.1 Problem formulation

Let $\Omega \subseteq \mathbb{R}^d$ be an open and bounded set, and let a measurable function χ denote a characteristic function of the first isotropic phase, with lower conductivity α (the other one is denoted by β). We shall denote the amount (measure) of the first phase α with q_α $(0 < q_\alpha < |\Omega|)$. The conductivity of the domain Ω can be expressed as $\mathbf{A}(\chi) := \alpha\chi\,\mathbf{I}+\beta(1-\chi)\,\mathbf{I}$, with restriction

$$\int_\Omega \chi(x)\,\mathrm{d}x = q_\alpha.$$

For given right-hand sides $f_1, \dots, f_m \in \mathrm{H}^{-1}(\Omega)$, the conductivity $\mathbf{A}$ uniquely determines state functions $u_1, \dots, u_m$ as the solutions of boundary value problems

$$-\operatorname{div}(\mathbf{A}\,\nabla u_i) = f_i\,,\ u_i \in \mathrm{H}^1_0(\Omega)\,, \qquad i = 1, \dots, m\,. \tag{1.1}$$

Equation (1.1) implies the following variational formulation, or weak form for $i = 1, ..., m$:

$$\int_\Omega \mathbf{A}\,\nabla u_i \cdot \nabla\varphi\,\mathrm{d}x = \langle f, \varphi\rangle_{\mathrm{H}^{-1},\mathrm{H}^1_0}\,,\ \varphi \in \mathrm{H}^1_0(\Omega).$$

where $\langle\ ,\ \rangle_{\mathrm{H}^{-1},\mathrm{H}^1_0}$ is the duality product between $H^{-1}(\Omega)$ and $\mathrm{H}^1_0(\Omega)$. For easier notation, we shall write it as $\int_\Omega f(x)\varphi(x)\,\mathrm{d}x$ which coincides with dual product when f is more regular. Observe that the mapping $\chi \mapsto u_i(\chi)$ is nonlinear. Next, we define a functional:

$$J(\chi) := \sum_{i=1}^m \mu_i \int_\Omega f_i(x)u_i(x)\,\mathrm{d}x. \tag{1.2}$$

for some given weights $\mu_1, \dots, \mu_m > 0$. Observe that the functional is a conic sum of the energy functionals for each respective state function u_i. We seek a solution χ of the optimal design problem

$$
\text{(O)} \qquad \begin{cases} \max & \displaystyle\sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}x \\ \text{s.t.} & \chi \in \mathrm{L}^\infty(\Omega; \{0,1\}) \,, \quad \displaystyle\int_\Omega \chi \, \mathrm{d}x = q_\alpha \,, \\ & \mathsf{u} = (u_1, \dots, u_m) \text{ solves (1.1) with } \mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I} \,, \end{cases}
$$

If such characteristic function χ exists we call it the *classical solution*. Generally there are no existence results of such solutions so first we need to relax the optimal design problem (O).

1.1.2 Relaxation through homogenization theory

Let us recall a standard formulation of relaxation which can be found in [41]. Optimization problem is usually written as a minimization problem:

$$
\begin{cases} F(x) \to \min \\ \quad x \in X. \end{cases} \tag{1.3}
$$

If X is a compact topological space and F a real valued, lower semicontinuous function then one can show that (1.3) admits at least one solution. If the space X fails to be compact or F fails to be a lower semicontinuous function, a proper relaxations for problem (1.3) is introduced

$$
\begin{cases} F_R(x) \to \min \\ \quad x \in X_R. \end{cases} \tag{1.4}
$$

where X_R is a compact topological space and F_R a lower semicontinuous function with following properties:

- X is dense in X_R, $F_R\big|_X = F$,
- for any sequence $(x_n)_{n\in\mathbb{N}} \subset X$ that converges to x

$$
F_R(x) \le \liminf_n F(x_n),
$$

- for any $x \in X_R$ there exists a sequence $(x_n)_{n\in\mathbb{N}} \subset X$ that converges to x and satisfies

$$
F_R(x) = \liminf_n F(x_n).
$$

One can then show that relaxed problem (1.4) has at least one solution. Furthermore,

$$\min_{x \in X_R} F_R(x) = \inf_{x \in X} F(x),$$

meaning that any accumulation point (in X_R) of a minimizing sequence of the problem (1.3) is a solution of the problem (1.4).

Before we continue with relaxation of the problem (O) let us recall several key results of the homogenization theory. We start by defining a set of admissible conductivities

$$(1.5) \qquad \begin{cases} \mathcal{M}(\alpha, \beta; \Omega) = \{\mathbf{A} \in \mathrm{L}^\infty(\Omega; \mathrm{M}_d(\mathbb{R})) \text{ such that for any} \xi \in \mathbb{R}^d \text{ and a.e. } x \in \Omega \\ \qquad \mathbf{A}(x)\xi \cdot \xi \geq \alpha|\xi|^2, \ \mathbf{A}^{-1}(x)\xi \cdot \xi \geq \dfrac{1}{\beta}|\xi|^2 \ \} \end{cases}$$

where $\mathbf{A}^{-1}(x)$ denotes the inverse matrix of $\mathbf{A}(x)$.

Remark 1.1.1. *A coercive matrix with coercive inverse is also bounded. By introducing* $\eta = \mathbf{A}^{-1}(x)\xi$ *we obtain*

$$(1.6) \qquad \mathbf{A}(x)\eta \cdot \eta \geq \frac{1}{\beta}|\,\mathbf{A}(x)\eta|^2.$$

Applying the Cauchy-Schwarz inequality we get

$$|\,\mathbf{A}(x)\eta| \leq \beta|\eta|, \quad \forall \eta \in \mathbb{R}^d.$$

Therefore, necessary condition for $\mathbf{A}$ *to belong to* $\mathcal{M}(\alpha, \beta; \Omega)$ *is that*

$$(1.7) \qquad \alpha|\xi|^2 \leq \mathbf{A}(x)\xi \cdot \xi \leq \beta|\xi|^2, \ \forall \xi \in \mathbb{R}^d, \ \textit{a.e. } x \in \Omega.$$

In the symmetric case when $\mathbf{A}(x) = \mathbf{A}(x)^\tau$ *almost everywhere in* Ω*, conductivity* $\mathbf{A}$ *satisfies* (1.7) *if and only if* $\mathbf{A}$ *belongs to* $\mathcal{M}(\alpha, \beta; \Omega)$.

If we take conductivity matrix $\mathbf{A} \in \mathcal{M}(\alpha, \beta; \Omega)$, the solutions of boundary value problems (1.1) are well defined. By the following Proposition one can see that the set $\mathcal{M}(\alpha, \beta; \Omega)$ is compact when equipped with weak $*$ L^∞ topology.

Proposition 1.1.2. *For a bounded set* $K \subset \mathbb{R}^d$*, let* $(\mathsf{u}_n)_{n \in \mathbb{N}} \subset \mathrm{L}^\infty(\Omega; K)$ *be a sequence that converges in weak* $*$ *topology to the function* u*. Then*

$$\mathsf{u}(x) \in \overline{\mathrm{conv} K} \quad \textit{a.e. } x \in \Omega,$$

and conversely, any function u *satisfying previous property can be obtained as a weak* $*$ *limit of sequence in* $\mathrm{L}^\infty(\Omega; K)$.

Unfortunately, weak $*$ L^∞ topology is not enough for our purposes since mapping

$$\mathbf{A} \mapsto \mathsf{u} = (u_1, ..., u_m) : \mathcal{M}(\alpha, \beta; \Omega) \to \mathrm{H}^1_0(\Omega; \mathbb{R}^d)$$

fails to be continuous. Indeed, if we take a sequence $(\mathbf{A}_n)_{n\in\mathbb{N}} \in \mathcal{M}(\alpha, \beta; \Omega)$ such that $\mathbf{A}_n$ converges to $\mathbf{A}^+$ in weak $*$ topology, the corresponding solutions of (1.1) $\mathsf{u}_n = (u^n_1, ..., u^n_m)$ with conductivity $\mathbf{A}_n$ converges (up to a subsequence) weakly in $\mathrm{H}^1_0(\Omega)$ to some $\mathsf{u}_0 = (u^0_1, ..., u^0_m)$ which in general may fail to be the solution to the (1.1) with conductivity $\mathbf{A}^+$. For that reason notion of H-convergence is introduced.

Definition 1.1.3. *We say that the sequence $\mathbf{A}_n \in \mathcal{M}(\alpha, \beta; \Omega)$ H-converges to the $\mathbf{A}^* \in \mathcal{M}(\alpha, \beta; \Omega)$ if for any $f \in \mathrm{H}^{-1}(\Omega)$ the solution $u_n \in \mathrm{H}^1_0(\Omega)$ of*

$$-\operatorname{div}(\mathbf{A}_n \nabla u_n) = f \ \textit{in } \Omega,$$

satisfies

$$\begin{cases} u_n \rightharpoonup u_0 \ \textit{weakly in } \mathrm{H}^1_0(\Omega) \\ \mathbf{A}_n \nabla u_n \rightharpoonup \mathbf{A}^* \nabla u_0 \ \textit{weakly in } \mathrm{L}^2(\Omega; \mathbb{R}^d) \end{cases}$$

Since $\mathbf{A}_n \nabla u_n \rightharpoonup \mathbf{A}^* \nabla u_0$ and $-\operatorname{div}(\mathbf{A}_n \nabla u_n) = f$ we conclude that $u_0 \in \mathrm{H}^1_0(\Omega)$ is a unique solution of the

$$-\operatorname{div}(\mathbf{A}^* \nabla u_0) = f \text{ in } \Omega.$$

The above definition makes sense because of the following sequential compactness theorem:

Theorem 1.1.4. *For any sequence $\mathbf{A}_n \in \mathcal{M}(\alpha, \beta; \Omega)$ there exists a subsequence, still denoted by $\mathbf{A}_n$ and $\mathbf{A}^* \in \mathcal{M}(\alpha, \beta; \Omega)$ such that $\mathbf{A}_n$ H-converge to $\mathbf{A}^*$.*

A useful result is that the topology induced by the H-convergence is metrizable. Following Proposition can be found in [5]:

Proposition 1.1.5. *Let $(f_n)_{n\in\mathbb{N}}$ be a dense countable family in $\mathrm{H}^{-1}(\Omega)$. Let $\mathbf{A}$ and $\mathbf{B}$ be two matrices in $\mathcal{M}(\alpha, \beta; \Omega)$. Define u_n and v_n the respective unique solutions in $\mathrm{H}^1_0(\Omega)$ of*

$$-\operatorname{div}(\mathbf{A} \nabla u_n) = f_n \ \textit{in } \Omega$$

and

$$-\operatorname{div}(\mathbf{B} \nabla v_n) = f_n \ \textit{in } \Omega.$$

We define a distance function in $\mathcal{M}(\alpha, \beta; \Omega)$ by

$$d(\mathbf{A}, \mathbf{B}) = \sum_{n=1}^{+\infty} 2^{-n} \frac{\|u_n - v_n\|_{\mathrm{L}^2(\Omega)} + \|\mathbf{A} \nabla u_n - \mathbf{B} \nabla v_n\|_{\mathrm{H}^{-1}(\Omega)^d}}{\|f_n\|_{\mathrm{H}^{-1}(\Omega)}}.$$

Then, $\mathcal{M}(\alpha, \beta; \Omega)$ is a metric space with this distance d, and the H-convergence is equivalent to the sequential convergence with respect to d.

The map defined by (1.1):

$$\mathbf{A} \mapsto \mathsf{u} = (u_1, ..., u_m) : \mathcal{M}(\alpha, \beta; \Omega) \to \mathrm{H}_0^1(\Omega; \mathbb{R}^d)$$

is continuous with respect to H-topology on $\mathcal{M}(\alpha, \beta; \Omega)$ and weak topology on $\mathrm{H}_0^1(\Omega; \mathbb{R}^d)$. By Proposition 1.1.5 it is enough to check the sequential continuity. Let us take a sequence $(\mathbf{A}_n)_{n\in\mathbb{N}} \subset \mathcal{M}(\alpha, \beta; \Omega)$ that H-converges to $\mathbf{A}^*$. Definition 1.1.3 then implies that a sequence u_n converges weakly in $\mathrm{H}_0^1(\Omega; \mathbb{R}^d)$ to u_0 which is a solution of (1.1) with conductivity $\mathbf{A}^*$.

The next fundamental step is to characterize the H-closure (closure with respect to H-topology) of some given set. Particularly, we are interested in characterization of H-closure of the set of conductivities of the form

$$\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$$

Proposition 1.1.6. *Assume that $\mathbf{A}_n = \chi_n\alpha\mathbf{I} + (1-\chi_n)\beta\mathbf{I} \xrightarrow{H} \mathbf{A}^*$ and that $\chi_n \overset{*\mathrm{L}^\infty}{\rightharpoonup} \vartheta$ where $\vartheta(x)$ denotes the local volume fraction at the point x. Then*

$$\mathbf{A}^*(x) \in \mathcal{K}(\vartheta(x)), \quad a.e.\ x \in \Omega$$

where for $\theta \in [0,1]$, the set $\mathcal{K}(\theta)$ is defined in the following way. A symmetric matrix belongs to $\mathcal{K}(\theta)$ if and only if its eigenvalues $(\lambda_1, ..., \lambda_d)$ satisfy

$$\begin{cases} \lambda_-(\theta) \le \lambda_i \le \lambda_+(\theta),\ i = 1, 2, ..., d, \\ \displaystyle\sum_{i=1}^d \frac{1}{\lambda_i - \alpha} \le \frac{1}{\lambda_-(\theta) - \alpha} + \frac{d-1}{\lambda_+(\theta) - \alpha}, \\ \displaystyle\sum_{i=1}^d \frac{1}{\beta - \lambda_i} \le \frac{1}{\beta - \lambda_-(\theta)} + \frac{d-1}{\beta - \lambda_+(\theta)}, \end{cases} \tag{1.8}$$

where $\lambda_-(\theta) = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta}\right)^{-1}$ and $\lambda_+(\theta) = \theta\alpha + (1-\theta)\beta$.

Conversely, if a measurable function $\mathbf{A}^*$ satisfies $\mathbf{A}^*(x) \in \mathcal{K}(\vartheta(x))$, a.e. $x \in \Omega$ for a function $\vartheta \in \mathrm{L}^\infty(\Omega; [0,1])$, there exists a sequence of characteristic functions $(\chi_n)_{n\in\mathbb{N}} \subset \mathrm{L}^\infty(\Omega; \{0,1\})$ such that $\chi_n \overset{*\mathrm{L}^\infty}{\rightharpoonup} \vartheta$ and $\mathbf{A}_n = \chi_n\alpha\mathbf{I} + (1-\chi_n)\beta\mathbf{I} \xrightarrow{H} \mathbf{A}^*$

Now we introduced everything to write a proper relaxation of the problem (O). Instead of $\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$ we are using $\vartheta \in \mathrm{L}^\infty(\Omega; [0,1])$ equipped with weak $*$ L^∞ topology. Proposition 1.1.2 states that $\mathrm{L}^\infty(\Omega; \{0,1\})$ is dense inside $\mathrm{L}^\infty(\Omega; [0,1])$. For given $\vartheta \in \mathrm{L}^\infty(\Omega; [0,1])$ by Proposition 1.1.6 conductivity is determined by a set of effec-

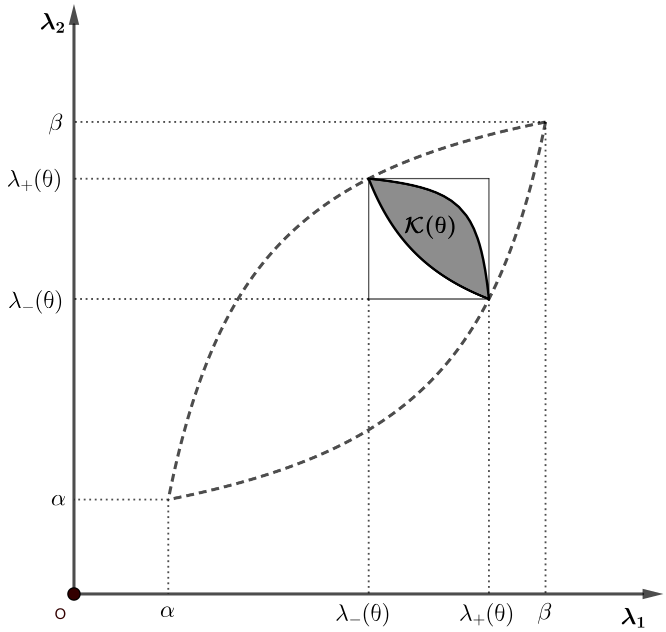


Figure 1.1: The set of effective conductivities $\mathcal{K}(\theta)$ in 2D

tive conductivities, so we can introduce a set of generalized designs:

$$\mathcal{A} = \left\{ (\vartheta, \mathbf{A}) \in \mathrm{L}^\infty(\Omega; [0,1] \times \mathrm{Sym}_d(\mathbb{R})) : \int_\Omega \vartheta \, dx = q_\alpha, \ \mathbf{A}(x) \in \mathcal{K}(\vartheta(x)), \ \text{a.e. } x \right\}.$$

Observe that $\mathrm{L}^\infty(\Omega; [0,1])$ is a weak $*\,\mathrm{L}^\infty$ compact and convex set. By Proposition 1.1.6 we can also conclude that $\mathcal{A}$ is compact in a product of weak $*$ L^∞ topology and H-topology. We shall also use natural extension of the functional J:

$$J_A(\vartheta, \mathbf{A}) = \sum_{i=1}^m \mu_i \int_\Omega f_i u_i \, \mathrm{d}x \tag{1.9}$$

where $\mathsf{u} = (u_1, ..., u_m)$ satisfies (1.1) with conductivity $\mathbf{A}$. Observe that the functional J_A can be understood as an extension of energy functional (1.2) since for any $\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$

$$J_A(\chi, \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I}) = J(\chi).$$

The relaxed problem then reads

$$\text{(A)} \qquad \left\{ \begin{array}{ll} \max & J_A(\vartheta, \mathbf{A}) = \displaystyle\sum_{i=1}^m \mu_i \int_\Omega f_i u_i \, \mathrm{d}x \\ \text{s.t.} & (\vartheta, \mathbf{A}) \in \mathcal{A}, \ \ \mathsf{u} = (u_1, \ldots, u_m) \text{ solves (1.1) with } \mathbf{A}. \end{array} \right.$$

Furthermore, one can check that the functional J_A is continuous on a set of relaxed designs $\mathcal{A}$ in a product of weak $*$ L^∞ topology and H-topology. Therefore, there exists at least one solution of the problem (A). One can also show that $\mathcal{K}(\vartheta)$ is convex for a fixed ϑ (see Figure 1.1) but this is not the case for the set of relaxed designs $\mathcal{A}$ as we can see in the following example.

Example 1.1.7. *Assume that $\Omega_0 \subset\subset \Omega$ is an open set chosen such that*

$$\mathrm{vol}(\Omega_0) < \min\{q_\alpha, \mathrm{vol}(\Omega) - q_\alpha\}.$$

Then one can easily construct two pairs $(\vartheta_1, \mathbf{A}_1), (\vartheta_2, \mathbf{A}_2) \in \mathcal{A}$ such that for any $x \in \Omega_0$ $\vartheta_1(x) = 1$ and $\vartheta_2(x) = 0$. From definition of the set $\mathcal{K}(\vartheta)$ one can conclude that for a.e. $x \in \Omega_0$ we have $\mathbf{A}_1(x) = \alpha\mathbf{I}$ and $\mathbf{A}_2(x) = \beta\mathbf{I}$. From this we can see that the pair $(\vartheta, \mathbf{A}) = (\frac{1}{2}(\vartheta_1 + \vartheta_2), \frac{1}{2}(\mathbf{A}_1 + \mathbf{A}_2))$ satisfies condition $\int_\Omega \vartheta \,\mathrm{d}x = q_\alpha$. On the other side one can show that the matrix $\mathbf{A} = \frac{1}{2}(\mathbf{A}_1 + \mathbf{A}_2)$ does not satisfy

$$\mathbf{A}(x) \in \mathcal{K}(\vartheta(x)) \text{ a.e. } x \in \Omega.$$

Indeed, since $\alpha < \beta$ the following holds

$$2d > \frac{\alpha}{\beta} + 1 + 2(d-1).$$

Multiplying by $\frac{1}{\beta - \alpha}$ we obtain

$$\frac{2d}{\beta - \alpha} > \frac{\alpha + \beta}{\beta(\beta - \alpha)} + \frac{2(d-1)}{\beta - \alpha}$$

which is equivalent to

$$\frac{d}{\beta - \frac{\alpha+\beta}{2}} > \frac{1}{\beta - \lambda_-(0.5)} + \frac{d-1}{\beta - \lambda_+(0.5)}.$$

This implies that $\frac{\alpha+\beta}{2}\mathbf{I} \notin \mathcal{K}(0.5)$ due to the last inequality in (1.8). Since for a.e. $x \in \Omega_0$ $\mathbf{A}(x) = \frac{1}{2}(\alpha\mathbf{I} + \beta\mathbf{I}) = \frac{\alpha+\beta}{2}\mathbf{I}$, we obtain the claim.

Remark 1.1.8. *As it was done in [55] one can easily characterize isotropic mixtures in the set $\mathcal{K}(\theta)$. For given $\theta \in [0,1]$, matrix $\gamma\mathbf{I}$ belongs to $\mathcal{K}(\theta)$ if and only if*

$$\alpha + \frac{d\alpha(\beta - \alpha)(1 - \theta)}{d\alpha + \theta(\beta - \alpha)} \leq \gamma \leq \beta - \frac{d\beta(\beta - \alpha)\theta}{(d-1)\beta + \alpha + \theta(\beta - \alpha)}.$$

The upper and lower bounds are strictly convex functions with respect to θ on $[0,1]$, in any dimension d. Therefore, a set

$$\{(\theta, \gamma) \in [0,1] \times [\alpha, \beta] : \gamma\mathbf{I} \in \mathcal{K}(\theta)\}$$

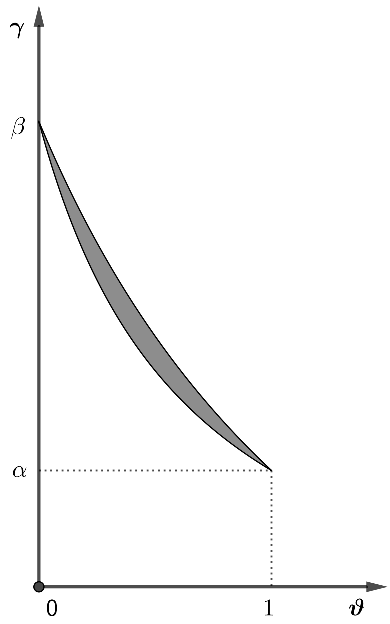


Figure 1.2: The set of all possible conductivities γ of isotropic mixtures in $\mathcal{K}(\theta)$

is not convex (see a Figure 1.2), which is explicitly proved in Example 1.1.7.

In order to amend this lack of convexity, we introduce a larger artificial design set

$$\begin{aligned}\mathcal{B} =&\{(\vartheta, \mathbf{A}) \in \mathrm{L}^\infty(\Omega; [0,1] \times \mathrm{Sym}_d(\mathbb{R}))\ :\ \textstyle\int_\Omega \vartheta \,\mathrm{d}x = q_\alpha, \\ &\lambda_-(\vartheta(x))|\xi|^2 \le \langle \mathbf{A}(x)\xi, \xi\rangle \le \lambda_+(\vartheta(x)|\xi|^2\ \ \forall \xi \in \mathbb{R}^d \text{ a.e. } x \in \Omega\}.\end{aligned}$$

Lemma 1.1.9. *The set $\mathcal{B}$ is convex and closed when equipped with a product of weak $*$ L^∞ topology and H-topology.*

Proof. One can show that the set $\mathcal{B}$ is closed using Proposition 1.1.2 and ordering property which holds for H-topology:

Lemma 1.1.10. *Let $(\mathbf{A}_n)_{n\in\mathbb{N}}$ and $(\mathbf{B}_n)_{n\in\mathbb{N}}$ be two sequences of symmetric matrices in $\mathcal{M}(\alpha, \beta; \Omega)$ that H-converge to the $\mathbf{A}^*$ and $\mathbf{B}^*$. If for all n*

$$\forall \xi \in \mathbb{R}^d \quad \langle \mathbf{A}_n\, \xi, \xi\rangle \le \langle \mathbf{B}_n\, \xi, \xi\rangle$$

then

$$\forall \xi \in \mathbb{R}^d \quad \langle \mathbf{A}^*\, \xi, \xi\rangle \le \langle \mathbf{B}^*\, \xi, \xi\rangle\,.$$

Proof. See Proposition 14 in [51] or Lemma 1.3.13 in [5]. □

To finish the proof of Lemma 1.1.9, convexity of the set $\mathcal{B}$ can be directly checked. Let $k \in [0,1]$, $(\vartheta_1, \mathbf{A}_1), (\vartheta_2, \mathbf{A}_2) \in \mathcal{B}$. Define a pair $(\vartheta, \mathbf{A}) = (k\nu_1 + (1-k)\vartheta_2, k\,\mathbf{A}_1 + (1-k)\,\mathbf{A}_2)$.

It is easy to check that it belongs to $\mathrm{L}^\infty(\Omega;[0,1]\times \mathrm{Sym}_d(\mathbb{R}))$. Furthermore, due to the linearity of the constraint

$$\int_\Omega \vartheta \,\mathrm{d}x = k\int_\Omega \vartheta_1 \,\mathrm{d}x + (1-k)\int_\Omega \vartheta \,\mathrm{d}x = q_\alpha.$$

For a.e. $x\in\Omega$ and $\xi\in\mathbb{R}^d$ we have:

$$k\lambda_-(\vartheta_1(x))|\xi|^2 \le \langle k\,\mathbf{A}_1(x)\xi,\xi\rangle \le k\lambda_+(\vartheta_1(x))|\xi|^2$$

$$(1-k)\lambda_-(\vartheta_2(x))|\xi|^2 \le \langle (1-k)\,\mathbf{A}_2(x)\xi,\xi\rangle \le (1-k)\lambda_+(\vartheta_2(x))|\xi|^2$$

By adding previous inequalities we get

$$\begin{aligned}(k\lambda_-(\vartheta_1(x)) + (1-k)\lambda_-(\vartheta_2(x)))|\xi|^2 &\le \langle (k\,\mathbf{A}_1(x) + (1-k)\,\mathbf{A}_2(x))\xi,\xi\rangle \\ &\le (k\lambda_+(\vartheta_1(x) + (1-k)\lambda_+(\vartheta_2(x))|\xi|^2\end{aligned} \tag{1.10}$$

Since $x\mapsto \frac{1}{x}$ is a convex function on $\langle 0,\infty\rangle$ we can conclude for the left inequality

$$\begin{aligned}k\left(\frac{\vartheta_1(x)}{\alpha}+\frac{1-\vartheta_1(x)}{\beta}\right)^{-1} + (1-k)\left(\frac{\vartheta_2(x)}{\alpha}+\frac{1-\vartheta_2(x)}{\beta}\right)^{-1} \ge \\ \left(\frac{k\nu_1(x)+(1-k)\vartheta_2(x)}{\alpha}+\frac{1-k\nu_1(x)-(1-k)\vartheta_2(x)}{\beta}\right)^{-1}\end{aligned}$$

thus $(k\lambda_-(\vartheta_1(x)) + (1-k)\lambda_-(\vartheta_2(x))) \ge \lambda_-(\vartheta(x))$. For the right inequality in (1.10) we can check that

$$k\lambda_+(\vartheta_1(x)) + (1-k)\lambda_+(\vartheta_2(x)) = \lambda_+(\vartheta(x)),$$

so we have obtained

$$\lambda_-(\vartheta(x))|\xi|^2 \le \langle \mathbf{A}(x)\xi,\xi\rangle \le \lambda_+(\vartheta(x))|\xi|^2$$

thus showing that $(\vartheta,\mathbf{A})\in\mathcal{B}$. □

One can also show in a similar manner that the set

$$\mathcal{C} = \{(\vartheta,\mathbf{B})\in \mathrm{L}^\infty(\Omega;[0,1]\times\mathrm{Sym}_d(\mathbb{R})) \;:\; (\vartheta,\mathbf{B}^{-1})\in\mathcal{B}\}$$

is convex. From Lemma 1.1.9 $\mathcal{B}$ is a compact set with respect to the introduced product topology, so the functional $J_B(\vartheta,\mathbf{B}) = \sum_{i=1}^m \mu_i \int_\Omega f_i u_i \,\mathrm{d}x$ where $(u_1,\dots,u_m)$ is the solution of (1.1) has a maximum point on $\mathcal{B}$, i.e. the optimal design problem

$$
\text{(B)} \qquad \begin{cases} \max & J_B(\vartheta, \mathbf{A}) = \displaystyle\sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \,\mathrm{d}x \\ \text{s.t.} & (\vartheta, \mathbf{A}) \in \mathcal{B}, \ \ \mathsf{u} = (u_1, \ldots, u_m) \text{ solves } (1.1) \text{ with } \mathbf{A}. \end{cases}
$$

admits at least one solution. Furthermore, $J_{B|\mathcal{A}} = J_A$ and since $\mathcal{A} \subset \mathcal{B}$ we can conclude

$$
\max_{(\vartheta,\mathbf{A})\in\mathcal{A}} J_A(\vartheta, \mathbf{A}) \leq \max_{(\vartheta,\mathbf{B})\in\mathcal{B}} J_B(\vartheta, \mathbf{B}).
$$

1.2 Interpretation as a Convex Optimization Problem

1.2.1 Theory of saddle points and minimax theory

We start this section with a short overview of classical results on saddle point theory. For details and proofs of some results see Chapter 6 in [25]. Let X, Y be Hausdorff topological vector spaces. We take a real valued function L defined on a set $A \times B \subset X \times Y$. Let us start with a definition of a saddle point:

Definition 1.2.1. *We say that a pair $(\tilde{u}, \tilde{p}) \in A \times B$ is a saddle point of L on $A \times B$ if*

$$
L(\tilde{u}, p) \leq L(\tilde{u}, \tilde{p}) \leq L(u, \tilde{p}), \quad u \in A, p \in B.
$$

Some important properties of a saddle point:

Proposition 1.2.2. *Let L be a real valued function defined on $A \times B$.*

1. *L has a saddle point if and only if*

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

   and this number is then equal to $L(\tilde{u}, \tilde{p})$, for any saddle point $(\tilde{u}, \tilde{p})$.

2. *The set of all saddle points of L is of the form $A_0 \times B_0$ where $A_0 \subset A$ and $B_0 \subset B$.*

We assume henceforth that

$$
A \subset X \text{ is convex, closed and non-empty,} \tag{1.11}
$$

$$
B \subset Y \text{ is convex, closed and non-empty,} \tag{1.12}
$$

and the function $L : A \times B \to \mathbb{R}$ satisfies

$$
\text{for any } u \in A,\ p \mapsto L(u, p) \text{ is concave and upper semicontinuous,} \tag{1.13}
$$

$$
\text{for any } p \in B,\ u \mapsto L(u, p) \text{ is convex and lower semicontinuous.} \tag{1.14}
$$

Proposition 1.2.3. *Under hypotheses* (1.11)-(1.14) *the set* $A_0 \times B_0$ *of the saddle points is convex.*

- *If* $p \mapsto L(u,p)$ *is strictly concave for all* $u \in A$ *then* B_0 *contains at most one point.*
- *If* $u \mapsto L(u,p)$ *is strictly convex for all* $p \in B$ *then* A_0 *contains at most one point.*

Proof of the following theorem is from [25].

Theorem 1.2.4. *Let* X, Y *be Hausdorff topological vector spaces such that one of them is also a reflexive Banach space. We assume that the conditions* (1.11)-(1.14) *are satisfied and additionally that* A *and* B *are compact sets. Then the function* L *possesses at least one saddle point* $(\tilde{u}, \tilde{p})$ *on* $A \times B$ *and*

$$L(\tilde{u}, \tilde{p}) = \min_{u \in A} \max_{p \in B} L(u,p) = \max_{p \in B} \min_{u \in A} L(u,p).$$

Proof. We consider the case where X is reflexive Banach space and for every $p \in B$ the map $u \mapsto L(u,p)$ is strictly convex. Then by the virtue of Proposition 1.2.3 the minimum of the function $u \mapsto L(u,p)$ is achieved for any $p \in B$ and is unique. We denote by $f(p)$ this minimum and the minimizer by $e(p) \in A$:

$$f(p) = \min_{u \in A} L(u,p) = L(e(p), p).$$

The function $p \mapsto f(p)$ is concave and upper semicontinuous as an infimum of such functions. It is therefore bounded above and attains its upper bound at a point $\tilde{p}$:

$$f(\tilde{p}) = \max_{p \in B} f(p) = \max_{p \in B} \min_{u \in A} L(u,p)$$

and

$$f(\tilde{p}) \le L(u, \tilde{p}), \quad u \in A.$$

Since for any $u \in A$ the map $p \mapsto L(u,p)$ is concave we have for any $u \in A$, $p \in B$ and $\lambda \in \langle 0, 1 \rangle$

$$L(u, (1-\lambda)\tilde{p} + \lambda p) \ge (1-\lambda) L(u, \tilde{p}) + \lambda L(u,p).$$

In particular, by taking $u = e_\lambda = e((1-\lambda)\tilde{p} + \lambda p)$, we obtain that

$$\begin{aligned} f(\tilde{p}) &\ge f((1-\lambda)\tilde{p} + \lambda p)) = L(e_\lambda, (1-\lambda)\tilde{p} + \lambda p) \\ &\ge (1-\lambda) L(e_\lambda, \tilde{p}) + \lambda L(e_\lambda, p) \\ &\ge (1-\lambda) f(\tilde{p}) + \lambda L(e_\lambda, p), \end{aligned}$$

meaning that

$$f(\tilde{p}) \geq L(e_\lambda, p). \tag{1.15}$$

Due to A being a compact set, for a sequence (λ_n) such that $\lambda_n \to 0$ there exists a subsequence, again denoted by (λ_n) such that e_{λ_n} converges to some limit $\tilde{u}$. One can see that the following inequality holds:

$$(1-\lambda_n)L(e_{\lambda_n}, \tilde{p}) + \lambda_n L(e_{\lambda_n}, p) \leq L(e_{\lambda_n}, (1-\lambda_n)\tilde{p} + \lambda_n p) \leq L(u, (1-\lambda_n)\tilde{p} + \lambda_n p),$$

for any $u \in A$ and therefore

$$\liminf_n \left[(1-\lambda_n)L(e_{\lambda_n}, \tilde{p}) + \lambda_n L(e_{\lambda_n}, p)\right] \leq \limsup_n L(u, (1-\lambda_n)\tilde{p} + \lambda_n p).$$

Since $L(e_{\lambda_n}, p) \geq f(p)$, we see that $\liminf_n \lambda_n L(e_\lambda, p) = 0 \cdot L(\tilde{u}, p) = 0$ due to L being lower semicontinuous in u and we can conclude

$$L(\tilde{u}, \tilde{p}) \leq \liminf_n L(e_{\lambda_n}, \tilde{p}) \leq \liminf_n (1-\lambda_n)L(e_{\lambda_n}, \tilde{p}) \leq \limsup_n L(u, (1-\lambda_n)\tilde{p} + \lambda p)$$

showing that for any $u \in A$ we have $L(\tilde{u}, \tilde{p}) \leq L(u, \tilde{p})$, which implies $e(\tilde{p}) = \tilde{u}$. We can now pass to the limit in (1.15) obtaining

$$f(\tilde{p}) \geq \liminf_n L(e_{\lambda_n}, p) \geq L(\tilde{u}, p), \quad \forall p \in B.$$

We have shown that for any $u \in A$ and $p \in B$:

$$L(\tilde{u}, p) \leq L(\tilde{u}, \tilde{p}) \leq L(u, \tilde{p}). \tag{1.16}$$

If the map $u \mapsto L(u, p)$ is not strictly convex, we introduce perturbed Lagrangians L_ε:

$$L_\varepsilon(u, p) = L(u, p) + \varepsilon \|u\|_X$$

for the norm $\|\cdot\|_X$ which is strictly convex. See Remark 1.2.5 for detail about the existence of such norm for a reflexive Banach space. Indeed, for L_ε we obtain the existence of a saddle point $(\tilde{u}_\varepsilon, \tilde{p}_\varepsilon) \in A \times B$ such that for any $u \in A$, $p \in B$:

$$L(\tilde{u}_\varepsilon, p) + \varepsilon \|\tilde{u}_\varepsilon\| \leq L(\tilde{u}_\varepsilon, \tilde{p}_\varepsilon) + \varepsilon \|\tilde{u}_\varepsilon\|_X \leq L(u, \tilde{p}_\varepsilon) + \varepsilon \|u\|_X.$$

Due to compactness of A and B, one can find a sequence ε_n converging to zero such that $\tilde{u}_{\varepsilon_n} \to \tilde{u}$ and $\tilde{p}_{\varepsilon_n} \to \tilde{p}$. By passing to a limit and using (1.13), (1.14) we can see that $(\tilde{u}, \tilde{p})$ satisfies (1.16), therefore is a saddle point for L. If X is not a reflexive Banach space, just change L with $-L$. □

Remark 1.2.5. *We say that a normed space is uniformly convex if given* $\varepsilon > 0$ *there exists* $\delta(\varepsilon) > 0$ *such that*

$$\frac{\|x+y\|}{2} \leq 1 - \delta(\varepsilon) \text{ whenever } \|x-y\| \geq \varepsilon, \text{ and } \|x\| = \|y\| = 1.$$

It is locally uniformly convex if given $\varepsilon > 0$ *and an element* x *such that* $\|x\| = 1$*, there exists* $\delta(\varepsilon, x) > 0$ *such that*

$$\frac{\|x+y\|}{2} \leq 1 - \delta(\varepsilon, x) \text{ whenever } \|x-y\| \geq \varepsilon, \text{ and } \|y\| = 1.$$

A normed linear space is strictly convex if $\|x+y\| = \|x\| + \|y\|$ *implies* $x = ty$, $t > 0$*, whenever* $x \neq 0$ *and* $y \neq 0$.

It is clear from the definitions that uniform convexity implies local uniform convexity, and local uniform convexity implies strict convexity. It is well known that every uniformly convex Banach space is reflexive, e.g. see Theorem 1.21 in [2]. The converse is not true, meaning there exist reflexive Banach spaces which are not uniformly convex. On the other hand every reflexive Banach space admits an equivalent locally uniform convex norm. For details and the proof see [53]. Therefore, every reflexive Banach space has equivalent strictly convex norm.

Remark 1.2.6. *The compactness of* A *and/or* B *in Theorem 1.2.4 can be replaced by coercivity of the function if the underlying space is also a reflexive Banach space:*

$$\begin{cases} \exists p_0 \in B \text{ such that} \\ \lim\limits_{u \in A\colon \|u\|_X \to \infty} L(u, p_0) = +\infty \end{cases} \tag{1.17}$$

and/or

$$\begin{cases} \exists u_0 \in A \text{ such that} \\ \lim\limits_{p \in B\colon \|p\|_Y \to \infty} L(u_0, p) = -\infty. \end{cases} \tag{1.18}$$

1.2.2 Necessary and Sufficient Conditions of Optimality

Denote with

$$\mathcal{S} = \{\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, ..., \boldsymbol{\sigma}_m) \in \mathrm{L}^2(\Omega; \mathbb{R}^d)^m \ : \ -\operatorname{div}(\boldsymbol{\sigma}_i) = f_i,\ i = 1, 2, ..., m\}.$$

Lemma 1.2.7. *Let* $\mathbf{A} \in \mathcal{M}(\alpha, \beta; \Omega)$ *and* $\mathsf{v} = (v_1, ..., v_m) \in \mathrm{H}_0^1(\Omega)^m$*. Then*

1. *The minimization problem*

$$\min_{\mathsf{v}\in \mathrm{H}_0^1(\Omega)^m} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}\,\nabla v_i\cdot\nabla v_i - 2 f_i v_i \,\mathrm{d}x \tag{1.19}$$

   admits a unique solution $\mathsf{v}^* \in \mathrm{H}_0^1(\Omega)^m$ *with minimum* $l_{\min}$*.*

2. *The maximization problem*

$$\max_{\boldsymbol{\sigma}\in\mathcal{S}} -\sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_i \,\mathrm{d}x \tag{1.20}$$

   dual to the (1.19) *admits a unique solution* $\boldsymbol{\sigma}^*$ *with maximum* $l_{\max}$*.*

3. *Values* $l_{\min}$ *and* $l_{\max}$ *are equal and optimal solutions* v^* *and* $\boldsymbol{\sigma}^*$ *satisfy:*

$$\mathbf{A}\,\nabla v_i^* = \boldsymbol{\sigma}_i^*, \quad i = 1, ..., m. \tag{1.21}$$

Proof. Let $\boldsymbol{\sigma}\in\mathcal{S}$ and $\mathsf{v}\in \mathrm{H}_0^1(\Omega)^m$. Then

$$\int_\Omega \boldsymbol{\sigma}_i\cdot\nabla\varphi\,\mathrm{d}x = \int_\Omega f_i\varphi\,\mathrm{d}x, \quad \varphi\in \mathrm{H}_0^1(\Omega). \tag{1.22}$$

One can easily check that the following inequalities hold almost everywhere in Ω:

$$(\nabla v_i - \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i)\cdot(\mathbf{A}\,\nabla v_i - \boldsymbol{\sigma}_i) \geq \frac{1}{\beta}|\,\mathbf{A}\,\nabla v_i - \boldsymbol{\sigma}_i|^2 \geq 0.$$

where the first inequality comes from (1.6) by replacing η with $\nabla v_i - \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i$. Integrating over Ω and dividing by β we obtain the inequality:

$$\int_\Omega \mathbf{A}\,\nabla v_i\cdot\nabla v_i - 2\boldsymbol{\sigma}_i\cdot\nabla v_i + \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_i\,\mathrm{d}x \geq 0$$

By (1.22) we conclude that for any $\mathsf{v}\in \mathrm{H}_0^1(\Omega)$ and $\boldsymbol{\sigma}\in\mathcal{S}$ the following inequality holds

$$\sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}\,\nabla v_i\cdot\nabla v_i - 2 f_i v_i\,\mathrm{d}x \geq -\sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_i\,\mathrm{d}x,$$

with equality if and only if $\mathbf{A}\,\nabla v_i = \boldsymbol{\sigma}_i$ for $i = 1, ..., m$ almost everywhere on Ω. Therefore we can conclude

$$\max_{\boldsymbol{\sigma}\in\mathcal{S}}\Big(-\sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_i\,\mathrm{d}x\Big) = \min_{\mathsf{v}\in \mathrm{H}_0^1(\Omega)^m} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}\,\nabla v_i\cdot\nabla v_i - 2 f_i v_i\,\mathrm{d}x. \tag{1.23}$$

since both problems (1.19) and (1.20) admit unique solutions with optimal values satisfying

$$-\sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{A}^{-1} \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^* \, \mathrm{d}x = \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{A} \nabla v_i^* \cdot \nabla v_i^* - 2 f_i v_i^* \, \mathrm{d}x.$$

As before, the last equality holds if and only if $\mathbf{A} \nabla v_i^* = \boldsymbol{\sigma}_i^*$ for $i = 1, ..., m$. □

Next theorem offers additional informations regarding optimal design problem (B). The first step will be to rewrite problem (B) as max-min problem and from there we will show that it is equivalent to a simpler problem which takes into account only the weak $*$ closure of the original set of characteristics functions $\mathrm{L}^\infty(\Omega; \{0,1\})$ denoted with

$$\mathcal{T} = \left\{ \vartheta \in \mathrm{L}^\infty(\Omega; [0,1]) \; : \; \int_\Omega \vartheta \, \mathrm{d}x = q_\alpha \right\}.$$

Theorem 1.2.8. *Let $(\vartheta^*, \mathbf{A}^*)$ be an optimal design for the problem (B) and u^* the corresponding state function. Then ϑ^* solves a simpler optimal design problem*

$$\text{(I)} \qquad \begin{cases} \max & J_I(\vartheta) = \displaystyle\sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}x \\ \text{s.t.} & \vartheta \in \mathcal{T}, \; \mathsf{u} = (u_1, \ldots, u_m) \textit{ solves} \\ & -\operatorname{div}(\lambda_-(\vartheta) \nabla u_i) = f_i, \; u_i \in \mathrm{H}_0^1(\Omega), \; i = 1, ..., m. \end{cases}$$

while $\mathbf{A}^*$ satisfies

$$\mathbf{A}^* \nabla u_i^* = \lambda_-(\vartheta^*) \nabla u_i^* = \boldsymbol{\sigma}_i^*, \; i = 1, ..., m, \tag{1.24}$$

where $\boldsymbol{\sigma}^* = (\boldsymbol{\sigma}_1, ..., \boldsymbol{\sigma}_m) \in \mathrm{L}^2(\Omega; \mathbb{R}^d)^m$ is uniquely determined. Consequently, the corresponding state function u^* is the same for both maximization problems.

Conversely, if $\tilde{\vartheta}$ is a solution of the optimal design problem (I), and $\tilde{\mathsf{u}}$ is the corresponding state function, then for any $\tilde{\mathbf{A}}$ such that $(\tilde{\vartheta}, \tilde{\mathbf{A}}) \in \mathcal{B}$ and

$$\tilde{\mathbf{A}} \nabla \tilde{u}_i = \lambda_-(\tilde{\vartheta}) \nabla \tilde{u}_i, \; i = 1, ..., m$$

almost everywhere on Ω, the pair $(\tilde{\vartheta}, \tilde{\mathbf{A}})$ is an optimal design for the problem (B).

Proof. Proof consists of several parts:

1. *Rewriting (B) as max-min problem.*
   Let $(\vartheta, \mathbf{A}) \in \mathcal{B}$ and u be a corresponding state function defined by (1.1). We

reformulate functional J_B in the following manner:

$$
\begin{aligned}
J_B(\vartheta, \mathbf{A}) &= \sum_{i=1}^m \mu_i \int_\Omega f_i u_i \,\mathrm{d}x \\
&= -\left(-\sum_{i=1}^m \mu_i \int_\Omega f_i u_i \,\mathrm{d}x \right) \\
&= -\left(\sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}\,\nabla u_i \cdot \nabla u_i - 2 f_i u_i \,\mathrm{d}x \right) \\
&= -\min_{\mathsf{v}\in \mathrm{H}_0^1(\Omega)^m} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}\,\nabla v_i \cdot \nabla v_i - 2 f_i v_i \,\mathrm{d}x \qquad (1.25)
\end{aligned}
$$

We use a dual formulation for the minimization problem above and by Lemma 1.2.7 we have:

$$
J_B(\vartheta, \mathbf{A}) = \min_{\boldsymbol{\sigma}\in\mathcal{S}} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \,\mathrm{d}x, \qquad (1.26)
$$

thus showing that the optimal design problem (B) can be understood as min-max problem:

$$
\begin{aligned}
\max_{(\vartheta,\mathbf{A})\in\mathcal{B}} J_B(\vartheta, \mathbf{A}) &= \max_{(\vartheta,\mathbf{A})\in\mathcal{B}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \,\mathrm{d}x \\
&= \max_{(\vartheta,\mathbf{B})\in\mathcal{C}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} \sum_{i=1}^m \mu_i \int_\Omega \mathbf{B}\,\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \,\mathrm{d}x. \qquad (1.27)
\end{aligned}
$$

2. *Application of the max-min theory.*
   We start by denoting a Lagrange functional

$$
L : (\vartheta, \mathbf{B}, \boldsymbol{\sigma}) \mapsto \sum_{i=1}^m \mu_i \int_\Omega \mathbf{B}\,\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \,\mathrm{d}x.
$$

For any pair $(\vartheta, \mathbf{B}) \in \mathcal{C}$ the map $\boldsymbol{\sigma} \mapsto L(\vartheta, \mathbf{B}, \boldsymbol{\sigma})$ is strictly convex (quadratic) function. It is also continuous in $\mathrm{L}^2(\Omega; \mathbb{R}^d)^m$ and one can observe that for any pair $(\vartheta, \mathbf{B}) \in \mathcal{C}$ the map is also coercive, meaning that

$$
\lim_{\|\boldsymbol{\sigma}\|_{\mathrm{L}^2}\to+\infty} L(\vartheta, \mathbf{B}, \boldsymbol{\sigma}) = +\infty.
$$

Observe that $\mathcal{S}$ is closed, convex, non-empty set.

For any $\boldsymbol{\sigma} \in \mathcal{S}$ map $(\vartheta, \mathbf{B}) \mapsto L(\vartheta, \mathbf{B}, \boldsymbol{\sigma})$ is linear (concave) function and continuous with respect to the weak $*$ L^∞ topology. The set $\mathcal{C}$ can be checked to be compact and convex set. By applying Theorem 1.2.4 and Remark 1.2.6 we can see that the set of saddle points is not-empty. Then by the virtue of Proposition 1.2.3 the set of all saddle points is of the form $\mathcal{C}_0 \times \mathcal{S}_0$ and due to strict convexity of $\boldsymbol{\sigma} \mapsto L(\vartheta, \mathbf{B}, \boldsymbol{\sigma})$ set $\mathcal{S}_0$ is singleton $\{\boldsymbol{\sigma}^*\}$. From the definition of the saddle point we have

$$(1.28) \qquad \begin{cases} \max_{(\vartheta,\mathbf{A})\in\mathcal{B}} J_B(\vartheta, \mathbf{A}) = \max_{(\vartheta,\mathbf{A})\in\mathcal{B}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{A}^{-1}\, \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^* \,\mathrm{d}x \\ \qquad\qquad\qquad\qquad = \max_{(\vartheta,\mathbf{B})\in\mathcal{C}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{B}\, \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^* \,\mathrm{d}x. \end{cases}$$

3. *Equivalence of problems* (B) *and* (I).

   For optimal pair $(\vartheta^*, \mathbf{A}^*) \in \mathcal{B}$, the flux $\boldsymbol{\sigma}^*$ is optimal for the minimization problem in (1.26) if and only if

$$\boldsymbol{\sigma}_i^* = \mathbf{A}^*\, \nabla u_i^*,\ i = 1, ..., m.$$

From (1.26) one can notice that if $(\vartheta^*, \mathbf{A}^*) \in \mathcal{B}$ is an optimal pair then pair $(\vartheta^*, \lambda_-(\vartheta^*)\,\mathbf{I}) \in \mathcal{B}$ is also optimal since

$$J_B(\vartheta^*, \mathbf{A}^*) \le \sum_{i=1}^{m} \mu_i \int_\Omega \frac{1}{\lambda_-(\vartheta^*)} \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^* \,\mathrm{d}x = J_B(\vartheta^*, \lambda_-(\vartheta^*)\,\mathbf{I})$$

and since $\boldsymbol{\sigma}^*$ is unique we know that

$$(1.29) \qquad \lambda_-(\vartheta^*)\nabla u_i^* = \boldsymbol{\sigma}_i^* = \mathbf{A}^*\, \nabla u_i^*,\ i = 1, ..., m.$$

For the proof of the first statement of the Theorem, let $(\vartheta^*, \mathbf{A}^*)$ be a maximizer of J_B over $\mathcal{B}$. Then $(\vartheta^*, \lambda_-(\vartheta^*)\,\mathbf{I})$ is also a maximizer. Since J_I can be understood as a restriction of the J_B to points of the form $(\vartheta^*, \lambda_-(\vartheta^*)\,\mathbf{I}) \in \mathcal{B}$ we conclude that ϑ^* is a maximizer of J_I over $\mathcal{T}$. Moreover, by (1.29) we have that u^* solves boundary value problem both in (1.1) for conductivity $\mathbf{A}^*$ and in (I).

For the proof of the converse statement, let $\tilde{\vartheta} \in \mathcal{T}$ be a maximizer of a problem (I). We can show that $(\tilde{\vartheta}, \lambda_-(\tilde{\vartheta})\,\mathbf{I}) \in \mathcal{B}$ is a maximizer of J_B over $\mathcal{B}$ and since the following holds

$$J_B(\tilde{\vartheta}, \lambda_-(\tilde{\vartheta})\,\mathbf{I}) = \sum_{i=1}^{m} \mu_i \int_\Omega \frac{1}{\lambda_-(\tilde{\vartheta})} \tilde{\boldsymbol{\sigma}}_i \cdot \tilde{\boldsymbol{\sigma}}_i \,\mathrm{d}x = \sum_{i=1}^{m} \mu_i \int_\Omega \tilde{\mathbf{A}}^{-1} \tilde{\boldsymbol{\sigma}}_i \cdot \tilde{\boldsymbol{\sigma}}_i \,\mathrm{d}x = J_B(\tilde{\vartheta}, \tilde{\mathbf{A}})$$

due to $\tilde{A}\nabla\tilde{u}_i = \tilde{\boldsymbol{\sigma}}_i = \lambda_-(\tilde{\vartheta})\nabla\tilde{u}_i$, $i = 1, ..., m$ we have shown that $(\tilde{\vartheta}, \tilde{\mathbf{A}})$ is an optimal design.

$\square$

Remark 1.2.9. *In previous theorem we have used the fact that $\mathcal{C}$ is compact with respect to weak $*$ L^∞ topology, but one can also utilize H-topology. We say that a sequence $(\vartheta_n, \mathbf{B}_n) \in \mathcal{C}$ converges to $(\vartheta_0, \mathbf{B}_0)$ if $\vartheta_n \rightharpoonup \vartheta_0$ in weak $*$ L^∞ and $\mathbf{B}_n^{-1} \rightharpoonup \mathbf{B}_0^{-1}$ in H-topology. Then $\mathcal{C}$ is again compact with the respect to the new topology and for any $\boldsymbol{\sigma}$ the map $(\vartheta, \mathbf{B}) \mapsto L(\vartheta, \mathbf{B}, \boldsymbol{\sigma})$ is continuous with respect to the new topology.*

We can also rewrite optimal problem (I) as a max-min problem since

$$\begin{aligned}\max_{\mathcal{T}} J_I &= \max_{\vartheta\in\mathcal{T}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} \sum_{i=1}^m \mu_i \int_\Omega \frac{1}{\lambda_-(\vartheta)} |\boldsymbol{\sigma}_i|^2 \, \mathrm{d}x \\ &= \min_{\boldsymbol{\sigma}\in\mathcal{S}} \max_{\vartheta\in\mathcal{T}} \sum_{i=1}^m \mu_i \int_\Omega \frac{1}{\lambda_-(\vartheta)} |\boldsymbol{\sigma}_i|^2 \, \mathrm{d}x\end{aligned}$$

By inserting the expression for $\lambda_-(\vartheta)$, we obtain

$$\max_{\mathcal{T}} J_I = \max_{\vartheta\in\mathcal{T}} \sum_{i=1}^m \mu_i \int_\Omega \frac{\beta-\alpha}{\alpha\beta} \vartheta |\boldsymbol{\sigma}_i^*|^2 \, \mathrm{d}x. \tag{1.30}$$

To simplify the expression, let us introduce $\Psi := \sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 \in \mathrm{L}^1(\Omega)$. We now appeal to a general theorem (see [33] Chapter 1, Theorem 5):

Theorem 1.2.10. *Let X, Y be a linear spaces, let $f_0, ..., f_n$ be convex functions on X, let $F : X \to Y$ be an affine mapping, and let A be a convex set. Consider the following problem:*

$$\left\{ \begin{array}{c} \inf_{x\in M} f_0(x) \\ M = \{x \,:\, F(x) = 0,\ f_1(x) \le 0, ..., f_n(x) \le 0,\ x \in A\} \end{array} \right. \tag{1.31}$$

If x^* is a solution of the problem (1.31), then there exist Lagrange multipliers $\lambda_0 \ge 0, ..., \lambda_n \ge 0$, $y^* \in Y'$ and map

$$\mathcal{L}(x, \lambda_0, ..., \lambda_n, y^*) := \sum_{i=0}^n \lambda_i f_i(x) + \langle y^*, F(x)\rangle_{Y',Y}$$

such that

$$\begin{gathered}\mathcal{L}(x^*, \lambda_0, ..., \lambda_n, y^*) = \min_{x\in A} \mathcal{L}(x, \lambda_0, ..., \lambda_n, y^*), \\ \lambda_i f_i(x^*) = 0, \quad i = 1, ..., n.\end{gathered}$$

If moreover, the image of the set A under the mapping $x \mapsto F(x)$ contains a neighbourhood *of the origin of Y, and if there exists a vector $x \in A$ such that*

$$F(x) = 0,\ f_i(x) < 0,\ i = 1, ..., n,$$

then $\lambda_0 \neq 0$ and one can set $\lambda_0 = 1$. In the last case, the relations written above are sufficient for the point x^* to be a solution of the problem (1.31).

Therefore, for convex programming problem (1.30) the classical Lagrange multiplier rule reads: $\vartheta^* \in \mathcal{T}$ is optimal if and only if there exists a Lagrange multiplier $c \in \mathbb{R}$ such that

$$G : \vartheta \mapsto \int_\Omega \frac{\beta - \alpha}{\alpha\beta} \vartheta \Psi \, \mathrm{d}x - c \frac{\beta - \alpha}{\alpha\beta} \int_\Omega \vartheta \, \mathrm{d}x$$

achieves maximum over $\mathrm{L}^\infty(\Omega; [0, 1])$ at ϑ^*. Then we can see that G is a linear function:

$$G(\vartheta) = \int_\Omega \vartheta \frac{\beta - \alpha}{\alpha\beta} (\Psi - c) \, \mathrm{d}x$$

and since $G(\vartheta^*) \geq G(\vartheta)$ for any $\vartheta \in \mathrm{L}^\infty(\Omega; [0, 1])$ we conclude the following necessary and sufficient conditions of optimality:

$$\int_\Omega (\vartheta - \vartheta^*) \frac{\beta - \alpha}{\alpha\beta} (\Psi - c) \, \mathrm{d}x \leq 0 \tag{1.32}$$

for any $\vartheta \in \mathrm{L}^\infty(\Omega; [0, 1])$. By considering $\vartheta = \vartheta^*$, except on a small measurable set in Ω, we come to a pointwise constraint

$$(\vartheta - \vartheta^*)(\Psi - c) \leq 0, \quad \text{a.e. on } \Omega. \tag{1.33}$$

We have shown the following lemma:

Lemma 1.2.11. *The necessary and sufficient condition of optimality for solution $\vartheta^* \in \mathcal{T}$ of optimal design problem* (I) *simplifies to the existence of a Lagrange multiplier $c \geq 0$ such that*

$$\begin{cases} \vartheta^* = 0 & \Longrightarrow \displaystyle\sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 \leq c, \\ \vartheta^* \in \langle 0, 1 \rangle & \Longrightarrow \displaystyle\sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 = c, \\ \vartheta^* = 1 & \Longrightarrow \displaystyle\sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2 \geq c, \end{cases} \tag{1.34}$$

or equivalently

$$\begin{cases} \sum_{i=1}^{m} \mu_i |\boldsymbol{\sigma}_i^*|^2 < c & \Longrightarrow \vartheta^* = 0, \\ \sum_{i=1}^{m} \mu_i |\boldsymbol{\sigma}_i^*|^2 > c & \Longrightarrow \vartheta^* = 1. \end{cases} \tag{1.35}$$

1.3 Problem with uniform heat source on annulus

1.3.1 Existence of classical solution

So far we have shown that

$$\max_{\mathcal{A}} J_A \leq \max_{\mathcal{B}} J_B = \max_{\mathcal{T}} J_I.$$

The idea is to use problem (I) to present some examples in which a relaxed optimal design is classical. Observe, if we have found a classical solution of optimal design problem (I) denoted with $\chi \in \mathrm{L}^\infty(\Omega\{0,1\})$ then we have also found optimal solutions of all three optimal design problems: χ for original problem (O) and $(\chi, \alpha\chi\mathbf{I}+\beta(1-\chi)\mathbf{I})$ for both relaxed problem (A) and enlarged convex problem (B). Generally, classical solutions are rare and the following strict inequality holds

$$\max_{\mathcal{A}} J_A < \max_{\mathcal{B}} J_B,$$

while problem (O) fails to yield any solution. But if we introduce spherically symmetry to the problem:

Assumption 1.3.1. $\Omega \subset \mathbb{R}^d$ *is spherically symmetric. The right-hand sides in* (1.1) *are radial functions,*

then our maximization problems become equivalent (for details see Theorem 3.2 in [55]):

$$\max_{\mathcal{A}} J_A = \max_{\mathcal{B}} J_B = \max_{\mathcal{T}} J_I.$$

Furthermore, one can also prove that the fluxes $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, ..., \boldsymbol{\sigma}_m) \in \mathcal{S}$ are all radial functions. Indeed, if $(\vartheta^*, \mathbf{B}^*, \boldsymbol{\sigma}^*)$ is a given saddle point of L defined in the Theorem 1.2.8, due to Assumption 1.3.1 one can demonstrate that

$$(\vartheta^* \circ \mathcal{R}^{-1}, \nabla\mathcal{R}(\mathbf{B}^* \circ \mathcal{R}^{-1})\nabla\mathcal{R}^{-1}, \nabla\mathcal{R}\boldsymbol{\sigma}^* \circ \mathcal{R}^{-1})$$

is again a saddle point of the L for any rotation $\mathcal{R}$. Since flux is unique, we have that

$$\nabla\mathcal{R}\boldsymbol{\sigma}^* \circ \mathcal{R}^{-1} = \boldsymbol{\sigma}^* \quad \text{for any rotation } \mathcal{R},$$

thus demonstrating that $\boldsymbol{\sigma}^*$ must be a radial function.

Henceforth, we will treat only spherically symmetric case which is essentially a one-dimensional problem. In literature, there is a well known optimal design problem with classical solution ([41], Remark 40), in case of maximization of energy with one state equation on a ball and a constant right-hand side: the better conductor should be placed inside a smaller (concentric) ball, whose radius can easily be calculated from the constraint on given amounts of materials. For multiple state optimal design problems this was done in [55] where examples of classical solutions were shown to exists on the ball for different right-hand sides.

In this Section we first consider a single state optimal design problem on an annulus $\Omega = B(0,r_2) \setminus \overline{B(0,r_1)}$ with a constant right-hand side. Single state equation states:

$$\left\{ \begin{array}{cc} -\operatorname{div}(\lambda_-(\vartheta)\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{array} \right. \tag{1.36}$$

and problem (I) in this case reads:

$$\left\{ \begin{array}{ll} \max & J_I(\vartheta) = \int_\Omega u \,\mathrm{d}x \\ \text{s.t.} & \vartheta \in \mathrm{L}^\infty(\Omega;[0,1]), \int_\Omega \vartheta \,\mathrm{d}x = q_\alpha,\ u \text{ satisfies } (1.36). \end{array} \right. \tag{1.37}$$

Observe that the radial flux $\boldsymbol{\sigma} = \sigma(r)\vec{e}_r = \lambda_-(\vartheta)\nabla u$ from the (1.36) if rewritten in polar coordinates then satisfies first order ODE:

$$-\frac{1}{r^{d-1}}(r^{d-1}\sigma)' = 1 \text{ in } \langle r_1, r_2\rangle \tag{1.38}$$

and solutions are given by

$$\sigma = -\frac{r}{d} + \frac{\gamma}{r^{d-1}},$$

where γ is unknown integration constant. Since for any γ the corresponding σ is not equal to a constant on any interval, we conclude by necessary and sufficient conditions of optimality from Lemma 1.2.11 that optimal design ϑ^* for problem (1.37) is unique, radial and classical (i.e. it attains only values 0 and 1, almost everywhere). Consequently, a solution of the original relaxation problem (A) is unique and classical.

Due to the uniqueness of the optimal design, the corresponding state function u^* is also a unique radial function. It is calculated from the equation $\sigma(r) = \lambda_-(\vartheta(r))u'(r)$, by the formula:

$$u^*(r) = \int_{r_1}^{r} \frac{1}{\lambda_-(\vartheta^*(\rho))}\left(\frac{\gamma}{\rho^{d-1}} - \frac{\rho}{d}\right) d\rho\,. \tag{1.39}$$

Here, the boundary condition $u^*(r_1) = 0$ is satisfied, and the other boundary condition $u^*(r_2) = 0$ gives a constraint on γ. For the beginning, we conclude that constant γ should

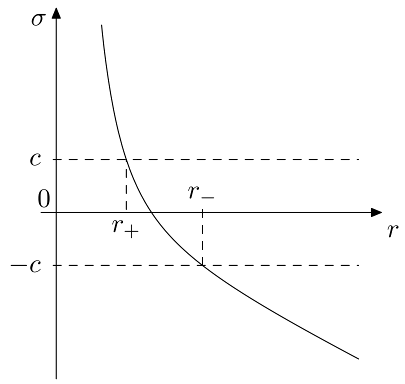


Figure 1.3: Typical graph of flux σ.

be positive.

This means that σ is a strictly decreasing function whose range is entire set of real numbers (Figure 1.3). For a constant $c_0 \geq 0$ appearing in Lemma 1.2.11 we introduce $r_+, r_- > 0$ as the unique solutions of the equations $\sigma(r_+) = c$ and $\sigma(r_-) = -c$, respectively, where c denotes $\sqrt{c_0}$.

Depending whether $r_\pm$ belongs to the interval $\langle r_1, r_2 \rangle$, by the necessary and sufficient condition of optimality the optimal ϑ^* has one of the following three configurations:

$$1)\ \ \vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_2\rangle \,, \end{cases}$$

$$2)\ \ \vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_-\rangle \\ 1, & r \in [r_-, r_2] \,, \end{cases}$$

$$3)\ \ \vartheta^*(r) = \begin{cases} 0, & r \in [r_1, r_-\rangle \\ 1, & r \in [r_-, r_2\rangle \,. \end{cases}$$

We shall speak about three possible optimal configurations: $\alpha - \beta$ in the first case, $\alpha - \beta - \alpha$ in the second case, and $\beta - \alpha$ in the third case. Our aim is to determine which configuration (out of three) is optimal, and to calculate the solution.

To summarise, for the optimal design ϑ^* the following system (with unknowns $\gamma, c, r_+ r_-$) holds:

$$S_d \int\limits_{r_1}^{r_2} \rho^{d-1} \vartheta^*(\rho)\, d\rho = q_\alpha \tag{1.40a}$$

$$\gamma \int_{r_1}^{r_2} \left(\frac{1}{\lambda_-(\vartheta^*(\rho))\rho^{d-1}} \right) d\rho = \int_{r_1}^{r_2} \frac{\rho}{\lambda_-(\vartheta^*(\rho))}\, d\rho \tag{1.40b}$$

$$\sigma(r_+) = c, \;\; \sigma(r_-) = -c, \, c > 0 \,, \tag{1.40c}$$

where (1.40a) is the constraint on the amount of the first phase (S_d is the surface measure of the unit sphere in $\mathbb{R}^d$), (1.40b) comes from condition $u^*(r_2) = 0$ and (1.40c) is given by the necessary and sufficient condition of optimality from the Lemma 1.2.11.

1.3.2 Analysis of solution configuration $\beta - \alpha$

Lemma 1.3.2. *If d equals 2 or 3 then for any admissible amount q_α of the first phase, the solution ϑ^* does not belong to the third case $\beta - \alpha$.*

Proof. Let us assume the opposite, namely that there exist some γ, c, r_+ and r_- satisfying nonlinear system (1.40a)–(1.40c), such that $r_+ < r_1 < r_- < r_2$. Since σ is a strictly decreasing function one can conclude that $\sigma(r_1) < c$ and $\sigma(r_2) < -c$ which implies

$$\sigma(r_1) + \sigma(r_2) < 0. \tag{1.41}$$

From (1.40b) one can express γ in terms of r_- with respect to space dimension d:

$$\begin{aligned} \gamma = \Gamma_2(r_-) &:= \frac{1}{4}\frac{\frac{r_2^2}{\alpha} - \frac{r_1^2}{\beta} - \left[\frac{1}{\alpha} - \frac{1}{\beta}\right] r_-^2}{\frac{\ln(r_2)}{\alpha} - \frac{\ln(r_1)}{\beta} - \left[\frac{1}{\alpha} - \frac{1}{\beta}\right]\ln(r_-)}, \quad \text{for } d = 2\,, \quad \text{and} \\ \gamma = \Gamma_3(r_-) &:= \frac{1}{6}\frac{\frac{r_2^2}{\alpha} - \frac{r_1^2}{\beta} - \left[\frac{1}{\alpha} - \frac{1}{\beta}\right] r_-^2}{\frac{1}{\beta r_1} - \frac{1}{\alpha r_2} + \left[\frac{1}{\alpha} - \frac{1}{\beta}\right]\frac{1}{r_-}}, \qquad \text{for } d = 3\,. \end{aligned} \tag{1.42}$$

Let us first consider the three-dimensional case. One can easily show that

$$\Gamma_3(r_-) > \Gamma_3(r_1) = \Gamma_3(r_2) = \frac{1}{6} r_1 r_2 (r_1 + r_2)\,,\ r_- \in \langle r_1, r_2\rangle\,. \tag{1.43}$$

From (1.41) one obtains

$$\Gamma_3(r_-)\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) < \frac{r_1 + r_2}{3}\,,$$

and by multiplying this inequality with $r_1 r_2/2$ one gets the following inequality

$$\Gamma_3(r_-) \le \Gamma_3(r_-)\left(\frac{\frac{r_1}{r_2} + \frac{r_2}{r_1}}{2}\right) < \frac{1}{6}(r_1 + r_2) r_1 r_2\,, \tag{1.44}$$

which is in contradiction with (1.43).

For the two-dimensional case the proof goes in the similar manner. A simple analysis leads to

$$\Gamma_2(r_-) > \Gamma_2(r_1) = \Gamma_2(r_2) = \frac{1}{4}\frac{r_2^2 - r_1^2}{\ln(r_2) - \ln(r_1)}\,,\ r_- \in \langle r_1, r_2\rangle\,. \tag{1.45}$$

On the other side, from (1.41) one obtains $\Gamma_2(r_-) < r_1 r_2/2$, which gives a contradiction due to the inequality

$$\mu^2 - 1 \geq 2\mu \ln(\mu)\,,\ \mu \geq 1\,,$$

where equality holds only for $\mu = 1$. Indeed, by substituting $\mu = r_2/r_1 > 1$ one gets

$$\frac{r_1 r_2}{2} < \frac{1}{4}\frac{r_2^2 - r_1^2}{\ln(r_2) - \ln(r_1)}\,.$$

□

Remark 1.3.3. *Unfortunately, the higher dimensional case $d > 3$ cannot be treated in the same manner unless additional assumptions on the radii are given.*

Lemma 1.3.2 proves that only two optimal configurations $\alpha - \beta - \alpha$ and $\alpha - \beta$ can appear. As we shall see in the next section, each of these two configurations is indeed optimal for particular q_α.

1.3.3 Analysis of configurations $\alpha - \beta$ and $\alpha - \beta - \alpha$

In the following results, we consider only two- and three-dimensional case. The amount q_α of the first phase will be replaced by the overall proportion of the first phase $\eta := \frac{q_\alpha}{\mathrm{vol}(\Omega)} \in \langle 0, 1\rangle$. The following result can be easily proved.

Lemma 1.3.4. *There exist positive constants $0 < \eta_1 \leq \eta_2 < 1$ such that for $\eta \in \langle 0, \eta_1\rangle$ the optimal design is of the form $\alpha - \beta$, while for $\eta \in \langle \eta_2, 1\rangle$ the configuration $\alpha - \beta - \alpha$ is optimal.*

In the next theorem, we claim that η_1 and η_2 from the previous Lemma can be taken to be equal. The proof is based on a more precise analysis of the optimality conditions

Theorem 1.3.5. *If Ω is an annulus, $m = 1$ and $f \equiv 1$, then the optimal design problem (I) has the unique solution ϑ^*, which is a radial function. Depending on given parameters α, β, and radii of annulus Ω, there exists a critical value $\eta_{crit} \in \langle 0, 1\rangle$ such that*

(a) if $\eta > \eta_{crit}$ then $$\vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_-\rangle \\ 1, & r \in [r_-, r_2] \end{cases}\,,$$

(b) if $\eta \leq \eta_{crit}$ then $$\vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_2\rangle\,. \end{cases}$$

The critical value η_{crit} can be calculated only numerically. For example, if $\alpha = 1, \beta = 2, r_1 = 1, r_2 = 2$ in the two-dimensional case the critical value η_{crit} approximately equals $0.032\,207\,2$, while in three-dimensional case it is approximately $0.035\,456\,1$. In general, for $\eta \leq \eta_{\text{crit}}$ optimal radius r_+ is simply calculated from (1.40a): it equals $\sqrt{(1-\eta)r_1^2 + \eta r_2^2}$

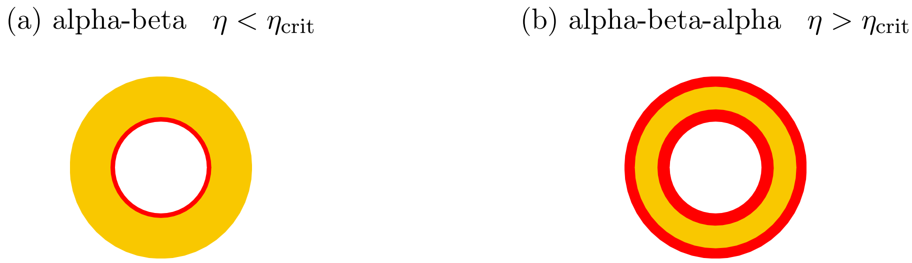


Figure 1.4: Two possible configurations

in the two-dimensional case, and $\sqrt[3]{(1-\eta)r_1^3 + \eta r_2^3}$ in the three-dimensional case. In the case $\eta > \eta_{\text{crit}}$ the values for radii r_+ and r_- which determine the optimal design can be obtained only numerically, by solving the system (1.40a)–(1.40c). The approximate solution for $\alpha = 1, \beta = 2, r_1 = 1, r_2 = 2$, and various values of volume fraction η is presented in Tables 1.1 and 1.2, in the two-dimensional and the three-dimensional case, respectively.

Table 1.1: Approximate values for radii r_+ and r_- for the single state problem with $f \equiv 1$ (Subsection 2.2), $d = 2$, $\alpha = 1$, $\beta = 2$, $r_1 = 1$ and $r_2 = 2$. The critical value η_{crit} from Theorem 1.3.5 approximately equals 0.032 207 2.

η	γ	r_+	r_-	J
0.01	1.070 03	1.014 89	/	0.410 799
0.02	1.059 14	1.029 56	/	0.424 053
0.03	1.049 26	1.044 03	/	0.435 758
0.04	1.047 99	1.050 23	1.995 74	0.446 422
0.05	1.048 98	1.054 11	1.990 27	0.456 850
0.10	1.053 69	1.073 64	1.962 83	0.505 929
0.20	1.061 78	1.113 18	1.907 66	0.589 525
0.30	1.068 23	1.153 49	1.852 17	0.655 297
0.40	1.073 19	1.194 75	1.796 51	0.705 212
0.50	1.076 83	1.237 14	1.740 84	0.741 310
0.60	1.079 33	1.280 82	1.685 38	0.765 712
0.70	1.080 87	1.325 93	1.630 36	0.780 622
0.80	1.081 68	1.372 61	1.576 09	0.788 324
0.90	1.081 98	1.420 97	1.522 88	0.791 173
0.99	1.082 02	1.465 98	1.476 18	0.791 581

Proof of Lemma 1.3.4 . We present the proof for the two-dimensional case. The three-dimensional case can be proved in the same manner.

Contrary to the first claim, let us assume that there exists a sequence (η^n) converging to zero, such that the optimal design has the form $\alpha - \beta - \alpha$. Therefore, for each n, system (1.40a)-(1.40c) has unique solution $\gamma^n, c^n, r_+^n, r_-^n$. Using (1.40b) one obtains expression for

Table 1.2: Approximate values for radii r_+ and r_- for the single state problem with $f \equiv 1$ (Subsection 2.2), $d = 3$, $\alpha = 1$, $\beta = 2$, $r_1 = 1$ and $r_2 = 2$. The critical value η_{crit} from Theorem 1.3.5 approximately equals 0.035 456 1.

η	γ	r_+	r_-	J
0.01	0.972 026	1.022 81	/	1.244 41
0.02	0.949 289	1.044 64	/	1.289 47
0.03	0.930 589	1.065 60	/	1.325 05
0.04	0.922 590	1.077 92	1.997 70	1.353 89
0.05	0.924 381	1.080 61	1.992 63	1.381 39
0.10	0.933 061	1.094 25	1.966 98	1.512 56
0.20	0.948 982	1.122 44	1.914 22	1.743 75
0.30	0.962 877	1.152 13	1.859 47	1.934 37
0.40	0.974 615	1.183 70	1.802 73	2.086 02
0.50	0.984 081	1.217 64	1.744 10	2.200 92
0.60	0.991 209	1.254 48	1.683 84	2.282 16
0.70	0.996 032	1.294 85	1.622 47	2.333 90
0.80	0.998 758	1.339 35	1.560 84	2.361 60
0.90	0.999 839	1.388 44	1.500 23	2.372 12
0.99	1.000 000	1.436 66	1.447 88	2.373 65

γ^n:

$$\gamma^n = \frac{1}{4}\frac{((r_+^n)^2 - r_1^2)/\alpha + ((r_-^n)^2 - (r_+^n)^2)/\beta + (r_2^2 - (r_-^n)^2)/\alpha}{\ln(r_+^n/r_1)/\alpha + \ln(r_-^n/r_+^n)/\beta + \ln(r_2/r_-^n)/\alpha}.$$

Since $\lim_n q_\alpha^n = 0$, we have $r_+^n \to r_1$ and $r_-^n \to r_2$, which implies

$$\gamma^n \to \frac{1}{4}\frac{r_2^2 - r_1^2}{\ln r_2 - \ln r_1}.$$

From (1.40c) by eliminating c one gets

$$\gamma^n = \frac{r_+^n r_-^n}{2} \to \frac{r_+ r_-}{2},$$

and by the same reasoning one concludes $\gamma^n \to r_1 r_2/2$. By the proof of Lemma 1.3.2 this is possible only if $r_1 = r_2$, which is a contradiction.

For the proof of the second claim, we again argue by contradiction. Suppose that there exists a sequence (η^n) which converges to 1 such that corresponding optimal design has the form $\alpha - \beta$. This means that, for given n and $q_\alpha = \eta^n \operatorname{vol}(\Omega)$, system (1.40a)-(1.40c) has a unique solution $\gamma^n, c^n, r_+^n, r_-^n$ such that $r_1 < r_+^n < r_2 < r_-^n$. The Lagrange multiplier c^n is given by (1.40c): $c^n = \sigma^n(r_+^n) = \frac{\gamma^n}{r_+^n} - \frac{r_+^n}{d}$, and to ensure the condition $r_-^n > r_2$ it is necessary and sufficient to assume $\sigma^n(r_+^n) + \sigma^n(r_2) > 0$. This is equivalent to

$$\gamma^n > \frac{r_+^n r_2}{2}. \tag{1.46}$$

From (1.40b) it follows

$$\gamma^n = \frac{1}{4}\frac{((r_+^n)^2 - r_1^2)/\alpha + (r_2^2 - (r_+^n)^2)/\beta}{\ln(r_+^n/r_1)/\alpha + \ln(r_2/r_+^n)/\beta},$$

and since $\eta^n \to 1$ we have $r_+^n \to r_2$, which implies that γ^n converges to $\dfrac{1}{4}\dfrac{r_2^2 - r^2}{\ln r_2 - \ln r_1}$.

According to (1.46), we obtain the inequality $\dfrac{1}{4}\dfrac{r_2^2 - r^2}{\ln r_2 - \ln r_1} \geq \dfrac{r_2^2}{2}$, which leads us to a contradiction since the inequality holds if and only if $r_1 = r_2$. □

Lemma 1.3.6. *For fixed η, system (1.40a)–(1.40c) admits a solution for only one of the configurations $\alpha - \beta$ and $\alpha - \beta - \alpha$.*

Proof. $d = 2$

Assume that the opposite holds. Then for some η there exists solution to system (1.40a)-(1.40c) with configuration $\alpha - \beta$ and $\alpha - \beta - \alpha$:

$$\begin{array}{rl} \alpha - \beta & \gamma, c, r_+, \\ \alpha - \beta - \alpha & \hat{\gamma}, \hat{c}, \hat{r}_+, \hat{r}_-. \end{array}$$

Observe that, if η is the same for both configurations, then

$$\hat{r}_+ < r_+ \quad \text{and} \quad \hat{r}_- < r_2. \tag{1.47}$$

From (1.40c) for $\hat{\gamma}$ and (1.46) for γ we conclude:

$$\hat{\gamma} = \frac{\hat{r}_+\hat{r}_-}{2} < \frac{r_+ r_2}{2} < \gamma\,. \tag{1.48}$$

In particular, (1.40b) for both configuration gives

$$\frac{1}{4}\frac{(\hat{r}_+^2 - r_1^2)/\alpha + (\hat{r}_-^2 - \hat{r}_+^2)/\beta + (\hat{r}_2^2 - \hat{r}_-^2)/\alpha}{\ln(\hat{r}_+/r_1)/\alpha + \ln(\hat{r}_-/\hat{r}_+)/\beta + \ln(r_2/\hat{r}_-)/\alpha} = \hat{\gamma} < \gamma = \frac{1}{4}\frac{(r_+^2 - r_1^2)/\alpha + (r_2^2 - r_+^2)/\beta}{\ln(r_+/r_1)/\alpha + \ln(r_2/r_+)/\beta}.$$

Observe that the numerators above are equal, since

$$(\hat{r}_+^2 - r_1^2) + (\hat{r}_2^2 - \hat{r}_-^2) = (r_+^2 - r_1^2), \tag{1.49}$$

$$\hat{r}_-^2 - \hat{r}_+^2 = r_2^2 - r_+^2. \tag{1.50}$$

With this simplification, after a short calculation, we obtain the following inequality from (1.48):

$$\ln(\hat{r}_+/\hat{r}_-) > \ln(r_+/r_2),$$

or better $\hat{r}_+/\hat{r}_- > r_+/r_2$. This is clearly a contradiction because from (1.50) we get:

$$(1 - r_+^2/r_-^2) = \frac{\hat{r}_-^2}{r_2^2}(1 - \hat{r}_+^2/\hat{r}_-^2) < (1 - \hat{r}_+^2/\hat{r}_-^2),$$

meaning $\hat{r}_+/\hat{r}_- < r_+/r_2$.

□

Proof of Theorem 1.3.5. The proof is again presented only in the two-dimensional case. The same approach can be applied for the three-dimensional case.

Let us suppose that configuration $\alpha - \beta$ is optimal. This means that, as in the previous proof, for given η, system (1.40a)–(1.40c) has an unique solution γ, c, r_+, r_- such that $r_1 < r_+ < r_2 < r_-$.

The first condition (1.40a) is simply rewritten as

$$r_+^2 - r_1^2 = \eta(r_2^2 - r_1^2)\,, \tag{1.51}$$

while the second one gives γ in terms of r_+:

$$\gamma = \frac{1}{4}\frac{(r_+^2 - r_1^2)/\alpha + (r_2^2 - r_+^2)/\beta}{\ln(r_+/r_1)/\alpha + \ln(r_2/r_+)/\beta}\,,$$

and the third one is equivalent to $\gamma > \dfrac{r_+ r_2}{2}$.

Therefore, a configuration $\alpha - \beta$ satisfies the optimality conditions if and only if inequality

$$\frac{1}{4}\frac{(r_+^2 - r_1^2)/\alpha + (r_2^2 - r_+^2)/\beta}{\ln(r_+/r_1)/\alpha + \ln(r_2/r_+)/\beta} > \frac{r_+ r_2}{2} \tag{1.52}$$

has solution $r_+ \in \langle r_1, r_2\rangle$. By simple manipulations, inequality (1.52) reads

$$f(r_+) := c_1 r_+^2 + c_2 - 2r_+ r_2(c_2 \ln r_+ + c_3) > 0\,,$$

where

$$\begin{aligned} c_1 &= \left(\frac{1}{\alpha} - \frac{1}{\beta}\right) \\ c_2 &= \frac{r_2^2}{\beta} - \frac{r_1^2}{\alpha} \\ c_3 &= \frac{1}{\beta}\ln(r_2) - \frac{1}{\alpha}\ln(r_1)\,. \end{aligned}$$

It is easy to check that $f(r_1) > 0$ and $f(r_2) < 0$, so function f has zero in $[r_1, r_2]$. Moreover, f is decreasing on $[r_1, r_2]$, which follows easily since $f'' < 0$ and $f'(r_1) < 0$. Therefore, there exists $r_0 \in \langle r_1, r_2\rangle$ such that (1.52) is equivalent to $r_+ \in \langle r_1, r_0\rangle$. Due to (1.51) this means that configuration $\alpha - \beta$ is optimal if and only if $0 \leq \eta < \eta_{\mathrm{crit}}$ (by Lemma 1.3.4 we know that $\eta_{\mathrm{crit}} \in \langle 0, 1\rangle$). Otherwise, configuration $\alpha - \beta - \alpha$ is optimal due to Lemma 1.3.6. □

1.4 Multiple State Optimal Design Problem

Let us now consider the optimal design problem with two state equations for dimension $d = 2$:

$$\left\{ \begin{aligned} -\operatorname{div}(\lambda_-(\vartheta)\nabla u_1) &= 1 =: f_1 && \text{in } \Omega \\ u_1 &= 0 && \text{on } \partial\Omega\,, \end{aligned} \right. \tag{1.53}$$

$$\left\{ \begin{aligned} -\operatorname{div}(\lambda_-(\vartheta)\nabla u_2) &= \tfrac{b}{r(b-r)^2} =: f_2 && \text{in } \Omega \\ u_2 &= 0 && \text{on } \partial\Omega, \end{aligned} \right. \tag{1.54}$$

where $b > r_2$. Functional J_I is then given as

$$J_I(\vartheta) = \mu_1 \int_\Omega f_1 u_1 \,dx + \mu_2 \int_\Omega f_2 u_2 \,dx \tag{1.55}$$

with $\mu_1, \mu_2 > 0$.

We shall follow the approach presented in the last Section, so the first step is to determine the set $\mathcal{S} = \{\boldsymbol{\sigma} \in \mathrm{L}^2(\Omega; \mathbb{R}^2)^2 : -\operatorname{div} \boldsymbol{\sigma}_i = f_i, i = 1, 2\}$. The calculation is easily done in polar coordinates (we seek for the unique *radial* function $\boldsymbol{\sigma}^* \in \mathcal{S}$ which appears in the optimality condition).

By solving the corresponding ordinary differential equations, one can easily obtain all radial solutions σ_1 and σ_2 such that $\boldsymbol{\sigma} = (\sigma_1(r)e_r, \sigma_2 e_r)$ belongs to $\mathcal{S}$:

$$\sigma_1(r) = -\frac{r}{2} + \frac{\gamma_1}{r}\,, \qquad \sigma_2(r) = -\frac{1}{b-r} + \frac{\gamma_2}{r}\,,$$

so the problem is to determine the unique constants γ_1^* and γ_2^* which lead to $\boldsymbol{\sigma}^*$.

The corresponding states u_1^* and u_2^* (radial functions, as well) are determined by $\lambda_-(\vartheta)u_i^{*\prime} = \sigma_i^*$, $i = 1, 2$. Therefore, the boundary conditions imply

$$\gamma_1 \int_{r_1}^{r_2} \left(\frac{1}{\lambda_-(\vartheta(\rho))\rho} \right) \mathrm{d}\rho = \int_{r_1}^{r_2} \frac{\rho}{2\lambda_-(\vartheta(\rho))} \,\mathrm{d}\rho \tag{1.56}$$

$$\gamma_2 \int_{r_1}^{r_2} \left(\frac{1}{\lambda_-(\vartheta(\rho))\rho} \right) \mathrm{d}\rho = \int_{r_1}^{r_2} \frac{1}{(b-\rho)\lambda_-(\vartheta(\rho))} \,\mathrm{d}\rho \tag{1.57}$$

As a consequence, by estimating $\lambda_-(\vartheta)$ from the below by α and from the above by β we can obtain rather precise estimates on γ_1 and γ_2.

If we define $\Psi : \langle 0, b\rangle \to \mathbb{R}$ as

$$\Psi := \mu_1 {\sigma_1}^2 + \mu_2 {\sigma_2}^2 ,$$

the optimality condition states (Ψ^* is determined by γ_1^* and γ_2^*): there exists $c > 0$ such that

$$\Psi^* > c \quad \Rightarrow \quad \theta^* = 1 ,$$

$$\Psi^* < c \quad \Rightarrow \quad \theta^* = 0 .$$

However, for any admissible γ_1 and γ_2 if $r \to 0$ or $r \to b$ then $\Psi(r) \to +\infty$. Moreover, one can show that Ψ has the unique stationary point in $\langle 0, b\rangle$. Therefore, for any c the equation $\Psi(r) = c$ has at most two solutions on $\langle 0, b\rangle$:

$$\Psi(r_*) = \Psi(r^*) = c \, , \; r_* \leq r^* . \tag{1.58}$$

Moreover, we can conclude (not knowing the exact γ_1^* and γ_2^*) that the solution ϑ^* is unique and radial, since Ψ^* is a radial function. The constraint on the amount of given materials is expressed by

$$2\pi \int_{r_1}^{r_2} \rho \vartheta^*(\rho) \, d\rho = q_\alpha . \tag{1.59}$$

Finally, depending on whether r_1 and r_2 belong to interval $\langle 0, r_*]$, $[r_*, r^*]$ or $[r^*, b\rangle$ the optimal solution has one of the three following configurations

$$1) \;\; \vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_*\rangle \\ 0, & r \in [r_*, r^*\rangle \\ 1, & r \in [r^*, r_2] \end{cases}$$

$$2) \;\; \vartheta^*(r) = \begin{cases} 1, & r \in [r_1, r_*\rangle \\ 0, & r \in [r_*, r_2] \end{cases}$$

$$3) \;\; \vartheta^*(r) = \begin{cases} 0, & r \in [r_1, r^*\rangle \\ 1, & r \in [r^*, r_2] \; . \end{cases}$$

The system (1.56)–(1.59) should be considered for each of the three possible configurations, and exactly one will provide us with the solution. Due to its high nonlinearity, this system with five unknowns r_*, r^*, c, γ_1 and γ_2 is solved numerically. Each of the three possible configurations of the optimal design can be achieved for appropriate choice of parameters η, α, β, r_1, r_2, μ_1, μ_2 and b. For example, if $\alpha = 1, \beta = 2, r_1 = 1, r_2 = 2, \mu_1 = \mu_2 = 0.5, b = 2.5$ the optimal configuration is $\beta - \alpha$ if volume fraction η is less than 0.040 101 6, and $\alpha - \beta - \alpha$, otherwise. In Table 1.3 we present approximate values for r_*, r^*, c, γ_1 and γ_2 for different values of the parameter η.

Table 1.3: Approximate values for radii r_* and r^* for the multiple state problem, $\alpha = 1$, $\beta = 2$, $r_1 = 1$, $r_2 = 2$, $\mu_1 = \mu_2 = 0.5$, $b = 2.5$.

η	γ_1	γ_2	r_*	r^*	J
0.01	1.086 94	1.597 81	/	1.992 49	1.011 15
0.02	1.091 76	1.610 21	/	1.984 94	1.046 98
0.03	1.096 48	1.622 19	/	1.977 37	1.080 62
0.04	1.101 11	1.633 75	/	1.969 77	1.112 20
0.05	1.099 02	1.632 76	1.005 82	1.965 11	1.142 30
0.06	1.096 98	1.631 66	1.011 68	1.960 49	1.171 49
0.10	1.089 78	1.627 44	1.035 05	1.941 99	1.279 66
0.20	1.077 41	1.618 18	1.092 74	1.895 80	1.497 75
0.30	1.070 80	1.610 57	1.149 36	1.849 60	1.655 72
0.40	1.068 04	1.604 37	1.204 94	1.803 30	1.767 66
0.50	1.067 85	1.599 33	1.259 50	1.756 80	1.844 25
0.60	1.069 37	1.595 24	1.313 07	1.710 01	1.893 89
0.70	1.071 96	1.591 91	1.365 67	1.662 84	1.923 42
0.80	1.075 17	1.589 19	1.417 33	1.615 19	1.938 63
0.90	1.078 62	1.586 92	1.468 08	1.566 92	1.944 61
0.99	1.081 69	1.585 15	1.512 97	1.522 85	1.945 98

CHAPTER 2

Calculations of shape derivative

2.1 Introduction

In this chapter we shall consider the same optimal design problem for the stationary diffusion equation in the case of two isotropic phases, aiming to maximize the energy functional. To simplify the notation, we shall focus only on single-state problems. Let us recall the original optimal design problem:

We seek for a distributions of materials such that the internal energy is maximized:

$$\left\{\begin{array}{ll} \max & J(\chi) = \displaystyle\int_\Omega f u \,\mathrm{d}x \\ \text{s.t.} & \chi \in L^\infty(\Omega, \{0,1\}), \quad \displaystyle\int_\Omega \chi \,\mathrm{d}x = q_\alpha, \\ & u \text{ solves (2.2) with } \mathbf{a} = \alpha\chi + \beta(1-\chi), \end{array}\right. \tag{2.1}$$

where (2.2) is the following boundary value problem:

$$\left\{\begin{array}{ll} -\mathrm{div}(\mathbf{a}\nabla u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{array}\right. \tag{2.2}$$

Henceforth we shall assume that the right-hand side f belongs to $\mathrm{L}^2(\Omega)$.

If such a characteristic function χ exists we call it a *classical solution*. In the previous chapter, the relaxation of the problem (2.1) through homogenization was used, by introducing relaxed designs.

A shape is a bounded set with well defined boundary (usually Lipschitz). If we were given a measurable set Ω_α representing the shape of the phase α then the map

$$\Omega_\alpha \mapsto J(\Omega_\alpha)$$

is well defined. In shape optimization the goal is to find an optimal shape Ω_α^* which maximizes the shape functional under the volume constraint. Such optimal shapes exist for the symmetrical cases, e.g. see Theorem 1.3.5 when the right-hand side is $f = 1$ and domain is annulus. This offers an important family of test examples which can be used for various numerical approaches based on shape sensitivity method [30], originally developed by Hadamard.

In this chapter we shall study the first and the second order shape derivatives for optimal design problem (2.1). This will be done extensively, using several different approaches to calculate the shape derivative. The results shall be used for the construction of descent methods of gradient type and "quasi-Newton" type in the following chapter.

2.1.1 Definition of Lipschitz domain and properties

We first start with the definition of a Lipschitz domain and some useful properties.

Definition 2.1.1. *Let ω be a bounded open set in $\mathbb{R}^d$ with boundary $\partial\omega$. We say that ω is a Lipschitz domain, whenever there exist $\delta, L > 0$, so that for any $z \in \partial\omega$ one can find:*

1. *a local coordinate system, denoting with $(x', x_d) = (x_1, x_2, ..., x_{d-1}, x_d)$ coordinates of a point x,*

2. *a rotation operator $\mathcal{R} : \mathbb{R}^{d-1} \times \mathbb{R} \to \mathbb{R}^d$ that maps the local coordinates to the global ones,*

3. *a Lipschitz continuous map $\varphi : \mathbb{R}^{d-1} \to \mathbb{R}$ (with the Lipschitz constant less then L),*

such that for the open cylinder $K(0; \delta, L) := \{(x', x_d) \ : \ |x'| < \delta, \ |x_d| < L\delta\}$ and the set $V_z := z + \mathcal{R}(K(0; \delta, L))$ the following holds:

- $\omega \cap V_z = z + \mathcal{R}(\{(x', x_d) \in K(0; \delta, L) \ : \ \varphi(x_d) > x_d\})$,
- $\partial\omega \cap V_z = z + \mathcal{R}(\{(x', x_d) \in K(0; \delta, L) \ : \ \varphi(x_d) = x_d\})$.

We say that ω is a domain of class C^k if each mapping φ is C^k.

Definition 2.1.1 implies that the boundary $\partial\omega$ can be locally represented (using proper rigid transformations) by the graph of a Lipschitz function. Sometimes boundedness assumption on a set ω is omitted in Definition 2.1.1 giving us definition of an open set with Lipschitz boundary. In the more regular case we are talking about sets with C^k boundary.

Remark 2.1.2. *In the literature a Lipschitz domain introduced in Definition 2.1.1 is also refereed to as a strongly Lipschitz domain. Weakly Lipschitz domain is such that for any $z \in \partial\omega$ there exists an open neighbourhood U of z and an open zero-neighbourhood V of $\mathbb{R}^d$ such that map $F : V \to U$ is bijective bi-Lipschitz function satisfying:*

- $F(V \cap (\mathbb{R}^{d-1} \times \mathbb{R}^+)) = U \cap \omega$,
- $F(V \cap (\mathbb{R}^{d-1} \times \{0\})) = U \cap \partial\omega$.

This definition is more general, i.e. there exists domains that are weakly Lipschitz but not strongly Lipschitz. See Figure 2.4 for classical "two-block" domain which is a standard example of weakly Lipschitz domain that is not a strongly Lipschitz domain. Generally, definition of Lipschitz domain may vary in the literature and one should be cautious which notion is used. For example in [2] strongly local Lipschitz property is defined for $\partial\omega$ which for the case of bounded ω gives equivalent definition (although, constants δ, L may have different values). A set (not necessarily bounded) that satisfies weakly Lipschitz condition in the literature is also known as a Lipschitz manifold (see e.g. Section 2.4 of [30]).

One can easily shown that every Lipschitz domain satisfies uniform cone property. We denote a cone as (see Figure 2.1):

$$C_{L,\delta} = \{x = (x', x_d) \in \mathbb{R}^{d-1} \times \mathbb{R} \ : \ x_d > L|x'|, |x| < \delta\}.$$

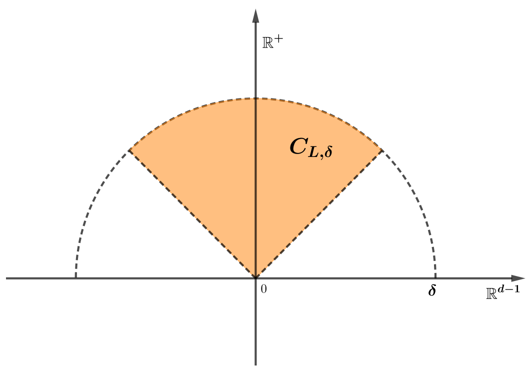


Figure 2.1: Cone $C_{L,\delta}$

Definition 2.1.3. *We say that an open bounded set ω satisfies the uniform cone property if there exists constants $\delta, L > 0$ such that for each $z \in \partial\omega$, there exists a rotation operator $\mathcal{R}$ with the following property:*

$$x \in \omega \cap B(z, \delta) \implies x + \mathcal{R}(C_{L,\delta}) \subset \omega.$$

Actually, the uniform cone property offers alternative, useful characterization of Lipschitz domain:

Lemma 2.1.4. *A bounded open set is a Lipschitz domain if and only if it satisfies the uniform cone property.*

Proof. see Theorem 1.2.2.2. in [27] or Theorem 2.4.7 in [30]. □

If we were given domain ω with C^k boundary and k-diffeomorphism $\Phi \in C^k(\mathbb{R}^d, \mathbb{R}^d)$ one can check using classical theory that $\Phi(\omega)$ remains domain with C^k boundary. When dealing with Lipschitz domain one should be cautious, because if we assume that we have bi-Lipschitz homeomorphism $\Phi : \mathbb{R}^d \to \mathbb{R}^d$, image $\Phi(\omega)$ may fail to be Lipschitz domain. In fact bi-Lipschitz functions may fail to map even bounded C^∞ planar domains into Lipschitz domain as can we see in the following example from [32]:

Example 2.1.5. *Consider the bi-Lipschitz homeomorphism:*

$$\Phi(x_1, x_2) = (x_1, \varphi(x_1) + x_2)$$

where $\varphi \in \mathrm{W}^{1,\infty}(\mathbb{R};\mathbb{R})$ *is given with (Figure 2.2):*

$$\varphi(t) = \begin{cases} 3|t| - \frac{1}{2^{2k-1}}, & t \in \left[\frac{1}{2^{2k+1}}, \frac{1}{2^{2k}}\right],\ k \in \mathbb{N} \\ -3|t| + \frac{1}{2^{2k}}, & t \in \left[\frac{1}{2^{2k+2}}, \frac{1}{2^{2k+1}}\right],\ k \in \mathbb{N}_0 \\ 3|t| - 2, & t \in \left[\frac{1}{2}, \frac{2}{3}\right] \\ 0, & t \in \mathbb{R} \setminus \left[0, \frac{2}{3}\right]. \end{cases}$$

Now consider the bounded Lipschitz domain $\omega \subset \mathbb{R}^2$:

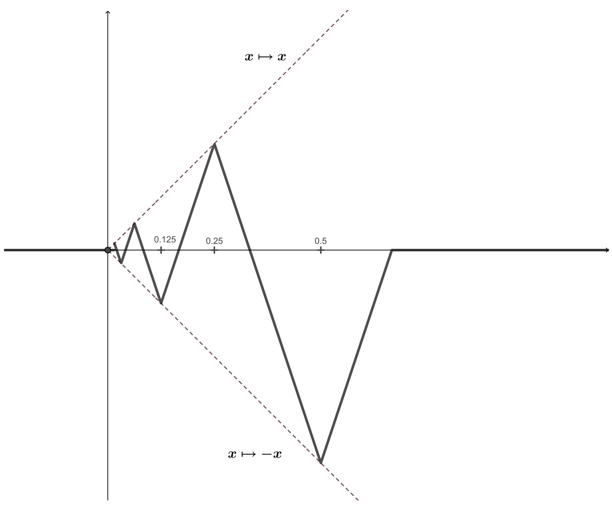


Figure 2.2: Lipschitz function φ

$$\omega = \{(x_1, x_2) \ :\ 0 < x_1 < 1,\ 0 < x_2 < x_1\}$$

Then $\Phi(\omega)$ *fails to be a Lipschitz domain, since the uniform cone property is not satisfied at* $(0,0)$*. See Figure 2.3. One can also create an example in which polyhedral three-dimensional domain represented in Figure 2.4 can be obtained as the image of a Lipschitz domain by a bi-Lipschitz mapping. For details we refer the reader to [36].*

The following theorem gives sufficient conditions for a class of Lipschitz homeomor-

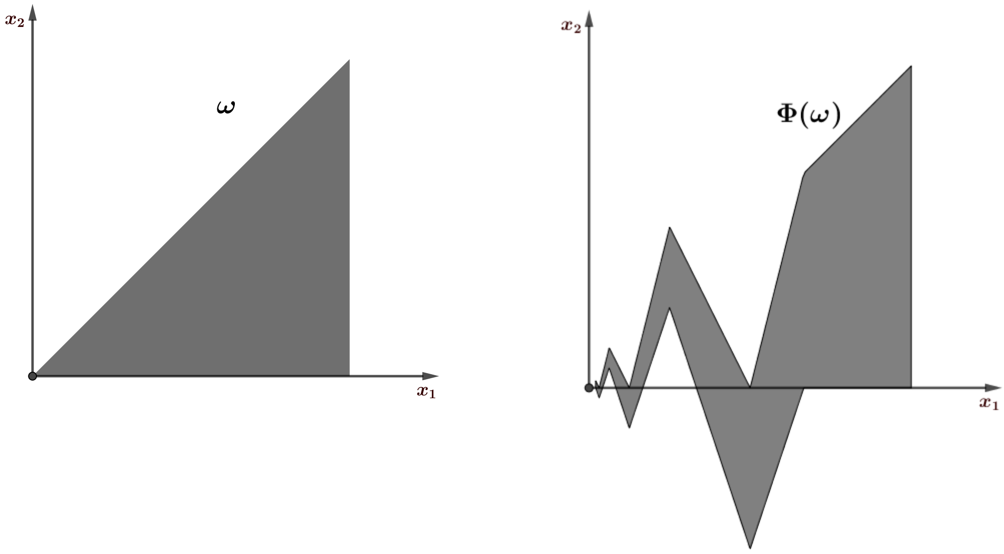


Figure 2.3: Left: Lipschitz domain ω. Right: Domain $\Phi(\omega)$ which fails to be Lipschitz under bi-Lipschitz mapping Φ.

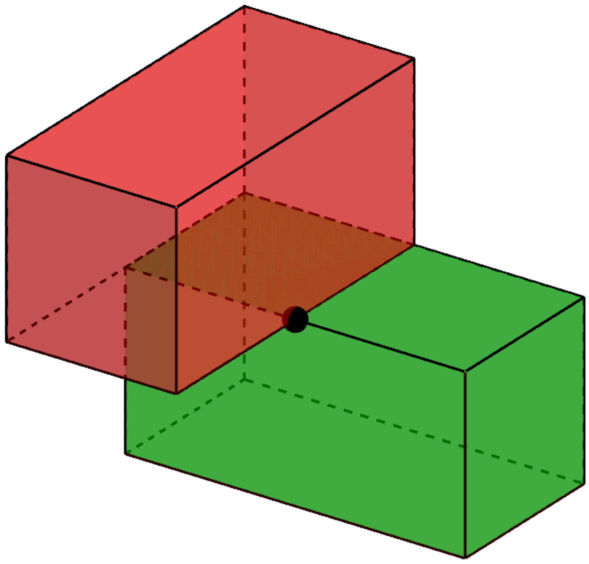


Figure 2.4: Polyhedral 3D so-called two-brick domain that is not represented by the graph of a Lipschitz function in a boundary of the marked point.

phisms, known as perturbation of identity:

$$\Phi_\theta := \mathrm{Id} + \theta, \quad \theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d),$$

to map Lipschitz domain onto a Lipschitz domain. The following result can be found in [11]:

Theorem 2.1.6. *Let ω be a bounded Lipschitz domain. There exists $c(\omega)$, $0 < c(\omega) < 1$, such that $\Phi_\theta(\omega)$ is a bounded Lipschitz domain for all $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, satisfying $\|\phi\|_{\mathrm{W}^{1,\infty}} \leq c(\omega)$.*

Proof of Theorem 2.1.6. First we prove a technical Lemma:

Lemma 2.1.7. *Assume that $\delta, L > 0$ are given. Then there exists $l > 0$ and $L_0, \delta_0 > 0$ such that for any $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ so that $\|\theta\|_{\mathrm{W}^{1,\infty}} \leq l$ and $\theta(0) = 0$ the following holds:*

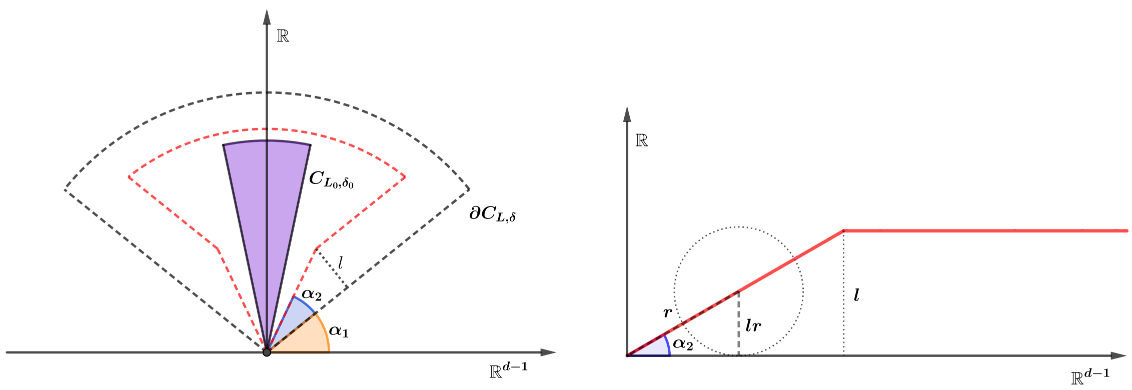
$$C_{L_0,\delta_0} \subset \Phi_\theta(C_{L,\delta}).$$

Proof. Fix $l \in \langle 0, 1\rangle$. Let $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ be such that $\|\theta\|_{\mathrm{W}^{1,\infty}} \leq l$ and $\theta(0) = 0$. Since $\theta(0) = 0$ we can conclude for any x that

$$|\theta(x)| = |\theta(x) - \theta(0)| \leq l|x|.$$

On the other side $|\theta(x)| \leq l$ since $\|\theta\|_{\mathrm{L}^\infty} < l$. Therefore for any $x \in \mathbb{R}^d$

$$|\theta(x)| \leq \min\{l|x|, l\}.$$



(a) Construction of C_{L_0,δ_0}.

(b) Construction of α_2.

Figure 2.5

Observe that every point x above the red line in Figure 2.5b will then satisfy $\Phi_\theta(x)_d = x_d + \theta(x)_d > 0$. This gives us angle $\alpha_2 = \arcsin(l)$. If we define $\alpha_1 = \arctan(L)$ then we can choose $\delta_0 \in \langle 0, \delta - l\rangle$ and $L_0 \in \langle \tan(\alpha_1 + \alpha_2), \infty\rangle$ such that the cone C_{L_0,δ_0} remains inside the red border in Figure 2.5a. One can easily check that everything inside the red border in Figure 2.5a has image under $\mathrm{Id} + \theta$ inside the cone $C_{\delta,L}$, thus proving the lemma. $\square$

Now we continue with the proof of theorem. For a fixed constant $c > 0$ we take an arbitrary $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ such that $\|\theta\|_{\mathrm{W}^{1,\infty}} \leq c$. Let ζ be in $\Phi_\theta(\partial\omega)$ and $\xi \in \Phi_\theta(\omega) \cap K(\zeta, \delta_0)$ for some $\delta_0 > 0$. Then there exists $x \in \omega$ and $z \in \partial\omega$ such that

$$\xi = x + \theta(x), \quad \zeta = z + \theta(z).$$

The goal is to prove that there exists $L_0 > 0$ such that

$$\xi + \mathcal{R}(C_{L_0,\delta_0}) \subset \Phi_\theta(\omega)$$

for some fixed rotation operator $\mathcal{R} = \mathcal{R}_\zeta$.

Let us take $\delta, L > 0$ as in definition of a for Lipschitz domain ω. The next step is to define a map ψ for a fixed $x \in \omega$:

$$\psi(y) = \theta(y + x) - \theta(x)$$

which clearly satisfies $\psi(x) = 0$ and $\|\psi\|_{W^{1,\infty}} \leq 2\|\theta\|_{W^{1,\infty}} \leq 2c$ (observe that the norm of ψ is independent of x). Obviously, c needs to be small enough so that there exists δ_2, L_2 from Lemma 2.1.7, applied for the Lipschitz mapping ψ.

For $z \in \partial\omega$ by Lemma 2.1.7 and Definition 2.1.3 there exists $\mathcal{R}$ such that for $x \in \omega \cap B(z, \delta)$:

$$x + \mathcal{R}(C_{L,\delta}) \subset \omega.$$

By using Lemma 2.1.7 we know that

$$\mathcal{R}(C_{L_2,\delta_2}) \subset \Phi_\psi(\mathcal{R}(C_{L,\delta})).$$

Therefore, for an arbitrary that for $\eta \in \mathcal{R}(C_{L_2,\delta_2})$ there exists $y \in \mathcal{R}(C_{L,\delta})$ such that

$$\eta = y + \psi(y) = y + \theta(y + x) - \theta(x).$$

By adding $\xi = x + \theta(x)$ we get

$$\xi + \eta = x + y + \theta(x + y)$$

which is in $\Phi_\theta(\omega)$ since $x + y \in \omega$. To conclude the proof, one only needs to show that $|x - z| < \delta$ (obviously, $x \in \omega$). We have

$$\delta_0 > |\xi - \zeta| = |x - z + \theta(x) - \theta(z)| \geq |x - z|(1 - c)$$

meaning $|x - z| < \frac{\delta_0}{1-c}$. By setting

$$\delta_0 = \min\{\delta_2, \delta(1 - c)\}, \quad L_0 = L_2,$$

we have proved that for any $\zeta \in \partial\omega$ there exists $\mathcal{R}$ such that for $\xi \in \Phi_\theta(\omega) \cap K(\zeta, \delta_0)$ we have

$$\xi + \mathcal{R}(C_{L_0,\delta_0}) \subset \Phi_\theta(\omega).$$

Since δ_0 and L_0 are independent of the choice ζ we have proved the statement of Theorem 2.1.6. $\square$

Remark 2.1.8. *If Φ_θ is a C^1-diffeomorphism from $\mathbb{R}^d$ onto $\mathbb{R}^d$ and ω a Lipschitz domain then the image $\Phi_\theta(\omega)$ is again a Lipschitz domain. Proof of that fact can become rather tedious, but intuitively one can show that the boundary $\partial\Phi_\theta(\omega) = \Phi_\theta(\partial\omega)$ will remain locally a Lipschitz graph since a composition of Lipschitz and C^1 maps is again a Lipschitz map.*

Another approach as presented in [32], characterize Lipschitz domain as those domains of locally finite perimeter for which there exist continuous vector fields that are transverse to the boundary and satisfies $\partial\omega = \partial\overline{\omega}$. For details see Theorem 4.1. in [32] which offers the proof that C^1-diffeomorphism maps a Lipschitz domain onto a Lipschitz domain.

2.1.2 Shape differentiation

General shape optimization problem is usually written as problem of minimization:

$$\min_{\omega\in\mathcal{O}} J(\omega), \tag{2.3}$$

where $\mathcal{O}$ is a class of Lipschitz domains which are subsets of some fixed, bounded "universe" set $D \subset \mathbb{R}^d$ and $J : \mathcal{O} \to \mathbb{R}$ is so called "shape functional". Unfortunately, $\mathcal{O}$ in general does not admit any "natural" topology.

Ideally, we would like to use Fréchet differentiability in classical sense. For that we need a structure of normed vector space, therefore we shall restrict ourselves to a special family of maps. Remember, we want to determine how does the shape functional behaves with respect to "small" changes of the domain $\omega \in \mathcal{O}$. A rather convenient way to represent small movements (perturbations) of domains is by a family of homeomorphisms on $\mathbb{R}^d$.

There are two standard ways for construction of such families of homeomorphisms:

- The *perturbation of identity method* constructs homemorphisms explicitly:

  $$\Phi_\theta(x) = x + \theta(x), \quad (\Phi = \mathrm{Id} + \theta).$$

  where θ belongs to $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, $k \in \mathbb{N}$ and $\|\theta\|_{\mathrm{W}^{k,\infty}}$ is chosen small enough so that the mapping Φ_θ is bijective.
  Sometimes, for simplicity, one can introduce real parameter t and denote homeomorphism with

  $$\Phi_{t\theta} = \mathrm{Id} + t\theta$$

  for fixed θ.

- The *velocity method* constructs a family of homeomorphism $(T(t,\cdot))_t$ implicitly using initial value problems for every $x \in \mathbb{R}^d$:

$$\partial_t T(t,x) = \theta(T(t,x)),$$
$$T(0,x) = x.$$

where θ belongs to $\mathrm{W}^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, $k \in \mathbb{N}$.

For details about first approach, which goes back to Hadamard, one can look in standard references of Murat and Simon [44] or [30]. For the second approach we refer to the well developed theory of velocity method in [21]. Henceforth, we will use homeomorphisms constructed by perturbations of identity.

One can easily see that the map $\mathcal{J} : \theta \mapsto J(\Phi_\theta(\omega))$ is well defined in a zero-neighborhood of space $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$. Therefore, we can talk about Fréchet differential in zero, i.e. existence of a continuous, linear functional $\mathcal{J}'(0) \in (\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d))'$ such that

$$J(\Phi_\theta(\omega)) - J(\omega) = \mathcal{J}(\theta) - \mathcal{J}(0) = \mathcal{J}'(0)[\theta] + o(\|\theta\|_{\mathrm{W}^{k,\infty}}).$$

Often, Fréchet differential of the functional $\mathcal{J}$ is calculated through the means of directional derivative meaning that the calculations are done with respect to a real parameter for some fixed direction $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$. If such directional derivative exists it is usually called *shape derivative*:

Definition 2.1.9 (Shape derivative)**.** *Let $J = J(\omega)$ be a shape functional and $k \in \mathbb{N}$. J is said to be shape differentiable at $\omega \in \mathcal{O}$ in direction $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ if*

$$J'(\omega; \theta) := \lim_{t \searrow 0} \frac{J(\Phi_{t\theta}(\omega)) - J(\omega)}{t}$$

exists and the mapping $\theta \mapsto J'(\omega, \theta)$ is linear and continuous.
$J'(\omega, \theta)$ is called the shape derivative of the functional J at ω in direction θ.

In most cases we shall also prove Fréchet differentiability of the shape functional in zero:

Definition 2.1.10. *Let $J = J(\omega)$ be a shape functional and $k \in \mathbb{N}$. J is said to be shape differentiable at $\omega \in \mathcal{O}$ if the map*

$$\mathcal{J} : \theta \mapsto J(\Phi_\theta(\omega))$$

is Fréchet differentiable at zero from $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ to $\mathbb{R}$. We denote $J'(\omega; \theta) = \mathcal{J}'(0)[\theta]$.

Remark 2.1.11. *The Definition 2.1.9 implies that the map $\mathcal{J}$ is Gateaux differentiable and its Gateaux derivative is linear or continuous, which is, in general not sufficient for*

Fréchet differentiability. On the other hand Fréchet differentiability of $\mathcal{J}$ implies Gateaux differentiability:

$$\mathcal{J}'(0)[\theta] = J'(\omega;\theta),\ \forall\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d),$$

thus the notation in Definition 2.1.10 is justified. In literature, directional derivative in sense of the Definiton 2.1.9 is also called Eulerian semi-derivative.

Let us start with so called "free PDE" shape functional

$$G(\omega) = \int_\omega f(x)\,\mathrm{d}x$$

where $f \in \mathrm{W}^{1,1}(\mathbb{R}^d)$. This type of functional is among the easiest one to consider. The following results can easily be checked (see [44],[30]):

Proposition 2.1.12. *Let $\omega \subset \mathbb{R}^d$ be a measurable bounded open set and $f \in \mathrm{W}^{1,1}_{loc}(\mathbb{R}^d)$. The functional $G(\omega) = \int_\omega f(x)\,\mathrm{d}x$ is shape differentiable and*

$$G'(\omega;\theta) = \int_\omega \mathrm{div}(f\theta)\,\mathrm{d}x, \quad \forall\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d).$$

If ω has a Lipschitz boundary, the shape derivative can be rewritten as:

$$G'(\omega;\theta) = \int_{\partial\omega} f\theta\cdot\boldsymbol{n}\,\mathrm{d}S, \quad \forall\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$$

where $\boldsymbol{n}$ is outer normal of the set ω.

As a special case, we have found the shape derivative of the volume:

Example 2.1.13 (Shape derivative of the volume)**.** *Let us consider the shape functional* $\mathrm{vol}(\omega) = \int_\omega \mathrm{d}x$. *This functional is shape differentiable at any bounded, measurable set ω: for any $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ we have the volume (distributed) representation of the shape derivative*

$$\mathrm{vol}'(\omega;\theta) = \int_\omega \mathrm{div}(\theta)\,\mathrm{d}x.$$

Note that the shape derivative can be expressed in the boundary representation if ω is a Lipschitz domain:

$$\mathrm{vol}'(\omega;\theta) = \int_{\partial\omega} \theta\cdot\boldsymbol{n}\,\mathrm{d}S.$$

We also state some technical results which will be used throughout this chapter:

Lemma 2.1.14. *Let $\omega \subset \mathbb{R}^d$ be an open set and $f \in \mathrm{W}^{m,p}(\omega)$, for $p \in [1,\infty\rangle$ where $m \in \mathbb{N}_0$ and $k \in N$. The following holds:*

1. *The mapping $p : \theta \mapsto |\det(I + \nabla\theta)| \in \mathrm{W}^{k-1,\infty}(\mathbb{R}^d;\mathbb{R})$ is continuously Fréchet differentiable at a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. Its directional derivative at zero*

is given by:

$$p'(0)[\theta] = \operatorname{div}(\theta), \quad \theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d).$$

2. *The mapping* $M : \theta \mapsto \nabla\Phi_\theta^{-1} = (I + \nabla\theta)^{-1} \in \mathrm{W}^{k-1,\infty}(\mathbb{R}^d; M_d(\mathbb{R}))$ *is continuously Fréchet differentiable at a zero-neighbourhood of* $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$*, with the directional derivative at zero is given by:*

$$M'(0)[\theta] = -\theta, \quad \theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d).$$

3. *The mapping* $r : \theta \mapsto f \circ (\mathrm{Id} + \theta) \in \mathrm{W}^{m-1,p}(\omega)$ *is continuously Fréchet differentiable at a zero-neighbourhood of* $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \cap \mathcal{C}_c(\omega;\mathbb{R}^d)$ *for* $k \geq \max\{1, m-1\}$ *and* $m \geq 1$*. Its directional derivative at zero is given with:*

$$r'(0)[\theta] = \nabla f \cdot \theta, \quad \theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d).$$

Moreover, the previous statement holds for $p = \infty$ *if we take* $f \in C^m(\omega)$*.*

Proof. The first two result are direct consequences of the general results which holds for space of matrices $M_d(\mathbb{R})$. For a regular matrix $A \in M_d(\mathbb{R})$ one can show:

$$\det(A + hB) - \det(A) = \det(A)\operatorname{tr}(A^{-1}B) + o(\|B\|).$$

Since

$$\theta \mapsto \nabla\theta : \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \to \mathrm{W}^{k-1,\infty}(\mathbb{R}^d; M_d(\mathbb{R}))$$

is linear and bounded, by composition we can see that $\theta \mapsto \det(\mathbf{I}+\nabla\theta) = |\det(\mathbf{I}+\nabla\theta)|$ is also continuously differentiable at the zero-neighbourhood with directional derivative

$$p'(\psi)[\theta] = \det(\mathbf{I}+\nabla\psi)\operatorname{tr}((\mathbf{I}+\nabla\psi)^{-1}\nabla\theta)$$

giving us $p'(0)[\theta] = \operatorname{div}(\theta)$. In the same way a map

$$m : A \mapsto (\mathbf{I}-A)^{-1} : M_d(\mathbb{R}) \to M_d(\mathbb{R})$$

is differentiable in the unit circle. Indeed, one can show that

$$m(A + B) - m(A) = m'(A)[B] + o(\|B\|)$$

where

$$m'(A)[B] = \sum_{k=1}^{+\infty}\sum_{l=0}^{k-1} A^l B A^{k-1-l}.$$

Again by composition we can obtain result that M is continuously Fréchet differentiable in the neighbourhood of zero. Furthermore, directional derivative is given with

$$M'(\psi)[\theta] = \sum_{k=1}^{\infty}\sum_{l=0}^{k-1}(-1)^k \nabla\psi^l \nabla\theta \nabla\psi^{k-1-l},$$

therefore, $M'(0)[\theta] = -\nabla\theta$. Proof of third result is rather technical and we omit it. One can adapt the proof of Lemma 5.2.6 for ω instead of $\mathbb{R}^d$ in [30] or Proposition 2.7 in [44]. $\square$

Using the previous Lemma we can easily prove:

Corollary 2.1.15. *Let $\omega \subset \mathbb{R}^d$ be an open set and $f \in \mathrm{H}^1(\omega)$, $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \cap \mathcal{C}_c(\omega;\mathbb{R}^d)$ for $k \in \mathbb{N}$. Then the following holds:*

1. *The map $\theta \mapsto p(\theta) f \circ \Phi_\theta \in \mathrm{L}^2(\omega)$ is well defined in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \cap \mathcal{C}_c(\omega;\mathbb{R}^d)$ and Fréchet differentiable at zero and*

$$p(\theta) f \circ \Phi_\theta - f = \mathrm{div}(\theta) f + \nabla f \cdot \theta + o(\|\theta\|_{\mathrm{W}^{k,\infty}}). \tag{2.4}$$

2. *The map $P : \theta \mapsto p(\theta)\nabla\Phi_\theta^{-\tau}\nabla\Phi_\theta^{-1} \in \mathrm{W}^{k-1,\infty}(\mathbb{R})$ is well defined in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \cap \mathcal{C}_c(\omega;\mathbb{R}^d)$ and Fréchet differentiable at zero and*

$$P(\theta) - P(0) = \mathrm{div}(\psi) I - \nabla\psi - \nabla\psi^t + o(\|\theta\|_{\mathrm{W}^{k,\infty}}). \tag{2.5}$$

2.1.3 Transmission model

In optimal design problem (2.1) we denote with $\Omega_\alpha, \Omega_\beta \subset \Omega$, sets occupied by two phases α and β, respectively. We assume that Ω_α and Ω_β are open sets with well defined continuous boundary, which is essential for the shape optimization. For that reason we will assume that the interface

$$\Gamma = \partial\Omega_\alpha \cap \partial\Omega_\beta$$

is at least Lipschitz regular, meaning that Ω_α is a Lipschitz domain. Notice that Ω_α is a Lipschitz domain if and only if Ω_β is a Lipschitz domains. Furthermore, we shall assume that Γ is compactly enclosed inside Ω. This is more for the mathematical convenience of avoiding detailed assumptions for possible regions where the interface can touch outer boundary $\partial\Omega$ and to ensure that both Ω_α and Ω_β are Lipschitz domains (see Figure 2.6).

Therefore, the following holds

$$\Omega = \Omega_\alpha \cup \Omega_\beta \cup \Gamma, \quad \Gamma \cap \partial\Omega = \emptyset.$$

The previous assumptions on the interface are summarized:

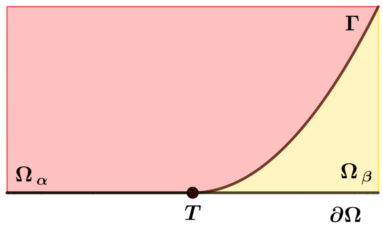


Figure 2.6: Locally around point $T(0,0)$ is given Ω_β between two curves: $x \mapsto x^2$ and $x \mapsto 0$ meaning that Ω_β fails to be a Lipschitz domain at point T.

Assumption 2.1.16. $\Omega \subset \mathbb{R}^d$ *is fixed, open set with smooth boundary. The phases are represented by a pair of open sets* $(\Omega_\alpha, \Omega_\beta)$ *where* Ω_α *is a Lipschitz domain and the interface* $\Gamma := \partial\Omega_\alpha \cap \partial\Omega_\beta$ *belongs to* Ω.

We say that $u \in \mathrm{H}^1_0(\Omega)$ is a weak solution of (2.2) if it is a solution to variational problem:

$$\begin{cases} \text{find } u \in \mathrm{H}^1_0(\Omega) \text{ such that} \\ (\forall \varphi \in \mathrm{H}^1_0(\Omega)) \quad \alpha \int\limits_{\Omega_\alpha} \nabla u \cdot \nabla \varphi \,\mathrm{d}x + \beta \int\limits_{\Omega_\beta} \nabla u \cdot \nabla \varphi \,\mathrm{d}x = \int\limits_{\Omega} f \varphi \,\mathrm{d}x \end{cases} \tag{2.6}$$

Due to Lax-Milgram weak solution of (2.6) exists and is unique.

If Assumption 2.1.16 is valid then the state solution of (2.2) satisfies something that is a solution of a *transmission problem*. Let us denote by $u_\alpha = u_{|\Omega_\alpha}, u_\beta = u_{|\Omega_\beta}$ restrictions of the solution u to the Ω_α, Ω_β respectively. For the moment let us assume that everything is regular enough for the following calculus:

$$\int\limits_{\Omega} f\varphi \,\mathrm{d}x = \int\limits_{\Omega_\alpha} \alpha \nabla u_\alpha \nabla \varphi \,\mathrm{d}x + \int\limits_{\Omega_\beta} \beta \nabla u_\beta \nabla \varphi$$

$$\int\limits_{\Omega} f\varphi \,\mathrm{d}x = \int\limits_{\Omega_\alpha} \mathrm{div}(\alpha \nabla u_\alpha \varphi) - \mathrm{div}(\alpha \nabla u_\alpha)\varphi \,\mathrm{d}x + \int\limits_{\Omega_\beta} \mathrm{div}(\beta \nabla u_\beta \varphi) - \mathrm{div}(\beta \nabla u_\beta)\varphi \,\mathrm{d}x$$

$$\int\limits_{\Omega} f\varphi \,\mathrm{d}x = \int\limits_{\partial\Omega_\alpha} \alpha \nabla u_\alpha \cdot \boldsymbol{n}_\alpha \varphi \,\mathrm{d}S + \int\limits_{\partial\Omega_\beta} \beta \nabla u_\beta \cdot \boldsymbol{n}_\beta \varphi \,\mathrm{d}S + \int\limits_{\Omega} -\mathrm{div}(\mathbf{a}\nabla u)\varphi \,\mathrm{d}x$$

where $\boldsymbol{n}_\alpha, \boldsymbol{n}_\beta$ are outer normals for $\Omega_\alpha, \Omega_\beta$, respectively. We can conclude by taking φ with support $\operatorname{supp}\varphi \subset\subset \Omega_\alpha \cup \Omega_\beta$ that

$$-\mathrm{div}(\mathbf{a}\nabla u) = f \text{ in } \Omega_\alpha \cup \Omega_\beta.$$

From there due to $\varphi \in \mathrm{H}_0^1(\Omega)$ we conclude:

$$\int_\Gamma (\alpha \nabla u_\alpha \cdot \boldsymbol{n}_\alpha + \beta \nabla u_\beta \cdot \boldsymbol{n}_\beta)\varphi \,\mathrm{d}S = 0.$$

Whenever u is continuous restriction of a function on a Lipschitz interface Γ is well defined and equalities $u_{|\Gamma} = u_{\alpha|\Gamma} = u_{\beta|\Gamma}$ hold. Therefore, we have obtained the following transmission conditions:

$$\begin{cases} u_\alpha = u_\beta & \text{on } \Gamma, \\ \alpha \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} + \beta \frac{\partial u_\beta}{\partial \boldsymbol{n}_\beta} = 0 & \text{on } \Gamma. \end{cases} \tag{2.7}$$

This conditions are sometimes called perfect transmission conditions: continuity of the state function and the flux on the interface is a standard hypothesis in the theory of materials and fluid dynamics.

To summarize, we have shown that the restrictions u_α and u_β of the weak solution u of (2.6) solve the following transmission system:

$$\begin{cases} -\alpha \Delta u_\alpha = f, & \text{in } \Omega_\alpha \\ u_\alpha = 0, & \text{on } \partial\Omega \cap \partial\Omega_\alpha \\ -\beta \Delta u_\beta = f, & \text{in } \Omega_\beta \\ u_\beta = 0, & \text{on } \partial\Omega \cap \partial\Omega_\beta \\ u_\alpha = u_\beta & \text{on } \Gamma \\ \alpha \nabla u_\alpha \cdot \boldsymbol{n}_\alpha = \beta \nabla u_\beta \cdot \boldsymbol{n}_\alpha & \text{on } \Gamma \end{cases} \tag{2.8}$$

Remark 2.1.17. *Conversely,* (2.8) *implies* (2.2)*. It is important to note that if u_α and u_β are solutions to* (2.8) *then the following holds:*

$$\int_{\Omega_\alpha} \alpha \nabla u_\alpha \nabla \varphi \,\mathrm{d}x + \int_{\Omega_\beta} \beta \nabla u_\beta \nabla \varphi \,\mathrm{d}x = \int_\Omega f\varphi \,\mathrm{d}x,$$

where we have used that fluxes are continuous. In order to show that a function $u := u_\alpha \chi_{\Omega_\alpha} + u_\beta \chi_{\omega_\beta}$ is a solution to (2.6) *we only have to prove it belongs to $\mathrm{H}_0^1(\Omega)$. Using the trace theory we know that there exists extension $w \in \mathrm{H}_0^1(\Omega)$ such that $w_{|\Gamma} = u_{\alpha|\Gamma} = u_{\beta|\Gamma}$. From w we can define two functions:*

$$w_1 = \begin{cases} w - u_\alpha, & \textit{in } \Omega_\alpha \\ 0, & \textit{in } \Omega_\beta \end{cases},$$

$$w_2 = \begin{cases} 0, & \textit{in } \Omega_\alpha \\ w - u_\beta, & \textit{in } \Omega_\beta \end{cases}.$$

Since $w - u_\alpha \in \mathrm{H}_0^1(\Omega_\alpha)$ *we have that* w_1 *is an extension by zero of* $w - u_\alpha$ *belonging to* $\mathrm{H}_0^1(\Omega)$. *Analogously,* $w_2 \in \mathrm{H}_0^1(\Omega)$. *Therefore,* $u = w - w_1 - w_2 \in \mathrm{H}_0^1(\Omega)$ *thus proving the converse.*

Remark 2.1.18. *The previous formal calculations can be rigorously written using the standard trace theory. Let* $\mathcal{T}_{H^1(\omega)} : \mathrm{H}^1(\omega) \to \mathrm{H}^{1/2}(\partial\omega)$ *be the trace operator for open and bounded* ω *with Lipschitz boundary. Then the previous continuity condition on state function reads as:*

$$\mathcal{T}_{H^1(\Omega_\alpha)} u_\alpha = \mathcal{T}_{H^1(\Omega_\beta)} u_\beta \quad \text{in } \mathrm{H}^{1/2}(\Gamma).$$

To define the trace of the flux we need the graph space

$$\mathrm{L}^2_{\mathrm{div}}(\omega) = \left\{ w \in \mathrm{L}^2(\omega; \mathbb{R}^d) \ : \ \operatorname{div} w \in \mathrm{L}^2(\omega) \right\}$$

endowed with the following norm:

$$\|u\|_{\mathrm{L}^2_{\mathrm{div}}(\omega)} = \|u\|_{\mathrm{L}^2(\omega)} + \|\operatorname{div} u\|_{\mathrm{L}^2(\omega)}.$$

(for details see [52],[13]). Let w *be a smooth vector field, and* φ *a smooth scalar function on* Ω. *Using partial integration and divergence theorem the following holds:*

$$\int_\omega (w \cdot \nabla\varphi + \varphi \operatorname{div} w)\, \mathrm{d}x = \int_\omega \operatorname{div}(\varphi w)\, \mathrm{d}x = \int_{\partial\omega} \varphi w \cdot \boldsymbol{n}\, \mathrm{d}S = \int_{\partial\omega} \boldsymbol{n} \cdot \mathcal{T}_{\mathrm{H}^1} w \mathcal{T}_{\mathrm{H}^1} \varphi\, \mathrm{d}S$$

This motivates us to define a normal trace operator $\mathcal{T}_{\mathrm{div}}$ *for a vector valued* $w \in \mathrm{H}^1(\omega; \mathbb{R}^d)$ *by its action on a test function* $\varphi \in \mathrm{H}^{1/2}(\partial\omega)$*:*

$$\langle \mathcal{T}_{\mathrm{div}} w, \varphi \rangle := \int_{\partial\omega} \boldsymbol{n} \cdot \mathcal{T}_{\mathrm{H}^1} w \mathcal{T}_{\mathrm{H}^1} \varphi\, \mathrm{d}S \le c \|\varphi\|_{\mathrm{H}^{1/2}(\partial\omega)}$$

Using the fact that $\mathrm{H}^1(\omega; \mathbb{R}^d)$ *is dense in* $\mathrm{L}^2_{\mathrm{div}}(\omega)$ *(since test functions are dense in* $\mathrm{L}^2_{\mathrm{div}}(\omega)$*) we can define a bounded linear operator* $\mathcal{T}_{\mathrm{div}} : \mathrm{L}^2_{\mathrm{div}}(\omega) \to \mathrm{H}^{-1/2}(\partial\omega)$.

Since $\mathbf{a}\nabla u \in \mathrm{L}^2(\Omega)$ *and* $-\operatorname{div}(\mathbf{a}\nabla u) = f \in \mathrm{L}^2(\Omega)$ *we conclude that* $\mathbf{a}\nabla u \in \mathrm{L}^2_{\mathrm{div}}(\Omega)$. *Particularly, the second continuity condition in* (2.7) *could then be understood as:*

$$\mathcal{T}_{\mathrm{div},\Omega_\alpha}(\alpha \nabla u_\alpha) = -\mathcal{T}_{\mathrm{div},\Omega_\beta}(\beta \nabla u_\beta) \quad \text{in } \mathrm{H}^{-1/2}(\Gamma).$$

Notice that minus in the previous equality comes from the fact that normals $\boldsymbol{n}_\alpha$ *and* $\boldsymbol{n}_\beta$ *have opposite orientation.*

We can now state our optimal design problem with additional assumptions on the interface:

$$
\text{(2.9)} \qquad \begin{cases} \text{find partition } (\Omega_\alpha, \Omega_\beta) \text{ such that } J(\Omega_\alpha, \Omega_\beta) = \displaystyle\int_\Omega f u \, \mathrm{d}x \text{ is maximized} \\ \text{where } u \text{ is weak solution of (2.6)}, \mathrm{vol}(\Omega_\alpha) = q_\alpha, \\ \text{and partition } (\Omega_\alpha, \Omega_\beta) \text{ satisfies Assumption 2.1.16} \end{cases}
$$

Observe that (2.9) admits solution due to Theorem 1.3.5 when $f = 1$ and domain Ω being an annulus.

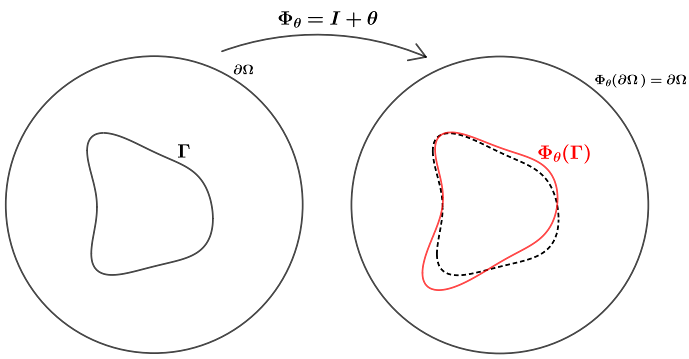


Figure 2.7: Changes to the interface Γ

Usually, in shape optimization, a shape functional is expressed in the following form:

$$
J(\omega) = \int_\omega F(x, u(x), \nabla u(x)) \, \mathrm{d}x
$$

where u is a solution to some boundary value problem defined on the domain ω. Optimal design problem (2.9) is different in that regard because we are not interested in movement of the outer boundary $\partial\Omega$ but only of the interface Γ (see Figure 2.7). For that reason when denoting shape functional for problem (2.9) we will a use shorter notation for the shape functional

$$
J(\Omega_\alpha) := J(\Omega_\alpha, \Omega_\beta) = \int_\Omega f u(\Omega_\alpha) \, \mathrm{d}x,
$$

where $u(\Omega_\alpha)$ is a solution of (2.6) for given partition $(\Omega_\alpha, \Omega_\beta)$. Observe that Ω_β could also be used since there is no reason to prefer one phase over the other.

A perturbed state $u(\theta) := u(\Phi_\theta(\Omega_\alpha))$ for $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ is defined as a solution (in the weak sense) of a transmission problem (2.8) where Ω_α and Ω_β are replaced by $\Phi_\theta(\Omega_\alpha)$

and $\Phi_\theta(\Omega_\beta)$, respectively:

$$\begin{cases} -\alpha\Delta u_\alpha(\theta) = f & \text{in } \Phi_\theta(\Omega_\alpha), \\ u_\alpha(\theta) = 0 & \text{on } \partial\Omega \cap \partial\Phi_\theta(\Omega_\alpha), \\ -\beta\Delta u_\beta(\theta) = f & \text{in } \Phi_\theta(\Omega_\beta), \\ u_\beta(\theta) = 0 & \text{on } \partial\Omega \cap \partial\Phi_\theta(\Omega_\beta), \\ u_\alpha(\theta) = u_\beta(\theta) & \text{on } \Phi_\theta(\Gamma), \\ \alpha\nabla u_\alpha(\theta)\cdot \boldsymbol{n}_\alpha(\theta) = \beta\nabla u_\beta(\theta)\cdot \boldsymbol{n}_\alpha(\theta) & \text{on } \Phi_\theta(\Gamma), \end{cases} \tag{2.10}$$

where $\boldsymbol{n}_\alpha(\theta), \boldsymbol{n}_\beta(\theta)$ are outer normals of $\Phi_\theta(\Omega_\alpha)$ and $\Phi_\theta(\Omega_\beta)$. $u_\alpha(\theta), u_\beta(\theta)$ are restrictions of $u(\theta)$ on $\Phi_\theta(\Omega_\alpha)$ and $\Phi_\theta(\Omega_\beta)$. Observe that transmission conditions defined in (2.10) make sense only if Γ is regular enough. But $\Phi_\theta(\Omega_\alpha)$ and $\Phi_\theta(\Omega_\beta)$ are not necessarily Lipschitz domain (see Example 2.1.5). Even if Φ_θ is bi-Lipschitz homeomorphism, this may not be satisfied. Generally, this lack of regularity can be solved in two standard ways:

- by choosing perturbation θ to be in $\mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ thus C^1 function, ensuring that Φ_θ is a C^1-diffeomorphism and therefore preserving the class of bounded Lipschitz domains (see Remark 2.1.8),
- by admitting an upper bound for the norm $\|\theta\|_{\mathrm{W}^{1,\infty}} < c(\Omega_\alpha)$, as introduced in Theorem 2.1.6.

The second way, although technically more complex, may be more appropriate especially for the theoretical framework since we are interested in the shape derivatives. The choice that θ belongs to $\mathrm{W}^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)$ is somewhat standard in literature: in variety of examples shape functionals are shape differentiable with $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)$. If a boundary representation of the shape derivatives is required, one only needs to assume higher regularity of domain (see Example 2.1.13). Numerically, the uniform boundedness of vector function θ is also a standard hypothesis.

Taking into the account that $\Phi_\theta(\Omega_\alpha)$ is a Lipschitz domain, the perturbed state $u(\theta)$ satisfies the following following variational problem:

$$\begin{cases} \text{find } u(\theta) \in \mathrm{H}^1_0(\Omega) \text{ such that} \\ \alpha \displaystyle\int_{\Phi_\theta(\Omega_\alpha)} \nabla u(\theta)\cdot\nabla\varphi \,\mathrm{d}x + \beta \int_{\Phi_\theta(\Omega_\beta)} \nabla u(\theta)\cdot\nabla\varphi \,\mathrm{d}x = \int_{\Phi_\theta(\Omega)} f\varphi \,\mathrm{d}x, \quad \varphi \in \mathrm{H}^1_0(\Omega)). \end{cases} \tag{2.11}$$

Note that (2.11) is equivalent to (2.10) by the same arguments used before and in the Remark 2.1.17. Moreover, the following holds

$$u(\theta)_{|\Phi_\theta(\Omega_i)} \circ \Phi_\theta \in \mathrm{H}^1(\Omega_i) \quad \text{for } i = \alpha, \beta.$$

Notice that perturbed state $u(\theta) := u(\Phi_\theta(\Omega_\alpha))$ is defined for any small enough $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. This means that we allow that the outer boundary $\partial\Omega$ changes, meaning that the pair $(\Phi_\theta(\Omega_\alpha), \Phi_\theta(\Omega_\beta))$ will technically fail to satisfy Assumption 2.1.16 since $\Phi_\theta(\Omega)$ is not necessarily Ω. Therefore, notion of the energy functional is expanded for $u(\theta)$ in (2.11) by the following formula:

$$J(\Phi_\theta(\Omega_\alpha)) = J(\Phi_\theta(\Omega_\alpha), \Phi_\theta(\Omega_\beta)) = \int\limits_{\Phi(\Omega)} f u(\theta)\,\mathrm{d}x.$$

From the perspective of shape analysis there is no reason to restrict ourselves to spaces like $\mathrm{W}_0^{k,\infty}(\Omega;\mathbb{R}^d)$ for several reasons. Firstly, we obtain more general results in a simpler notation. Secondly, since $u(\theta)$ belongs to $\mathrm{H}_0^1(\Omega)$ for small enough $\theta \in \mathrm{W}_0^{k,\infty}(\Omega;\mathbb{R}^d)$ one may be inclined to a conjecture that a map $\theta \mapsto u(\theta)$ is Fréchet differentiable at the zero from $\mathrm{W}_0^{k,\infty}(\Omega;\mathbb{R}^d)$ to $\mathrm{H}_0^1(\Omega)$. As we will see by the end of the following section this is not true. On the other hand, one can demonstrate that a map

$$\theta \mapsto u(\theta) \circ \Phi_\theta \in \mathrm{H}_0^1(\Omega)$$

is well defined in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\Omega;\mathbb{R}^d)$ and Fréchet differentiable at the zero.

2.2 First order shape derivative for transmission problem

2.2.1 Material derivative

Let ω be an open subset of $\mathbb{R}^d$. For a small $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, $k \in \mathbb{N}$, a set $\Phi_\theta(\omega)$ is open. Assume that y is a map such that for any θ in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ $y(\theta)$ belongs to $\mathrm{W}^{m,p}(\Phi_\theta(\omega))$, where $m \in \mathbb{N}$ and $p \in [1,\infty\rangle$. Let the map

$$\theta \mapsto y(\theta) \circ \Phi_\theta \in \mathrm{W}^{m,p}(\omega)$$

be Fréchet differentiable at the zero of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. Its directional derivative at zero in direction θ is usually denoted with $\dot{y}(\theta)$ and we shall call it *material derivative* of the map y.

In order to calculate the material derivative of the map $\theta \mapsto u(\theta)$ defined by (2.11) we need the implicit function theorem on Banach spaces. Let us recapitulate this result. The proof can be found in [24].

Theorem 2.2.1 (Implicit Function Theorem)**.** *Suppose that X, Z and W are Banach spaces, $k \geq 1$, $A \subset X \times Z$ is an open set, (x_0, z_0) is a point in A, and $f : A \to W$ is a C^k-map such $f(x_0, y_0) = 0$. Assume that $D_z f(x_0, z_0) := D(f(x_0, \cdot))(z_0) : Z \to W$ is a* *bounded invertible linear operator. Then there is an open neighbourhood U_0 of x_0 in X and a unique continuous function $u : U_0 \to Z$ such that $u(x_0) = z_0$, and $f(x, u(x)) = 0$ for all $x \in U_0$. Moreover u is C^k function and*

$$Du(x) = -D_z f(x, u(x))^{-1} D_x f(x, u(x)), \text{ for all } x \in U.$$

□

Let us also recall a characterization of dual space $\mathrm{H}^{-1}(\Omega)$:

Theorem 2.2.2. *Assume that $f \in \mathrm{H}^{-1}(\Omega)$. Then there exists unique functions $f_0 \in \mathrm{L}^2(\Omega), f_1 \in \mathrm{L}^2(\Omega; \mathbb{R}^d)$ such that for any $\varphi \in \mathrm{H}^1_0(\Omega)$*

$$\langle f, \varphi \rangle_{\mathrm{H}^{-1}(\Omega), \mathrm{H}^1_0(\Omega)} = \int\limits_\Omega f_1 \cdot \nabla\varphi \,\mathrm{d}x + \int\limits_\Omega f_0 \varphi \,\mathrm{d}x.$$

and $\|f\|^2_{H^{-1}} = \|f_0\|^2_{\mathrm{L}^2(\Omega)} + \|f_1\|^2_{\mathrm{L}^2(\Omega)^d}$.

Proof. The proof can be found in [2]. □

The following theorem says that map $\theta \mapsto u(\theta) \circ \Phi_\theta$ is Fréchet differentiable at zero.

Theorem 2.2.3 (Material derivative $\dot{u}(\theta)$)**.** *Let $f \in \mathrm{H}^1(\Omega)$. The mapping*

$$\theta \mapsto u(\theta) \circ \Phi_\theta \in \mathrm{H}^1_0(\Omega)$$

is well defined in a zero-neighbourhood of $\mathrm{W}^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$, where $u(\theta)$ is a solution of (2.11). It is Fréchet differentiable at zero and directional derivative at zero in direction θ, denoted with $\dot{u}(\theta) \in \mathrm{H}^1_0(\Omega)$, satisfies:

$$\text{(2.12)} \quad \begin{cases} (\forall \varphi \in \mathrm{H}^1_0(\Omega)) \displaystyle\int\limits_\Omega \mathbf{a} \nabla \dot{u}(\theta) \cdot \nabla\varphi \,\mathrm{d}x & = \displaystyle\int\limits_\Omega \mathbf{a}(\nabla\theta + \nabla\theta^{\mathcal{T}} - \mathrm{div}(\theta) I) \nabla u \cdot \nabla\varphi \mathrm{d}x \\ & \quad + \displaystyle\int\limits_\Omega \mathrm{div}(f\theta)\varphi \,\mathrm{d}x. \end{cases}$$

Proof.
1. *Defining a function for implicit function theorem.*
We start by transforming (2.11) to the domains Ω_α and Ω_β. First for the left hand-side phase α

$$\begin{aligned} \alpha \int\limits_{\Phi_\theta(\Omega_\alpha)} \nabla u(\theta) \cdot \nabla\varphi \,\mathrm{d}x &= \alpha \int\limits_{\Omega_\alpha} \nabla u(\theta) \circ \Phi_\theta \cdot \nabla\varphi \circ \Phi_\theta \; p(\theta) \,\mathrm{d}x \\ &= \alpha \int\limits_{\Omega_\alpha} \nabla\Phi_\theta^{-\mathcal{T}} \nabla(u(\theta) \circ \Phi_\theta) \cdot \nabla\Phi_\theta^{-\mathcal{T}} \nabla(\varphi \circ \Phi_\theta) \; p(\theta) \,\mathrm{d}x \end{aligned}$$

$$= \alpha \int\limits_{\Omega_\alpha} P(\theta)\nabla(u(\theta) \circ \Phi_\theta) \cdot \nabla(\varphi \circ \Phi_\theta)\,\mathrm{d}x$$

where

$$p(\theta) = |\det(\nabla\Phi_\theta)|, \quad P(\theta) = p(\theta)\nabla\Phi_\theta^{-1}\nabla\Phi_\theta^{-\mathcal{T}}.$$

The same holds for the phase β:

$$\beta \int\limits_{\Phi_\theta(\Omega_\beta)} \nabla u(\theta) \cdot \nabla\varphi\,\mathrm{d}x = \beta \int\limits_{\Omega_\beta} P(\theta)\nabla(u(\theta) \circ \Phi_\theta) \circ \nabla(\varphi \circ \Phi_\theta)\,\mathrm{d}x.$$

Similarly, by a change of variables in the integral on the right hand-side we have:

$$\int\limits_{\Phi_\theta(\Omega)} f\varphi\,\mathrm{d}x = \int\limits_{\Omega} f \circ \Phi_\theta\ \varphi \circ \Phi_\theta\ p(\theta)\,\mathrm{d}x,$$

giving us

$$\int\limits_{\Omega} \mathbf{a}P(\theta)\nabla(u(\theta) \circ \Phi_\theta) \circ \nabla(\varphi \circ \Phi_\theta)\,\mathrm{d}x = \int\limits_{\Omega} f \circ \Phi_\theta\ \varphi \circ \Phi_\theta\ p(\theta)\,\mathrm{d}x$$

Taking $\varphi \circ \Phi_\theta^{-1}$ instead of φ we get (2.11) written as a variational problem on the original domain Ω:

$$\int\limits_{\Omega} \mathbf{a}P(\theta)\nabla(u(\theta) \circ \Phi_\theta) \cdot \nabla\varphi\,\mathrm{d}x = \int\limits_{\Omega} p(\theta) f \circ \Phi_\theta\ \varphi\,\mathrm{d}x \quad \forall\varphi \in \mathrm{H}_0^1(\Omega). \tag{2.13}$$

Choose $\delta < c(\Omega_\alpha)$ for $c(\Omega_\alpha)$ introduced in Theorem 2.1.6 such that $p(\theta)$ and $P(\theta)$ are Fréchet differentiable in $K(0;\delta) \subset \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. Now we can define a map $F : K(0;\delta) \times \mathrm{H}_0^1(\Omega) \to \mathrm{H}^{-1}(\Omega)$:

$$\langle F(\theta, z), \varphi\rangle_{\mathrm{H}^{-1}(\Omega),\mathrm{H}_0^1(\Omega)} = \int\limits_{\Omega} \mathbf{a}P(\theta)\nabla z \cdot \nabla\varphi\,\mathrm{d}x - \int\limits_{\Omega} p(\theta) f \circ \Phi_\theta\ \varphi\,\mathrm{d}x.$$

From (2.9) it follows $F(\theta, u(\theta) \circ \Phi_\theta) = 0$.

2. *Application of the implicit function theorem:*

From Lemma 2.1.14 we can conclude that the maps:

$$\theta \mapsto \mathbf{a}P(\theta)\nabla z \in \mathrm{L}^2(\Omega;\mathbb{R}^d),$$

for any $z \in \mathrm{H}_0^1(\Omega)$ and

$$\theta \mapsto -p(\theta) f \circ \Phi_\theta \in \mathrm{L}^2(\Omega)$$

are well defined and Fréchet differentiable in a zero-neighbourhood of $\mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$.

Moreover, By Theorem 2.2.2 we conclude that $\theta \mapsto F(\theta, z)$ is Fréchet differentiable on a zero-neighbourhood of $\mathrm{W}^{1,\infty}(\Omega;\mathbb{R}^d)$ to $\mathrm{H}^{-1}(\Omega)$ and

$$\text{(2.14)} \qquad \begin{cases} \langle D_\theta F(0,u)[\theta], \varphi\rangle_{\mathrm{H}^{-1}(\Omega),\mathrm{H}^1_0(\Omega)} = \displaystyle\int_\Omega \mathbf{a}(-\nabla\theta - \nabla\theta^{\mathcal{T}} + \operatorname{div}\theta I)\nabla u \cdot \nabla\varphi \,\mathrm{d}x \\ \qquad\qquad - \displaystyle\int_\Omega \varphi f \operatorname{div}(\theta) + \varphi \nabla f \cdot \theta \,\mathrm{d}x. \end{cases}$$

For fixed θ in a zero-neighbourhood of $\mathrm{W}^{1,\infty}(\Omega;\mathbb{R}^d)$ the map $z \mapsto F(\theta, z)$ is continuous and affine from $\mathrm{H}^1_0(\Omega)$ to $\mathrm{H}^{-1}(\Omega)$, thus continuously differentiable at every point of $\mathrm{H}^1_0(\Omega)$ and

$$\langle D_z F(0,u)[h], \varphi\rangle_{\mathrm{H}^{-1}(\Omega),\mathrm{H}^1_0(\Omega)} = \int_\Omega \mathbf{a}\nabla h \cdot \nabla\varphi \,\mathrm{d}x.$$

Using the Poincaré inequality and the Lax-Milgram lemma we can conclude that the differential

$$D_z F(0,u) : \mathrm{H}^1_0(\Omega) \to \mathrm{H}^{-1}(\Omega)$$

is an isomorphism. By 2.2.1 this implies that there exists an open zero-neighbourhood of $\mathrm{W}^{1,\infty}(\Omega;\mathbb{R}^d)$ such that the function

$$\theta \mapsto u(\theta) \circ \Phi_\theta$$

is Fréchet differentiable.

3. *Proof of* (2.12): Using Theorem 2.2.1 we obtain that

$$\dot{u}(\theta) = -D_z F(0,u)^{-1} D_\theta F(0,u)[\theta]$$

or equivalently,

$$D_z F(0,u)[\dot{u}(\theta)] = -D_\theta F(0,u)[\theta] \quad \text{ in } \mathrm{H}^{-1}(\Omega).$$

Applying the last functional to a test function $\varphi \in \mathrm{H}^1_0(\Omega)$ we obtain on the left-hand side:

$$\langle D_z F(0,u)[\dot{u}(\theta)], \varphi\rangle_{\mathrm{H}^{-1}(\Omega),\mathrm{H}^1_0(\Omega)} = \int_\Omega \mathbf{a}\nabla\dot{u}(\theta) \cdot \nabla\varphi \,\mathrm{d}x,$$

and from (2.14) the right hand side thus proving the statement. □

Remark 2.2.4. *Previous approach based on the Implicit Function Theorem is rather standard in literature. See proof of Lemma 4.8 in [19] or Theorem 5.7.4 in [30] where material derivative is calculated in a similar manner but with different functional spaces and underlying problems. See also [17] for a two-phase eigenvalue problem.*

Remark 2.2.5. *The assumption that f belongs to $\mathrm{H}^1(\Omega)$ cannot be dropped. This is due to the fact that the map $\theta \mapsto f \circ \Phi_\theta : \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d) \to \mathrm{H}^{-1}(\Omega)$ fails to be differentiable even* *when* $f \in \mathrm{L}^2(\Omega)$*. Indeed, let* $\Omega = [-1,1]$ *and* $\Phi_t = \mathrm{Id} + t\theta$ *where* $\theta \in C_c^1(\Omega) \subset \mathrm{W}^{1,\infty}(\Omega)$ *such that* $\theta(0) = 1$*. If we define* $f \in \mathrm{L}^2(\Omega)$ *in the following manner*

$$f(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0, \end{cases}$$

then one can check that for any $\varphi \in \mathrm{H}_0^1(\Omega)$ *and* $t > 0$ *small enough following holds:*

$$\frac{1}{t}\int_{-1}^{1} (f \circ \Phi_t - f)\varphi \,\mathrm{d}x = \frac{1}{t}\int_{-t}^{0} \varphi(x)\,\mathrm{d}x.$$

Let us define a sequence of functions $(\varphi_n)_{n\in\mathbb{N}} \subset \mathrm{H}_0^1(\Omega)$*:*

$$\varphi_n(x) = \begin{cases} \frac{1}{n} + \frac{nx}{2}, & x \in \left[-\frac{-2}{n^2}, -\frac{1}{n^2}\right] \\ -\frac{nx}{2}, & x \in \left[-\frac{1}{n^2}, 0\right] \\ 0, & \textit{elsewhere.} \end{cases}$$

The sequence is bounded in $\mathrm{H}_0^1(\Omega)$ *since*

$$\|\varphi\|_{\mathrm{H}_0^1(\Omega)} = \int_{-1}^{1} |\varphi_n'(x)|^2, \mathrm{d}x = 2\int_{0}^{1/n^2} \frac{n^2}{4}\,\mathrm{d}x = \frac{1}{2}$$

On the other hand for $t = 1/n$ *we can see*

$$\frac{1}{t}\int_{-t}^{0} \varphi_n(x)\,\mathrm{d}x = n\int_{-1/n}^{0} \frac{-nx}{2}\,\mathrm{d}x = \frac{1}{2}.$$

thus

$$\frac{1}{t}\|f \circ \Phi_t - f\|_{\mathrm{H}^{-1}(\Omega)} = \sup_{\varphi \in \mathrm{H}_0^1(\Omega):\|\varphi\|_{\mathrm{H}_0^1} \leq 1} \left|\frac{1}{t}\int_{-1}^{1} (f \circ \Phi_t - f)\varphi\,\mathrm{d}x\right| \geq \frac{1}{2},$$

proving the statement. The previous counter-example can be found in the remark after Proposition 2.39 in [46].

2.2.2 Basic concepts in differential geometry

In the following sections we will need to use some results in differential geometry. Here we shall offer a short overview of well-known results which can be found in [30]. Henceforth, we shall assume Φ to be a C^1-diffeomorphism from $\mathbb{R}^n$ into itself and ω to be a bounded set with C^1 boundary denoted with $\partial\omega$.

Remark 2.2.6. *By Definition 2.1.1 there exists* $\delta, L > 0$ *such that for every* $z \in \partial\omega$ *one* *can found a local orthonormal system of coordinates $x = (x', x_d)$, a rotation operator $\mathcal{R}$, $\delta_z \in \langle 0, \delta\rangle$ and a C^1 map $\varphi : B(0;\delta_z) \subset \mathbb{R}^{d-1} \to \langle -L\delta_z, L\delta_z\rangle$ such that*

$$z + \mathcal{R}(\{(x', \varphi(x')) \,:\, |x'| < \delta_z\}) \subset \partial\omega.$$

Moreover, with

$$\psi_z(x) = \psi_z(x', x_d) = z + \mathcal{R}(x', \varphi(x') - x_d)$$

we can define a C^1-diffeomorphism from an open neighbourhood

$$\mathcal{O}_z = \{(x', x_d) : |x'| < \delta_z, |x_d| < L\delta_z\}$$

onto a $\psi_z(\mathcal{O}_z)$. Observe that

$$\{\psi_z(\mathcal{O}_z) : z \in \partial\omega\}$$

is an open covering of $\partial\omega$, which due to its compactness can be represented by a finite number of C^1-diffeomorphisms ψ_i, $i = 1, 2, ..., k$. Now we can define a non-negative partition of unity $\xi_i \in C_0^\infty(\psi_i(\mathcal{O}_i))$ such that $\sum_{i=1}^k \xi_i = 1$ on a neighbourhood of $\partial\omega$. Then any function $G \in C(\partial\omega; \mathbb{R}^q)$, $q \geq 1$ can be extended to the whole space $\mathbb{R}^d$ by the formula:

$$\tilde{G}(x) = \sum_{i=1}^{k} \xi_i(x) G \circ \psi_i \circ \pi_i \circ \psi_i^{-1}(x), \tag{2.15}$$

where π_i is the orthogonal projection $\pi_i(x', x_d) = (x', 0)$. This, in particular, allows us to define a continuous extension of the outer unit normal vector $\boldsymbol{n}$ of $\partial\omega$ to the whole $\mathbb{R}^d$.

Every vector field $G \in C(\mathbb{R}^d; \mathbb{R}^d)$ can be divided into two parts: tangential $G_{\partial\omega}$ and normal $(G\cdot\boldsymbol{n})\boldsymbol{n}$ such that $G = G_{\partial\omega} + (G\cdot\boldsymbol{n})\boldsymbol{n}$. We say that a function is of class C^1 on $\partial\omega$ if its extension defined by (2.15) is of class C^1. We denote by $C^1(\partial\omega)$ the corresponding space. Let $g \in C^1(\partial\omega)$. We define its tangential gradient by

$$\nabla_{\partial\omega} g := \nabla\tilde{g} - (\nabla\tilde{g}\cdot\boldsymbol{n})\boldsymbol{n} \quad \text{ on } \partial\omega,$$

where $\tilde{g}$ is an extension of g. We denote by $\mathrm{W}^{1,1}(\partial\omega)$ the closure of $C^1(\partial\omega)$ with respect to the norm

$$\|g\|_{\mathrm{W}^{1,1}(\partial\omega)} := \|g\|_{\mathrm{L}^1(\partial\omega)} + \|\nabla_{\partial\omega} g\|_{\mathrm{L}^1(\partial\omega)}.$$

The tangential divergence of a vector field $G \in C^1(\mathbb{R}^d; \mathbb{R}^d)$ is given by

$$\mathrm{div}_{\partial\omega}(G) := \mathrm{div}\, G - \boldsymbol{n}\cdot\nabla G\boldsymbol{n} \quad \text{ on } \mathbb{R}^d.$$

Now we can define *tangential divergence on $\partial\omega$*. Let $G \in C^1(\Gamma; \mathbb{R}^d)$. We define its tangential divergence by

$$\operatorname{div}_{\partial\omega}(G) = \operatorname{div} \tilde{G} - \nabla \tilde{G}\boldsymbol{n} \cdot \boldsymbol{n} \quad \text{ on } \partial\omega$$

where $\tilde{G} \in C^1(\mathbb{R}^d; \mathbb{R}^d)$ is an extension of G. Again, we can extend this definition to the space $\mathrm{W}^{1,1}(\partial\omega; \mathbb{R}^d)$.

There is another, perhaps more canonical way to define an extension of the outer unit normal $\boldsymbol{n}$. For this we need a distance function:

Definition 2.2.7. *Let ω be a domain with C^1 boundary. We define the signed distance function for the set ω by*

$$d(x) = d_\omega(x) := \begin{cases} \operatorname{dist}(x, \partial\omega) & x \in \mathbb{R}^d \setminus \omega \\ 0 & x \in \partial\omega \\ -\operatorname{dist}(x, \partial\omega) & x \in \omega. \end{cases}$$

If we assume that ω is an open set with at least C^2 boundary then ∇d_ω gives C^1 unitary extension of the outer normal around Γ which can be easily extended to the whole $\mathbb{R}^d$ (see Remark 2.2.6). Furthermore, if Φ is to be a C^1-diffeomorphism from $\mathbb{R}^n$ into itself then we can easily see that the preimage of $\{0\}$ under $d_\omega \circ \Phi^{-1}$ defines a boundary of a set $\Phi(\omega)$. This means that gradient of the $d_\omega \circ \Phi^{-1}$ on the boundary $\partial\Phi(\omega)$ is a multiple of the normal vector of a set $\Phi(\omega)$. The outer unit normal vector of a set $\Phi(\omega)$ is then given by

$$\frac{\nabla(d_\omega \circ \Phi^{-1})}{|\nabla(d_\omega \circ \Phi^{-1})|} = \frac{\nabla\Phi^{-\mathcal{T}}\boldsymbol{n} \circ \Phi^{-1}}{|\nabla\Phi^{-\mathcal{T}}\boldsymbol{n} \circ \Phi^{-1}|}. \tag{2.16}$$

Proposition 2.2.8. *Let ω be of class C^2. Let $N \in C^1(\mathbb{R}^d; \mathbb{R}^d)$ be an extension of the unit normal vector $\boldsymbol{n}$ to the boundary $\partial\omega$. Then with*

$$N(\theta) = \frac{\nabla\Phi_\theta^{-\mathcal{T}} N \circ \Phi_\theta^{-1}}{|\nabla\Phi_\theta^{-\mathcal{T}} N \circ \Phi_\theta^{-1}|}$$

is defined an extension of the normal to the boundary of the set $\Phi_\theta(\omega)$ and $\theta \mapsto N(\theta) \in \mathrm{W}^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ is well defined in a zero neighbourhood of $\mathrm{W}^{2,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ and it is Fréchet differentiable at zero. Its derivative $N'(\theta) := N'(0; \theta)$ is given with

$$N'(\theta) = -\nabla_{\partial\omega}(\theta \cdot \boldsymbol{n}) - (\theta \cdot \boldsymbol{n})\frac{\partial N(0)}{\partial \boldsymbol{n}}, \quad \text{in } \mathrm{L}^\infty(\partial\omega; \mathbb{R}^d).$$

Proof. See Proposition 5.4.14 in [30] or Theorem 4.1 in [44]. □

Henceforth, we shall always assume that our extension $\boldsymbol{n} \in C^1(\mathbb{R}^d; \mathbb{R}^d)$ of the outer unit normal to the $\partial\omega$ is obtained as the gradient of oriented distance function, i.e.

by extending $\nabla d_\omega \in C^1(\partial\omega;\mathbb{R}^d)$ to the whole $\mathbb{R}^d$. Then $\boldsymbol{n}\cdot\boldsymbol{n} = 1$ on Γ, therefore $\nabla\boldsymbol{n}^{\mathcal{T}}\boldsymbol{n} = 0$. Since $\nabla\boldsymbol{n} = \nabla^2 d_\omega$ we can conclude that $\nabla\boldsymbol{n}$ is symmetrical, showing that $0 = \nabla\boldsymbol{n}^{\mathcal{T}}\boldsymbol{n} = \nabla\boldsymbol{n}\,\boldsymbol{n}$ on Γ. Proposition 2.2.8 then states that for the map

$$\theta \mapsto \boldsymbol{n}(\theta) = \frac{\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}\circ\Phi_\theta^{-1}}{|\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}\circ\Phi_\theta^{-1}|}$$

we have

$$\boldsymbol{n}'(\theta) = -\nabla_{\partial\omega}(\theta\cdot\boldsymbol{n}). \tag{2.17}$$

In our calculations of the shape derivatives of the second order a mean curvature of a boundary will naturally appear:

Definition 2.2.9. *For an open set ω with the C^2 boundary we define the mean curvature of $\partial\omega$ by*

$$\mathrm{H} = \operatorname{div}_{\partial\omega}\boldsymbol{n} \text{ on } \partial\omega.$$

Actually, for the mean curvature H a stronger result holds:

Proposition 2.2.10. *Let ω be of class C^2. Then, for any C^1 extension N of outer unit normal $\boldsymbol{n}$, we have*

$$\operatorname{div} N = \mathrm{H} \quad \text{on } \partial\omega \quad \text{in } \mathrm{L}^\infty(\partial\omega;\mathbb{R}^d).$$

Proof. Due to $N\cdot\boldsymbol{n}$ being 1 on $\partial\omega$ we have $\nabla N^{\mathcal{T}}\boldsymbol{n} = 0$ on $\partial\omega$. By definition

$$\mathrm{H} = \operatorname{div}_{\partial\omega}\boldsymbol{n} = \operatorname{div} N - \nabla N\boldsymbol{n}\cdot\boldsymbol{n} = \operatorname{div} N - \boldsymbol{n}\cdot\nabla N^{\mathcal{T}}\boldsymbol{n} = \operatorname{div} N$$

thus obtaining the desired equality. □

We end this part with the notion of *tangential jacobian*. We introduce the tangential Jacobian of Φ on $\partial\omega$, denoted by $\mathrm{Jac}_{\partial\omega}(\Phi)$, as

$$\mathrm{Jac}_{\partial\omega}(\Phi) = |\nabla\Phi^{-\tau}\boldsymbol{n}||\det(\nabla\Phi)|.$$

Theorem 2.2.11 (Change of variables on surface)**.** *Let $f : \Phi(\partial\omega) \to \mathbb{R}$. Then $f \in \mathrm{L}^1(\Phi(\partial\omega))$ if and only if $f\circ\Phi \in \mathrm{L}^1(\partial\omega)$ and*

$$\int_{\Phi(\partial\omega)} f\,\mathrm{d}S = \int_{\partial\omega} f\circ\Phi\,\mathrm{Jac}_{\partial\omega}(\Phi)\,\mathrm{d}S$$

Proof. See Proposition 5.4.3 in [30]. □

2.2.3 Regularity of transmission problem and applications

Consider Sobolev space $\mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta)$ with norm

$$\|u\|^2_{\mathrm{H}^k(\Omega_\alpha\cup\Omega_\beta)} := \|u_{|\Omega_\alpha}\|^2_{\mathrm{H}^k(\Omega_\alpha)} + \|u_{|\Omega_\beta}\|^2_{\mathrm{H}^k(\Omega_\beta)}.$$

While $\mathrm{H}^1(\Omega_\alpha \cup \Omega_\beta) \subset \mathrm{L}^2(\Omega)$ it is not necessarily a subset of $\mathrm{H}^1(\Omega)$, more precisely a function in $\mathrm{H}^1(\Omega_\alpha \cup \Omega_\beta) \subset \mathrm{L}^2(\Omega)$ belongs to $\mathrm{H}^1(\Omega)$ if and only if it satisfies transmission conditions (2.7). The following theorem states that the restrictions of the solution of (2.6) to Ω_α and Ω_β have better regularity when the interface and the right hand-side are smooth enough.

Theorem 2.2.12 (Regularity of transmission problem)**.** *Let the Assumption 2.1.16 be satisfied, $k \in \mathbb{N}_0$ and $w \in \mathrm{H}^1_0(\Omega)$ be a solution of the variational equality:*

$$(\forall \varphi \in \mathrm{H}^1_0(\Omega)) \qquad \int_\Omega \mathbf{a}\nabla w \cdot \nabla\varphi \,\mathrm{d}xe = \int_\Omega f\varphi\,\mathrm{d}x \tag{2.18}$$

If the interface is of class $\mathcal{C}^{k+2}$ and $f \in \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta)$ then $w \in \mathrm{H}^{k+2}(\Omega_\alpha \cup \Omega_\beta)$ with the estimate:

$$\|w\|_{\mathrm{H}^{k+2}(\Omega_\alpha\cup\Omega_\beta)} \le C\left(\|f\|_{\mathrm{H}^k(\Omega_\alpha\cup\Omega_\beta)} + \|w\|_{\mathrm{H}^1(\Omega)}\right).$$

Proof. See Section 5.3 in [18] □

Theorem 2.2.13 (Higher regularity of material derivative $\dot{u}(\theta)$)**.** *Let $k \in \mathbb{N}, k \ge 2$. Assume that the interface between phases is of class $\mathcal{C}^k$ and satisfies Assumption 2.1.16. Let $f \in \mathrm{H}^{\max\{k-2,1\}}(\Omega)$. Then material derivative $\dot{u}(\theta)$ in direction $\theta \in \mathrm{W}^{k+1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ defined by (2.12) belongs to the space $\mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta) \cap \mathrm{H}^1_0(\Omega)$.*

Proof. Let $u(\theta)$ be the solution of (2.11). For small $\theta \in \mathrm{W}^{k+1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, we conclude that the interface between phases $\Phi_\theta(\Omega_\alpha)$ and $\Phi_\theta(\Omega_\beta)$ is of class $\mathcal{C}^k$. Then, using Theorem 2.2.12 we obtain

$$u(\theta) \in \mathrm{H}^k(\Phi_\theta(\Omega_\alpha) \cup \Phi_\theta(\Omega_\beta)) \cap \mathrm{H}^1_0(\Omega).$$

Again as in Theorem 2.2.3 by using change of variables in (2.11) we obtain the following variational equality:

$$\int_\Omega \mathbf{a}P(\theta)\nabla(u(\theta)\circ\Phi_\theta)\cdot\nabla(\varphi\circ\Phi_\theta)\,\mathrm{d}x = \int_\Omega \varphi\circ\Phi_\theta\ f\circ\Phi_\theta\ p(\theta)\,\mathrm{d}x, \quad \varphi \in \mathrm{H}^1_0(\Omega). \tag{2.19}$$

Observe that $u(\theta)\circ\Phi_\theta \in \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta)$. Therefore, we can apply the partial integration rule on the above integral over Ω_α and obtain

$$\alpha \int_{\Omega_\alpha} P(\theta)\nabla(u_\alpha(\theta)\circ\Phi_\theta)\cdot\nabla(\varphi\circ\Phi_\theta)\,\mathrm{d}x = \alpha\int_\Gamma P(\theta)\nabla(u_\alpha(\theta)\circ\Phi_\theta)\cdot\boldsymbol{n}_\alpha\,\varphi\circ\Phi_\theta\,\mathrm{d}S - \alpha\int_{\Omega_\alpha}\mathrm{div}\left(P(\theta)\nabla(u_\alpha(\theta)\circ\Phi_\theta)\right)\varphi\circ\Phi_\theta\,\mathrm{d}x.$$

Then

$$\begin{aligned}\int_\Gamma P(\theta)\nabla(u_\alpha(\theta)\circ\Phi_\theta)\cdot\boldsymbol{n}_\alpha\,\varphi\circ\Phi_\theta\,\mathrm{d}S &= \int_\Gamma \nabla\Phi_\theta^{-\mathcal{T}}\nabla(u_\alpha(\theta)\circ\Phi_\theta)\;\cdot\;\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}_\alpha\;\varphi\circ\Phi_\theta\,p(\theta)\,\mathrm{d}S\\ &= \int_\Gamma \nabla u_\alpha(\theta)\circ\Phi_\theta\cdot\frac{\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}_\alpha}{|\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}_\alpha|}\;\varphi\circ\Phi_\theta\,\mathrm{Jac}_\Gamma(\Phi_\theta)\,\mathrm{d}S.\end{aligned}$$

From (2.16) one can conclude that $\boldsymbol{n}_\alpha(\theta)\circ\Phi_\theta = \frac{\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}_\alpha}{|\nabla\Phi_\theta^{-\mathcal{T}}\boldsymbol{n}_\alpha|}$ and by applying Theorem 2.2.11 we have:

$$\int_\Gamma \nabla u_\alpha(\theta)\circ\Phi_\theta\cdot\boldsymbol{n}_\alpha(\theta)\circ\Phi_\theta\;\varphi\circ\Phi_\theta\mathrm{Jac}_\Gamma(\Phi_\theta)\,\mathrm{d}S = \int_{\Phi_\theta(\Gamma)}\nabla u_\alpha(\theta)\cdot\boldsymbol{n}_\alpha(\theta)\,\varphi\,\mathrm{d}S.$$

Therefore, we have showed that

$$\alpha\int_\Gamma P(\theta)\nabla(u_\alpha(\theta)\circ\Phi_\theta)\cdot\boldsymbol{n}_\alpha\,\varphi\circ\Phi_\theta\,\mathrm{d}S = \alpha\int_{\Phi_\theta(\Gamma)}\nabla u_\alpha(\theta)\cdot\boldsymbol{n}_\alpha(\theta)\,\varphi\,\mathrm{d}S.$$

Analogously, for the domain Ω_β we obtain:

$$\beta\int_\Gamma P(\theta)\nabla(u_\beta(\theta)\circ\Phi_\theta)\cdot\boldsymbol{n}_\beta\,\varphi\circ\Phi_\theta\,\mathrm{d}S = \beta\int_{\Phi_\theta(\Gamma)}\nabla u_\beta(\theta)\cdot\boldsymbol{n}_\beta(\theta)\,\varphi\,\mathrm{d}S,$$

Due to the transmission condition from (2.10):

$$\alpha\int_{\Phi_\theta(\Gamma)}\nabla u_\alpha(\theta)\cdot\boldsymbol{n}_\alpha(\theta)\,\varphi\,\mathrm{d}S + \beta\int_{\Phi_\theta(\Gamma)}\nabla u_\beta(\theta)\cdot\boldsymbol{n}_\beta(\theta)\,\varphi\,\mathrm{d}S = 0,$$

the boundary integrals in the above calculations disappear and the following holds if we replace $\varphi\circ\Phi_\theta$ by φ

$$-\int_\Omega \mathbf{a}\,\mathrm{div}\left(P(\theta)\nabla(u(\theta)\circ\Phi_\theta)\right)\varphi\,\mathrm{d}x = \int_\Omega f\circ\Phi_\theta\;\;p(\theta)\varphi\,\mathrm{d}x,\quad \varphi\in\mathrm{H}^1_0(\Omega). \tag{2.20}$$

Now for a zero-neighbourhood $\mathcal{U}\subset\mathrm{W}^{k+1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\theta\mapsto P(\theta), p(\theta)$ are continuously differentiable, we define a map $F_0 : \mathcal{U} \times \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta) \cap \mathrm{H}^1_0(\Omega) \to \mathrm{H}^{k-2}(\Omega_\alpha \cup \Omega_\beta)$

$$F_0(\theta, z) = -\mathbf{a}\,\mathrm{div}\,(P(\theta)\nabla z) - f \circ \Phi_\theta p(\theta) \tag{2.21}$$

and proceed as in the proof of Theorem 2.2.3. To show that the differential $D_z F(0, u)$: $\mathrm{H}\,\mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta) \cap \mathrm{H}^1_0(\Omega) \to \mathrm{H}^{k-2}(\Omega_\alpha \cup \Omega_\beta)$ is an isomorphism use regularity result from Theorem 2.2.12). Notice that in case of more regular interface, (2.20) is equivalent to (2.13) and therefore F_0 is a restriction of F from Theorem 2.2.3 to the Banach space set $\mathrm{W}^{k+1,\infty}(\mathbb{R}^d; \mathbb{R}^d) \times \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta) \cap \mathrm{H}^1_0(\Omega)$. □

Remark 2.2.14. *The choice for the mapping F_0 used above is not unique. We can use the partial integration rule prior to the change of variables in* (2.11)*:*

$$-\alpha \int\limits_{\Phi_\theta(\Omega_\alpha)} \varphi\,\mathrm{div}(\nabla u(\theta))\,\mathrm{d}x - \beta \int\limits_{\Phi_\theta(\Omega_\beta)} \varphi\,\mathrm{div}(\nabla u(\theta))\,\mathrm{d}x = \int\limits_{\Phi_\theta(\Omega)} f\varphi\,\mathrm{d}x.$$

By using the change of variables we obtain

$$-\alpha \int\limits_{\Omega_\alpha} p(\theta)\varphi\circ\Phi_\theta\,\mathrm{div}(\nabla u(\theta))\circ\Phi_\theta\,\mathrm{d}x - \beta \int\limits_{\Omega_\beta} p(\theta)\varphi\circ\Phi_\theta\,\mathrm{div}(\nabla u(\theta))\circ\Phi_\theta\,\mathrm{d}x = \int\limits_{\Omega} p(\theta)\varphi\circ\Phi_\theta f\circ\Phi_\theta.$$

Putting φ instead of $p(\theta)\varphi \circ \Phi_\theta \in \mathrm{H}^1_0(\Omega)$ in the previous equality we have simplified expression:

$$-\alpha \int\limits_{\Omega_\alpha} \varphi\ \mathrm{div}(\nabla u(\theta)) \circ \Phi_\theta\,\mathrm{d}x - \beta \int\limits_{\Omega_\beta} \varphi\ \mathrm{div}(\nabla u(\theta)) \circ \Phi_\theta\,\mathrm{d}x = \int\limits_{\Omega} \varphi\, f \circ \Phi_\theta.$$

Assuming that the interface and the right hand-side f is regular enough using Theorem 2.2.12 we can conclude that $u(\theta) \in \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta)$ i.e.

$$-\mathbf{a}\Delta u(\theta) \circ \Phi_\theta - f \circ \Phi_\theta = 0 \quad \text{in } \mathrm{H}^{k-2}(\Omega_\alpha \cup \Omega_\beta).$$

The hardest part is to rewrite the previous equality in terms of θ and $u(\theta) \circ \Phi_\theta$ in order to use the implicit function theorem. With some work one can show that

$$\Delta u(\theta) \circ \Phi_\theta = \nabla\Phi_\theta^{-\mathcal{T}} : \nabla(\nabla\Phi_\theta^{-\mathcal{T}}\nabla(u(\theta) \circ \Phi_\theta))$$

where $:$ $M_d(\mathbb{R}) \times M_d(\mathbb{R}) \to \mathbb{R}$ stands for the dot product of matrices. Then one may define $\mathcal{F} : \mathrm{W}^{k+1,\infty}(\Omega; \mathbb{R}^d) \times \mathrm{H}^k(\Omega_\alpha \cup \Omega_\beta) \cap \mathrm{H}^1_0(\Omega) \to \mathrm{H}^{k-2}(\Omega_\alpha \cup \Omega_\beta)$

$$\mathcal{F}(\theta, z) = -\mathbf{a}\nabla\Phi_\theta^{-\mathcal{T}} : \nabla(\nabla\Phi_\theta^{-\mathcal{T}}\nabla z) - f \circ \Phi_\theta.$$

A similar approach may be found in [44].

Remark 2.2.15. *The calculation of variational equality* (2.12) *from the implicit function theorem can be tedious (especially for the functions defined in the previous theorem and remark). On the other hand we can directly obtain it by subtracting* (2.13) *and* (2.6) *and dividing the result by* $t \neq 0$*:*

$$\int_\Omega \mathbf{a}\nabla\varphi \cdot \left[\frac{P_\theta(t)\nabla(u(t\theta)\circ\Phi_{t\theta}) - \nabla u}{t}\right] \mathrm{d}x = \int_\Omega \varphi \left[\frac{p_\theta(t) f\circ\Phi_{t\theta} - f}{t}\right] \mathrm{d}x,$$

where we use the notation $P_\theta(t) = P(t\theta), p_\theta(t) = p(t\theta)$*. Since the following holds:*

$$P_\theta(t)\nabla(u(t\theta)\circ\Phi_{t\theta}) - \nabla u = t\left((-\nabla\theta - \nabla\theta^{\mathcal{T}} + \operatorname{div}(\theta))\nabla u + u'(\theta)\right) + o(t) \quad \textit{in } \mathrm{H}^{k-1}(\Omega_\alpha \cup \Omega_\beta),$$

and

$$p_\theta(t) f\circ\Phi_{t\theta} - f = t(f\operatorname{div}\theta + \theta\cdot\nabla f) + o(t) \qquad \textit{in } \mathrm{L}^2(\Omega)$$

we obtain (2.12) *by taking the limit as* t *goes to zero.*

Let

$$J(\Omega_\alpha) = \int_\Omega f\, u(\Omega_\alpha)\,\mathrm{d}x$$

be the energy functional where u is the unique solution of the boundary value problem (2.6). Using the information on the material derivative $\dot{u}(\theta)$ we can easily calculate the shape derivative $J'(\Omega_\alpha;\theta)$, such that following holds:

$$J(\Phi_\theta(\Omega_\alpha)) = J(\Omega_\alpha) + J'(\Omega_\alpha;\theta) + o(\|\theta\|_{\mathrm{W}^{1,\infty}}).$$

Observe that

$$u(\theta)\circ\Phi_\theta = u + \dot{u}(\theta) + o(\|\theta\|_{\mathrm{W}^{1,\infty}}), \qquad \text{in } \mathrm{H}^1(\Omega),$$

and

$$f\circ\Phi_\theta p(\theta) = f + \nabla f\cdot\theta + f\operatorname{div}(\theta) + o(\|\theta\|_{\mathrm{W}^{1,\infty}}), \qquad \text{in } \mathrm{L}^2(\Omega).$$

Furthermore, by using the Leibnitz product rule we can conclude that

$$\begin{aligned} J(\Phi_\theta(\Omega_\alpha)) &= \int_{\Phi_\theta(\Omega)} f u(\theta)\,\mathrm{d}x = \int_\Omega f\circ\Phi_\theta u(\theta)\circ\Phi_\theta\, p(\theta)\,\mathrm{d}x \\ &= \int_\Omega fu + f\dot{u}(\theta) + (\nabla f\cdot\theta + f\operatorname{div}(\theta))u\,\mathrm{d}x + o(\|\theta\|_{\mathrm{W}^{1,\infty}}) \\ &= J(\Omega) + \int_\Omega f\dot{u}(\theta) + (\nabla f\cdot\theta + f\operatorname{div}(\theta))u\,\mathrm{d}x + o(\|\theta\|_{\mathrm{W}^{1,\infty}}) \end{aligned}$$

Since $\dot{u}(\theta) \in \mathrm{H}_0^1(\Omega)$, by (2.11) and (2.12):

$$\int_\Omega f\dot{u}(\theta)\,\mathrm{d}x = \int_\Omega \mathbf{a}\nabla u \cdot \nabla \dot{u}(\theta)\,\mathrm{d}x$$
$$= \int_\Omega \mathbf{a}(\nabla\theta + \nabla\theta^\tau - \operatorname{div}(\theta)I)\nabla u \cdot \nabla u + \operatorname{div}(f\theta)u\,\mathrm{d}x.$$

Therefore,

$$J'(\Omega_\alpha;\theta) = \int_\Omega \mathbf{a}(\nabla\theta + \nabla\theta^\tau - \operatorname{div}(\theta)I)\nabla u \cdot \nabla u + 2\operatorname{div}(f\theta)u\,\mathrm{d}x.$$

With this we have proved the first part of the following theorem:

Theorem 2.2.16 (First derivative of the energy functional)**.** *Let the pair* $(\Omega_\alpha, \Omega_\beta)$ *satisfies Assumption 2.1.16,* $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *and the right hand side* $f \in \mathrm{H}^1(\Omega)$*. Then,*

1. *The shape functional*
$$\theta \mapsto \int_{\Phi_\theta(\Omega)} f u(\theta)\,\mathrm{d}x$$
is well defined in a zero-neighbourhood in $\mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *and Fréchet differentiable at zero. Directional derivative at zero in the direction* θ *is given with*
$$J'(\Omega_\alpha;\theta) = \int_\Omega \mathbf{a}(\nabla\theta + \nabla\theta^\tau - \operatorname{div}(\theta)I)\nabla u \cdot \nabla u + 2\operatorname{div}(f\theta)u\,\mathrm{d}x, \tag{2.22}$$
where u *is a solution of* (2.6)*.*

2. *Whenever the interface* Γ *is of* C^2 *the shape derivative of the energy functional in the boundary form for any* $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *such that* $\operatorname{supp}\theta \subset\subset \Omega$ *is given with:*
$$J'(\Omega_\alpha;\theta) = \int_\Gamma \theta\cdot\boldsymbol{n}_\alpha\Big[2\Big\{\alpha\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - \beta\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2\Big\} - \big\{\alpha|\nabla u_\alpha|^2 - \beta|\nabla u_\beta|^2\big\}\Big]\,\mathrm{d}S. \tag{2.23}$$

Proof. Let us prove the second part. By Theorem 2.2.12 $u_\alpha \in \mathrm{H}^2(\Omega_\alpha)$ and $u_\beta \in \mathrm{H}^2(\Omega_\beta)$ We divide shape derivative (2.22) into two terms $J'(\Omega_\alpha,\theta) = I_\alpha + I_\beta$ where

$$I_\alpha = \int_{\Omega_\alpha} 2\alpha(\nabla\theta\nabla u_\alpha)\cdot\nabla u_\alpha\,\mathrm{d}x + \int_{\Omega_\alpha} 2u_\alpha\operatorname{div}\theta f + 2u_\alpha\nabla f\cdot\theta - \alpha\operatorname{div}\theta|\nabla u_\alpha|^2\,\mathrm{d}x$$

and

$$I_\beta = \int_{\Omega_\beta} 2\beta(\nabla\theta\nabla u_\beta)\cdot\nabla u_\beta \,\mathrm{d}x + \int_{\Omega_\beta} 2u_\beta \operatorname{div}\theta f + 2u_\beta\nabla f\cdot\theta - \beta\operatorname{div}\theta|\nabla u_\beta|^2 \,\mathrm{d}x.$$

Integrating by parts we obtain:

$$\begin{aligned}\int_{\Omega_\alpha} 2u_\alpha \operatorname{div}\theta f + 2u_\alpha\nabla f\cdot\theta - \alpha\operatorname{div}\theta|\nabla u_\alpha|^2 \,\mathrm{d}x &= \int_{\Omega_\alpha} \operatorname{div}\left[\theta\left(2fu_\alpha - \alpha|\nabla u_\alpha|^2\right)\right]\,\mathrm{d}x \\ &+ \int_{\Omega_\alpha} -2f\theta\cdot\nabla u_\alpha + \alpha\theta\cdot\nabla|\nabla u_\alpha|^2\,\mathrm{d}x \\ &= \int_{\Gamma} \theta\cdot\boldsymbol{n}_\alpha\left(2fu_\alpha - \alpha|\nabla u_\alpha|^2\right)\,\mathrm{d}S \\ &+ \int_{\Omega_\alpha} -2f\theta\cdot\nabla u_\alpha + \alpha\theta\cdot\nabla|\nabla u_\alpha|^2\,\mathrm{d}x.\end{aligned}$$

Using the fact that

$$2\nabla u_\alpha\cdot\nabla(\theta\cdot\nabla u_\alpha) = 2(\nabla\theta\nabla u_\alpha)\cdot\nabla u_\alpha + \theta\cdot\nabla|\nabla u_\alpha|^2$$

we can conclude that

$$I_\alpha = \int_{\Omega_\alpha} 2\alpha\nabla u_\alpha\cdot\nabla(\theta\cdot\nabla u_\alpha) - 2f(\theta\cdot\nabla u_\alpha)\,\mathrm{d}x + \int_{\Gamma}\theta\cdot\boldsymbol{n}_\alpha\left(2fu_\alpha - \alpha|\nabla u_\alpha|^2\right)\,\mathrm{d}S.$$

Analogously, we get

$$I_\beta = \int_{\Omega_\alpha} 2\beta\nabla u_\beta\cdot\nabla(\theta\cdot\nabla u_\beta) - 2f(\theta\cdot\nabla u_\beta)\,\mathrm{d}x + \int_{\Gamma}\theta\cdot\boldsymbol{n}_\beta\left(2fu_\beta - \beta|\nabla u_\beta|^2\right)\,\mathrm{d}S.$$

Observe that

$$\begin{aligned}\int_{\Omega_\alpha} 2\alpha\nabla u\cdot\nabla(\theta\cdot\nabla u_\alpha)\,\mathrm{d}x &= \int_{\Omega_\alpha} 2\operatorname{div}[\alpha\nabla u_\alpha(\theta\cdot\nabla u_\alpha)]\,\mathrm{d}x - \int_{\Omega_\alpha} 2\operatorname{div}(\alpha\nabla u_\alpha)(\theta\cdot\nabla u_\alpha)\,\mathrm{d}x \\ &= \int_{\Gamma} 2\alpha\nabla u_\alpha\cdot\boldsymbol{n}_\alpha(\theta\cdot\nabla u_\alpha)\,\mathrm{d}S + \int_{\Omega_\alpha} 2f(\theta\cdot\nabla u_\alpha)\,\mathrm{d}x.\end{aligned}$$

The same can be done for domain Ω_β, therefore,

$$J'(\Omega_\alpha,\theta) = I_\alpha + I_\beta = 2\int_{\Gamma}\alpha\nabla u_\alpha\cdot n_\alpha(\theta\cdot\nabla u_\alpha) + \beta\nabla u_\beta\cdot n_\beta(\theta\cdot\nabla u_\beta)\,\mathrm{d}S$$

$$+\int_{\Gamma} \theta \cdot \boldsymbol{n}_\alpha \left(2fu_\alpha - 2fu_\beta - \alpha|\nabla u_\alpha|^2 + \beta|\nabla u_\beta|^2\right) \,\mathrm{d}S$$

$fu \in \mathrm{H}_0^1(\Omega)$, thus $fu_{\alpha|\Gamma} = fu_{\beta|\Gamma}$ meaning that this terms disappears. Using continuation of the fluxes on Γ and continuation of the tangential derivative:

$$\begin{aligned} \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha = \beta\nabla u_\beta \cdot \boldsymbol{n}_\alpha, &\quad \text{in } \mathrm{H}^{1/2}(\Gamma) \\ \nabla_\Gamma u_\alpha = \nabla_\Gamma u_\beta, &\quad \text{in } \mathrm{H}^{1/2}(\Gamma) \end{aligned}$$

we can conclude that

$$\nabla u_\alpha - \nabla u_\beta = \nabla_\Gamma u_\alpha + (\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)\boldsymbol{n}_\alpha - \nabla_\Gamma u_\beta - (\nabla u_\beta \cdot \boldsymbol{n}_\alpha)\boldsymbol{n}_\alpha = (\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)\boldsymbol{n}_\alpha - (\nabla u_\beta \cdot \boldsymbol{n}_\alpha)\boldsymbol{n}_\alpha$$

and multiplying with $\theta = \theta_\Gamma + \theta \cdot \boldsymbol{n}_\alpha \boldsymbol{n}_\alpha$ we get

$$\theta \cdot (\nabla u_\alpha - \nabla u_\beta) = (\theta \cdot \boldsymbol{n}_\alpha)((\nabla u_\alpha - \nabla u_\beta) \cdot \boldsymbol{n}_\alpha).$$

The following identity holds:

$$\begin{aligned} (\theta \cdot \nabla u_\alpha)\alpha\nabla u_\alpha \cdot n_\alpha + (\theta \cdot \nabla u_\beta)\beta\nabla u_\beta \cdot n_\beta &= \theta \cdot (\nabla u_\alpha - \cdot\nabla u_\beta)\alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha \\ &= (\theta \cdot \boldsymbol{n}_\alpha)\left[\alpha(\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)^2 - \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha \nabla u_\beta \cdot \boldsymbol{n}_\alpha\right] \\ &= (\theta \cdot \boldsymbol{n}_\alpha)\left[\alpha(\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)^2 - \beta(\nabla u_\beta \cdot \boldsymbol{n}_\alpha)^2\right] \end{aligned}$$

thus proving the theorem. □

2.2.4 Direct calculations of a shape derivative without a material derivative

We shall provide an alternative way of calculating shape derivative (2.22). We recommend consulting [50] for details, where the same method was applied even for the non-linear PDE problems. In essence, the following Lagrange methods starts by construction of a Lagrange functional. This Lagrange functional is a priori unknown but it generally consists of shape functional coupled with a linear penalization of the state equation (we have both state and adjoint functions). The need for such approach arises naturally in shape optimization where a computation of Fréchet derivatives often become technical and complex. In general, one important benefit of such approach is avoidance of material derivative in calculations. We can observe that the material derivative does not appear in the final expression of (2.22), so there is a possibility to calculate it without employing the material derivative. However, one should be cautious when using this approach and rigorous in justification of all calculations since it is well known that usage of wrong functional could lead to erroneous result.

For a given set Ω_α occupied by the first phase we denote the Lagrange functional by the following formula:

$$\text{(L)} \qquad \mathcal{L}(\Omega_\alpha, u, v) = \int_\Omega fu - \left(\alpha \int_{\Omega_\alpha} \nabla u \cdot \nabla v + \beta \int_{\Omega_\beta} \nabla u \cdot \nabla v - \int_\Omega fv \right),$$

where the first term is the energy functional and the second term comes from (2.6).

Henceforth we shall assume that $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ is fixed. For simpler notation we will be using

$$\begin{aligned} \Phi_t &= \mathrm{Id} + t\theta, \\ p(t) &= p(t\theta) = \det(\nabla \Phi_t), \\ P(t) &= P(t\theta) = p(t) \nabla \Phi_t^{-1} \nabla \Phi_t^{-\mathcal{T}}. \end{aligned}$$

$$\begin{aligned} \mathcal{L}(\Phi_t(\Omega_\alpha), u, v) &= \int_{\Phi_t(\Omega)} fu - \left(\alpha \int_{\Phi_t(\Omega_\alpha)} \nabla u \cdot \nabla v + \beta \int_{\Phi_t(\Omega_\beta)} \nabla u \cdot \nabla v - \int_{\Phi_t(\Omega)} fv \right) \\ &= \int_\Omega p(t) f \circ \Phi_t \, u \circ \Phi_t \, \mathrm{d}x - \alpha \int_{\Omega_\alpha} P(t)(\nabla u \circ \Phi_t) \cdot (\nabla v \circ \Phi_t) \, \mathrm{d}x \\ &\quad - \beta \int_{\Omega_\beta} P(t)(\nabla u \circ \Phi_t) \cdot (\nabla v \circ \Phi_t) \, \mathrm{d}x + \int_\Omega p(t) f \circ \Phi_t \, v \circ \Phi_t \, \mathrm{d}x \\ &= \int_\Omega p(t) f \circ \Phi_t \, u \circ \Phi_t \, \mathrm{d}x - \int_\Omega \mathbf{a} P(t)(\nabla u \circ \Phi_t) \cdot \nabla v \, \mathrm{d}x \\ &\quad + \int_\Omega p(t) f \circ \Phi_t \, v \circ \Phi_t \, \mathrm{d}x. \end{aligned}$$

From the above it can be seen that homeomorphism Φ_t actually introduces non-linearity in Lagrange functional $\mathcal{L}$ if written from the perspective of fixed Ω_α. With this in mind we introduce a new functional $G : [0, \tau] \times \mathrm{H}_0^1(\Omega) \times \mathrm{H}_0^1(\Omega) \to \mathbb{R}$:

$$G(t, u, v) = \mathcal{L}(\Phi_t(\Omega_\alpha), u \circ \Phi_t^{-1}, v \circ \Phi_t^{-1})$$

which simplifies to

$$G(t, u, v) = \int_\Omega p(t) f \circ \Phi_t u \, \mathrm{d}x - \int_\Omega \mathbf{a} P(t) \nabla u \cdot \nabla v \, \mathrm{d}x + \int_\Omega p(t) f \circ \Phi_t v \, \mathrm{d}x.$$

Observe that G is linear in both u and v. Let $u(t) \in \mathrm{H}_0^1(\Omega)$ represents a solution of the boundary value problem:

$$\begin{cases} -\operatorname{div}(\mathbf{a}\circ\Phi_t\nabla u(t)) = f, & \text{in } \Omega_t \\ u(t) = 0 & \text{on } \partial\Omega_t \end{cases} \tag{2.24}$$

Notice that $u(t) = u(t\theta)$, where $u(t\theta)$ is the perturbed state introduced in (2.11). Let us define $u^t := u(t)\circ\Phi_t$. One can easily verify that

$$J(\Phi_t(\Omega_\alpha)) = G(t, u^t, v), \quad v \in H_0^1(\Omega).$$

Let $u^0 = u(0)$ represents the solutions of (2.24) for $t = 0$. The following result may be proved in much the same way as it was done in [35]. We should note that the following method is used to show existence and to calculate the shape derivative $J'(\Omega_\alpha;\theta)$ in the sense of the Definition 2.1.9. For Fréchet differentiability see Theorem 2.2.16.

Theorem 2.2.17. *Let a pair $(\Omega_\alpha, \Omega_\beta)$ satisfies Assumption 2.1.16 and $\theta \in \mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. For $f \in \mathrm{H}^1(\Omega)$ the shape derivative (in the sense of the Definition 2.1.9) of the energy functional $J(\Omega_\alpha) = \int_\Omega f u \,\mathrm{d}x$ exists and*

$$J'(\Omega_\alpha;\theta) = \int\limits_\Omega \mathbf{a}(\nabla\theta + \nabla\theta^{\mathcal{T}} - \operatorname{div}(\theta)I)\nabla u\cdot\nabla u + 2\operatorname{div}(f\theta)u\,\mathrm{d}x.$$

Proof. Let us define a family $(v^t) \subset \mathrm{H}_0^1(\Omega)$ for $t \in \langle 0, \delta\rangle$

$$\begin{cases} \text{find } v^t \in \mathrm{H}_0^1(\Omega) \text{ such that} \\ \int\limits_\Omega \mathbf{a}P(t)\nabla v^t\nabla\varphi\,\mathrm{d}x = \int\limits_\Omega p(t) f\circ\Phi_t\varphi\,\mathrm{d}x, \end{cases} \tag{2.25}$$

where $\delta > 0$ is such that (2.25) has a unique solution v^t, i.e. the left hand side in the equation is coercive. One can conclude

$$\begin{aligned} J(\Phi_t(\Omega_\alpha)) - J(\Omega_\alpha) &= G(t, u^t, v^t) - G(0, u^0, v^t) \\ &= G(t, u^t, v^t) - G(t, u^0, v^t) + G(t, u^0, v^t) - G(0, u^0, v^t) \\ &= G(t, u^0, v^t) - G(0, u^0, v^t) \end{aligned}$$

where (2.25) is used:

$$G(t, u^t, v^t) - G(t, u^0, v^t) = \int\limits_\Omega p(t) f\circ\Phi_t(u^t - u^0)\,\mathrm{d}x - \int\limits_\Omega P(t)\mathbf{a}\nabla(u^t - u^0)\cdot\nabla v^t\,\mathrm{d}x = 0.$$

The following technical result is needed for the final conclusion:

Lemma 2.2.18. *The function v^t defined with (2.25) converges to u^0 in $\mathrm{H}_0^1(\Omega)$ as t decreases to zero. Moreover, there exists $c > 0$ such that $\|v^t - u\|_{\mathrm{H}^1} \leq ct$, as $t \to 0^+$.*

Proof. We shall prove lemma in several steps:

1. *(v^t) is bounded in* $\mathrm{H}_0^1(\Omega)$.

   Since mapping $t \mapsto P(t)$ is continuous there exists $\delta > 0$ such that for any $t \in \langle 0, \delta\rangle$ we have $\|P(t) - I\|_{\mathrm{L}^\infty} < \alpha/2$. By using the Poincaré inequality

$$\frac{\alpha}{2}\|\nabla v^t\|_{\mathrm{L}^2}^2 \leq \int\limits_\Omega P(t)\mathbf{a}\nabla v^t \cdot \nabla v^t \,\mathrm{d}x = \int\limits_\Omega p(t) f \circ \Phi_t \, v^t \mathrm{d}x \leq \|p(t) f \circ \Phi_t\|_{\mathrm{L}^2}\|v^t\|_{\mathrm{L}^2},$$

   we can conclude that for all $t \in \langle 0, \delta\rangle$ a family is bounded: $\|v^t\|_{\mathrm{H}_0^1} \leq C$.

2. *v^t converges weakly to u^0, in* $\mathrm{H}^1(\Omega)$.

   Due to v^t being bounded for $t \in \langle 0, \delta\rangle$ for any sequence t_n tending to zero one can find a subsequence, again denoted with (t_n) such that $v^{t_n} \rightharpoonup \overline{u} \in \mathrm{H}_0^1(\Omega)$. From (2.25) for any $\varphi \in \mathrm{H}_0^1(\Omega)$:

$$\int\limits_\Omega P(t)\mathbf{a}\nabla v^{t_n} \cdot \nabla\varphi \,\mathrm{d}x \;\to\; \int\limits_\Omega \mathbf{a}\nabla\overline{u} \cdot \nabla\varphi \mathrm{d}x$$

   and due to continuity of the map $t \mapsto p(t) f \circ \Phi_t$ we have

$$\int\limits_\Omega p(t) f \circ \Phi_t \varphi \,\mathrm{d}x \to \int\limits_\Omega f\varphi \,\mathrm{d}x,$$

   thus showing that $\overline{u}$ satisfies variational equality:

$$\int\limits_\Omega \mathbf{a}\nabla\overline{u} \cdot \nabla\varphi \mathrm{d}x = \int\limits_\Omega f\varphi \,\mathrm{d}x, \quad \forall\varphi \in \mathrm{H}_0^1(\Omega),$$

   and therefore $\overline{u} = u^0$. Due to the uniqueness of the accumulation point, we have $v^t \rightharpoonup u^0$ as $t \to 0^+$.

3. *v^t converges strongly to u^0 in* $\mathrm{H}^1(\Omega)$.

   One can show

$$\int\limits_\Omega P(t)\mathbf{a}\nabla(v^t - u^0) \cdot \nabla w \,\mathrm{d}x = \int\limits_\Omega p(t) f \circ \Phi_t \, w \,\mathrm{d}x - \int\limits_\Omega \mathbf{a}P(t)\nabla u^0 \cdot \nabla w \,\mathrm{d}x + \int\limits_\Omega \mathbf{a}\nabla u^0 \cdot \nabla w \,\mathrm{d}x - \int\limits_\Omega f w \,\mathrm{d}x$$

$$= \int_\Omega w\left(p(t) f \circ \Phi_t - f\right) \mathrm{d}x - \int_\Omega \mathbf{a}\left(I - P(t)\right) \nabla u^0 \cdot \nabla w \,\mathrm{d}x$$

Taking $w = v^t - u^0$ and using Lemma 2.1.14 and Corollary 2.1.15 we obtain

$$\begin{aligned}\frac{\alpha}{2}\|\nabla v^t - \nabla u\|_{\mathrm{L}^2}^2 &\leq C_1 t\|v^t - u\|_{\mathrm{L}^2} + \alpha C_2 t\|\nabla u\|_{\mathrm{L}^2}\|\nabla v^t - \nabla u\|_{\mathrm{L}^2}\\ &\leq Ct\end{aligned}$$

since $\|v^t\|$ is bounded in $\mathrm{H}^1(\Omega)$.

□

Thanks to Proposition 2.2.18 and Corollary 2.1.15 we can easily verify the following steps:

$$\begin{aligned}&\lim_{t\to 0^+} \frac{J(\Phi_t(\Omega_\alpha)) - J(\Omega_\alpha)}{t} = \lim_{t\to 0^+} \frac{1}{t}\left[G(t, u, v^t) - G(0, u, v^t)\right]\\ &= \lim_{t\to 0^+}\left[\int_\Omega \frac{j(t) f\circ\Phi_t - f}{t} u \,\mathrm{d}x + \int_\Omega \frac{j(t) f\circ\Phi_t - f}{t} v^t \,\mathrm{d}x\right.\\ &\quad\left. - \int_\Omega \mathbf{a}\frac{J(t) - I}{t}\nabla u \nabla v^t \,\mathrm{d}x\right]\\ &= \int_\Omega \left[\operatorname{div}(\theta) f + \nabla f \theta\right] 2u \,\mathrm{d}x - \int_\Omega \mathbf{a}(\operatorname{div}(\theta) I - \nabla\theta - \nabla\theta^\tau)\nabla u \nabla u \,\mathrm{d}x\end{aligned}$$

which finishes the proof. □

Remark 2.2.19. *In the previous theorem the adjoint state is equal to the original state. This simplifies the calculation significantly, since there is no additional analysis of the adjoint state. We will use this approach to the full extent in a calculation of the second order shape derivative in the following chapter. In essence, we shall define a family of adjoint states (v_t) with the following property:*

$$G(t, u^t, v^t) - G(t, u^0, v^t) = 0. \tag{2.26}$$

The previous equation could be satisfied in several different ways. First we will require that the the map $s \mapsto G(t, su^t + (1-s)u^0, v)$ is absolutely continuous for every $v \in \mathrm{H}_0^1(\Omega)$, therefore

$$G(t, u^t, v) - G(t, u^0, v) = \int_0^1 D_u G(t, su^t + (1-s)u^0, v)\,\mathrm{d}s.$$

Then we can replace (2.26) *with the following:*

$$\int_0^t D_u G(t, (1-s)u^0 + su^t, v^t)\,\mathrm{d}s = 0. \tag{2.27}$$

For more complex problems existence and uniqueness of v^t such that (2.27) *holds may be false. In our case* (2.27) *will end up with the coercive linear elliptic operator, therefore by Lax-Milgram lemma we shall always find a unique solution for any small enough t. See the beginning of the Section 4.3.4 in [50] for the other possible types of adjoint equations. Since v^t is averaged in some sense we shall refer to it as* averaged adjoint method *for calculating shape derivative.*

For the state and the adjoint solutions we should not necessarily consider the strong topology. Observe that in order to find the limit in the last part of the proof of Theorem 2.2.17, the fact that v^t weakly converges to u^0 was enough to pass to the limit. Therefore, the application of the method could still be developed, e.g. see extension of the Correa-Seeger results in Chapter 4 of [50].

2.2.5 Local derivative of the transmission problem

Key approach for calculation of the shape derivative of the energy functional was to make change of variables to the fixed domain. More precisely, we have analysed the map

$$\theta \mapsto u(\theta) \circ \Phi_\theta \in \mathrm{H}^1_0(\Omega)$$

defined in a zero-neighbourhood $\mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, where $u(\theta)$ is the state function for the perturbed problem (2.11) under homeomorphism Φ_θ. Its directional derivative also known as material derivative has offered an easy way to calculate the shape derivative of the energy functional (see Theorem 2.2.16). But what about shape differentiability of the map $\theta \mapsto u(\theta)$? For that we need to define a notion of local derivative.

Consider the following type of mapping:

$$\omega \mapsto y(\omega) \in \mathrm{H}^1(\omega).$$

For example, $\Omega_\alpha \mapsto u_\alpha(\Omega_\alpha)$ is one such map. As before, we restrict ourselves only on the map $\theta \mapsto y(\Phi_\theta(\omega))$, taking ω fixed. An obvious problem when dealing with such map is the fact that the codomain lacks the structure of the vector space. In the literature this can be remedied in several different ways but the most natural one is to consider its restriction to any compact subset K of the open set ω.

If we take $K \subset\subset \omega$ then for $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, $k \in \mathbb{N}$ such that $\|\theta\|_k$ is small enough the following holds

$$K \subset\subset (\mathrm{Id} + \theta)\omega.$$

Now we can define a local derivative of the function $\theta \mapsto y(\theta) := y(\Phi_\theta(\omega))$:

Definition 2.2.20 (local derivative)**.** *Mapping $\theta \mapsto y(\theta)$ is said to be locally differentiable in zero if for every $K \subset\subset \omega$ the function $\theta \mapsto y(\theta)\big|_K \in \mathrm{H}^m(K), m \in \mathbb{N}$ (which is well defined on a $W^{k,\infty}(\omega; R^d)$ neighbourhood of zero) is Fréchet differentiable at zero. The coresponding derivative (at zero) in direction theta is called local derivative and denoted by $y'(\theta) \in \mathrm{H}^{\mathrm{m}}_{loc}(\omega)$.*

The following proposition gives an existence result for the local derivative $u'(\theta)$:

Proposition 2.2.21. *Let $\theta \mapsto y(\theta) \circ \Phi_\theta$ be well defined in a $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ neighbourhood of zero with values in $\mathrm{H}^m(\omega), m \in \mathbb{N}$ and Fréchet differentiable at zero. Then $\theta \mapsto y(\theta)$ is well defined in a $\mathrm{W}^{k,\infty}(R^d; R^d)$ neighbourhood of zero with values in $\mathrm{H}^m(\omega)$ and locally differentiable at 0. The following identity holds for all $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$:*

$$y'(\theta) = \dot{y}(\theta) - \nabla y(0) \cdot \theta.$$

Proof. The proof can be found in [44], v. Theorem 2.13. □

Remark 2.2.22. *The equality*

$$y'(\theta) = \dot{y}(\theta) - \nabla y(0) \cdot \theta$$

is sometimes taken to be a definition of the local derivative. Furthermore, it is a key aspect of proving a better regularity of the local derivative, e.g. if $\dot{y}(\theta) \in \mathrm{H}^1(\omega)$ this implies that $y'(\theta) \in \mathrm{L}^2(\omega)$.

If y belongs to a Sobolev space which is embedded in the space of continuously differentiable functions it should be noted that the following holds

$$y'(\theta)(x) = \lim_{t \to 0} \frac{y(t\theta)(x) - y(0)(x)}{t} \quad x \in \omega,$$

thus explaining the choice for notation.

Due to Lemma 2.2.3 and Proposition 2.2.21 we can conclude that the local derivative $u'(\theta)$ for the transmission problem exists and

$$u'(\theta) = \dot{u}(\theta) - \nabla u \cdot \theta \in \mathrm{L}^2(\Omega).$$

As before, let $u_\alpha = u_{|\Omega_\alpha}$ and $u_\beta = u_{|\Omega_\beta}$ be the restrictions of a u on Ω_α and Ω_β. The next theorem gives some light on the structure of $u'(\theta)$. A similar conclusion can be found in [3],[4].

Theorem 2.2.23 (Local derivative $u'(\theta)$)**.** *Let a pair* $(\Omega_\alpha, \Omega_\beta)$ *satisfies Assumption 2.1.16 and the interface* Γ *be of class* C^3*. Let* $f \in \mathrm{H}^1(\Omega)$ *and* $\theta \in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *such that* $supp\, \theta \subset\subset \Omega$*. Then local derivative* $u'(\theta) \in \mathrm{H}^1(\Omega_\alpha \cup \Omega_\beta)$ *is a solution of the following transmission problem with discontinuous jumps on the interface:*

$$\begin{cases} \Delta u'(\theta) = 0 & \text{in } \Omega_\alpha \cup \Omega_\beta, \\ u'_\alpha(\theta) - u'_\beta(\theta) = \frac{\alpha-\beta}{\beta}(\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)(\theta \cdot \boldsymbol{n}_\alpha) & \text{on } \Gamma, \\ \alpha \nabla u'_\alpha(\theta) \cdot \boldsymbol{n}_\alpha - \beta \nabla u'_\beta(\theta) \cdot \boldsymbol{n}_\alpha = (\alpha - \beta) \operatorname{div}_\Gamma((\theta \cdot \boldsymbol{n}_\alpha)\nabla_\Gamma u) & \text{on } \Gamma, \\ u'(\theta) = 0 & \text{on } \partial\Omega. \end{cases} \tag{2.28}$$

Proof. Using regularity Theorem 2.2.12 we can conclude that $u \in \mathrm{H}^3(\Omega_\alpha \cup \Omega_\beta)$. Proposition 2.2.21 combined with Theorem 2.2.3 shows that $u'(\theta)$ exists, is unique and

$$u'(\theta) = \dot{u}(\theta) - \nabla u \cdot \theta \in \mathrm{H}^1(\Omega_\alpha \cup \Omega_\beta).$$

For any $\varphi \in \mathrm{H}^1_0(\Omega)$ and $f \in \mathrm{H}^1(\Omega)$ the following holds:

$$0 = \int\limits_{\partial\Omega} \varphi f \theta \cdot \boldsymbol{n} \, \mathrm{d}S = \int\limits_{\Omega} \operatorname{div}(\varphi f \theta) \, \mathrm{d}x = \int\limits_{\Omega} \varphi \operatorname{div}(f\theta) \, \mathrm{d}x + \int\limits_{\Omega} f\theta \cdot \nabla\varphi \, \mathrm{d}x.$$

This means that (2.12) can be written as:

$$\int\limits_{\Omega} \mathbf{a} \nabla \dot{u}(\theta) \cdot \nabla\varphi \, \mathrm{d}x = \int\limits_{\Omega} \mathbf{a}(\nabla\theta + \nabla\theta^{\mathcal{T}} - \operatorname{div}(\theta) I)\nabla u \cdot \nabla\varphi \mathrm{d}x - \int\limits_{\Omega} f\theta \cdot \nabla\varphi \, \mathrm{d}x.$$

Assume that $\varphi \in \mathrm{H}^2(\Omega)$ for the moment. Then $\theta \cdot \nabla\varphi \in \mathrm{H}^1_0(\Omega)$ is a test function for (2.6) and we have

$$\int\limits_{\Omega} \mathbf{a} \Delta u(\theta \cdot \nabla\varphi) \, \mathrm{dx} = -\int\limits_{\Omega} f(\theta \cdot \nabla\varphi) \, \mathrm{dx}.$$

Therefore

$$\begin{aligned} \int\limits_{\Omega} \mathbf{a} \nabla \dot{u}(\theta) \cdot \nabla\varphi \, \mathrm{d}x &= \int\limits_{\Omega} \mathbf{a}(\nabla\theta + \nabla\theta^{\mathcal{T}} - \operatorname{div}(\theta) I)\nabla u \cdot \nabla\varphi \mathrm{d}x + \int\limits_{\Omega} \operatorname{div}(\mathbf{a}u)\theta \cdot \nabla\varphi \, \mathrm{d}x, \\ &= \int\limits_{\Omega} \mathbf{a}(\nabla\theta\nabla u \cdot \nabla\varphi + \nabla\theta^{\mathcal{T}}\nabla u \cdot \nabla\varphi - (\nabla u \cdot \nabla\varphi) \operatorname{div}\theta + (\theta \cdot \nabla\varphi)\Delta u) \, \mathrm{d}x \\ &= I_\alpha + I_\beta \end{aligned}$$

Then using the following identity

$$\operatorname{div}((\theta \cdot \nabla\varphi)\nabla u) - \operatorname{div}((\nabla u \cdot \nabla\varphi)\theta) = \nabla\theta\nabla u \cdot \nabla\varphi - (\nabla^2 u)\theta \cdot \nabla\varphi$$

$$+ (\theta \cdot \nabla\varphi)\Delta u - (\nabla u \cdot \nabla\varphi)\operatorname{div}\theta$$

we get

$$\begin{aligned}
I_\alpha &= \alpha \int\limits_{\Omega_\alpha} \operatorname{div}((\theta \cdot \nabla\varphi)\nabla u) - \operatorname{div}((\nabla u \cdot \nabla\varphi)\theta) + (\nabla^2 u)\theta \cdot \nabla\varphi + \nabla\theta^{\mathcal{T}}\nabla u \cdot \nabla\varphi \,\mathrm{d}x \\
&= \alpha \int\limits_{\Omega_\alpha} \operatorname{div}((\theta \cdot \nabla\varphi)\nabla u) - \operatorname{div}((\nabla u \cdot \nabla\varphi)\theta) + \nabla(\theta \cdot \nabla u) \cdot \nabla\varphi \,\mathrm{d}x.
\end{aligned}$$

With this we have obtained a variational equality for $u'(\theta)$ since $u'(\theta) = \dot{u}(\theta) - \theta \cdot \nabla u$:

$$\int\limits_{\Omega} \mathbf{a}\nabla u'(\theta) \cdot \nabla\varphi \,\mathrm{d}x = \int\limits_{\Omega} \mathbf{a}(\operatorname{div}((\theta \cdot \nabla\varphi)\nabla u) - \operatorname{div}((\nabla u \cdot \nabla\varphi)\theta)) \,\mathrm{d}x.$$

Using the divergence theorem on parts Ω_α and Ω_β separately:

$$\begin{aligned}
\int\limits_{\Omega} \mathbf{a}\nabla u'(\theta) \cdot \nabla\varphi \,\mathrm{d}x = &\int\limits_{\Gamma} (\theta \cdot \nabla\varphi)(\alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha) - \alpha(\nabla u_\alpha \cdot \nabla\varphi)(\theta \cdot \boldsymbol{n}_\alpha) \,\mathrm{d}S \\
&- \int\limits_{\Gamma} (\theta \cdot \nabla\varphi)(\beta\nabla u_\beta \cdot \boldsymbol{n}_\alpha) - \beta(\nabla u_\beta \cdot \nabla\varphi)(\theta \cdot \boldsymbol{n}_\alpha)\mathrm{d}S
\end{aligned}$$

Due to $\alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha = \beta\nabla u_\beta \cdot \boldsymbol{n}_\alpha$ on Γ and since $\nabla v = \nabla_\Gamma v + (\nabla v \cdot \boldsymbol{n}_\alpha)\boldsymbol{n}_\alpha$ we can rewrite the last part as

$$\begin{aligned}
\int\limits_{\Omega} \mathbf{a}\nabla u'(\theta) \cdot \nabla\varphi \,\mathrm{d}x &= -(\alpha - \beta) \int\limits_{\Gamma} (\nabla_\Gamma u \cdot \nabla_\Gamma\varphi)(\theta \cdot \boldsymbol{n}_\alpha) \,\mathrm{d}S \\
&= (\alpha - \beta) \int\limits_{\Gamma} \operatorname{div}_\Gamma((\theta \cdot \boldsymbol{n}_\alpha)\nabla_\Gamma u)\varphi \,\mathrm{d}S
\end{aligned}$$

where we use the fact that the $u_\alpha = u_\beta$ in $\mathrm{H}^{5/2}(\Gamma)$ thus $\nabla_\Gamma u_\alpha = \nabla_\Gamma u_\beta$ in $\mathrm{H}^{3/2}(\Gamma)$ and $\nabla_\Gamma\varphi$ belongs to $\mathrm{H}^{1/2}(\Gamma)$ for $\varphi \in \mathrm{H}^2(\Omega)$. Since $\operatorname{div}_\Gamma((\theta \cdot \boldsymbol{n}_\alpha)\nabla_\Gamma u)$ belongs to $\mathrm{H}^{1/2}(\Gamma)$ and $\mathrm{H}^2(\Omega)$ is dense in $\mathrm{H}^1(\Omega)$ we conclude for any $\varphi \in \mathrm{H}^1_0(\Omega)$ the following variational equality:

$$\int\limits_{\Omega} \mathbf{a}\nabla u'(\theta) \cdot \nabla\varphi \,\mathrm{d}x = (\alpha - \beta) \int\limits_{\Gamma} \operatorname{div}_\Gamma((\theta \cdot \boldsymbol{n}_\alpha)\nabla_\Gamma u)\varphi \,\mathrm{d}S$$

By applying partial integration, we can then calculate jump of the fluxes on the interface Γ in (2.28).

Since $\dot{u}_\alpha(\theta) = \dot{u}_\beta(\theta)$ on Γ we conclude that

$$\begin{aligned} u'_\alpha(\theta) - u'_\beta(\theta) &= -\nabla u_\alpha \cdot \theta + \nabla u_\beta \cdot \theta \\ &= -(\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)(\theta \cdot \boldsymbol{n}_\alpha) + (\nabla u_\beta \cdot \boldsymbol{n}_\alpha)(\theta \cdot \boldsymbol{n}_\alpha) \\ &= \frac{\alpha - \beta}{\beta}(\nabla u_\alpha \cdot \boldsymbol{n}_\alpha)(\theta \cdot \boldsymbol{n}_\alpha) \end{aligned}$$

again by using that $\nabla_\Gamma u_\alpha = \nabla_\Gamma u_\beta$ and the transmission condition. Note that $u'(\theta) = -\nabla u \cdot \boldsymbol{n}$ on $\partial\Omega$ and since $\operatorname{supp}\theta \subset\subset \Omega$ we have $u'(\theta) = 0$ on $\partial\Omega$. This concludes the proof. $\square$

Remark 2.2.24. *One can see that (2.28) is a system of two elliptic partial differential equations coupled with jump conditions on the interface Γ. We continue by showing that (2.28) uniquely defines the local derivative. Let us denote more general Poisson's equations with interfacial jumps:*

$$\text{(2.29)} \qquad \begin{cases} -\operatorname{div}(\mathbf{a}\nabla v) = f, & \text{in } \Omega_\alpha \cup \Omega_\beta \\ v_\alpha - v_\beta = a, & \text{on } \Gamma \\ (\mathbf{a}\nabla v)_\alpha \cdot \boldsymbol{n}_\alpha - (\mathbf{a}\nabla v)_\beta \cdot \boldsymbol{n}_\alpha = b, & \text{on } \Gamma \\ v = 0, & \text{on } \partial\Omega \end{cases}$$

where $f \in \mathrm{L}^2(\Omega)$, $\mathbf{a} \in \mathrm{L}^\infty(\Omega) \cap C(\Omega_\alpha \cup \Omega_\beta)$ strictly positive coefficient with discontinuity on the interface Γ which is at least Lipschitz. For simplicity we assume that there exists $\tilde{a}, \tilde{b} \in \mathrm{H}^1_0(\Omega)$ such that $\tilde{a}|_\Gamma = a$ and $\tilde{b}|_\Gamma$.

For the moment assume that $a = 0$. Then weak formulation for (2.29) states that for any $\varphi \in \mathrm{H}^1_0(\Omega)$:

$$\text{(2.30)} \qquad \begin{aligned} \int_\Omega \mathbf{a}\nabla v_0 \cdot \nabla\varphi \,\mathrm{d}x &= \int_\Omega f\varphi \,\mathrm{d}x + \int_\Gamma b\varphi \,\mathrm{d}S \\ &= \int_\Omega f\varphi \,\mathrm{d}x + \int_{\Omega_\alpha} \operatorname{div}(\tilde{b}\varphi\boldsymbol{n}_\alpha) \,\mathrm{d}x \end{aligned}$$

By the Lax-Milgram lemma there exists unique $v_0 \in \mathrm{H}^1_0(\Omega)$.

Now, for general a, we need the following set

$$H(a) := \{v \in \mathrm{L}^2(\Omega) \;:\; v - \tilde{a}\chi_{\Omega_\alpha} \in \mathrm{H}^1_0(\Omega)\}.$$

We say that $v \in H(a)$ is a weak solution of (2.29) if $u = v + \tilde{a}\chi_{\Omega_\alpha}$ for any $\varphi \in \mathrm{H}^1_0(\Omega)$

satisfies

$$\int_{\Omega} \mathbf{a}\nabla u \cdot \nabla\varphi \,\mathrm{d}x = \int_{\Omega} f\varphi \,\mathrm{d}x + \int_{\Omega_\alpha} \mathrm{div}(\tilde{b}\varphi \boldsymbol{n}_\alpha) \,\mathrm{d}x + \int_{\Omega_\alpha} \mathbf{a}\nabla\tilde{a} \cdot \nabla\varphi \,\mathrm{d}x. \tag{2.31}$$

Again by the Lax-Milgram lemma there exists unique solution $u \in \mathrm{H}^1_0(\Omega)$ *and therefore unique* $v \in H(a)$.

This means that the local derivative $u'(\theta) \in \mathrm{H}^1(\Omega_\alpha \cup \Omega_\beta)$ *is well defined by* (2.28).

We end this section by a demonstration on how one may use the local derivative in order to calculate the shape derivative of the energy functional. For this we recall a standard result:

Proposition 2.2.25. *Let* ω *be an open set. Let* $\theta \mapsto y(\theta)$ *be well defined in a zero-neighbourhood of* $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, $k \in \mathbb{N}$ *such that* $y(\theta) \in L^1(\Phi_\theta(\omega))$ *and the mapping*

$$\theta \mapsto y(\theta) \circ \Phi_\theta \in \mathrm{L}^1(\omega)$$

Fréchet differentiable at zero. Assume that $y(0) \in \mathrm{W}^{1,1}(\omega)$.

Then for any $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *we have* $y'(\theta) \in \mathrm{L}^1(\omega)$ *and*

$$y'(\theta) + \mathrm{div}(\theta y(0)) \in \mathrm{L}^1(\omega).$$

Furthermore, the map

$$\theta \mapsto \int_{\Phi_\theta(\omega)} y(\theta) \,\mathrm{d}x$$

is well defined in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *and Fréchet differentiable at zero. Its directional derivative at zero in the direction* θ *is:*

$$\int_{\omega} y'(\theta) + \mathrm{div}(\theta y(0)) \,\mathrm{d}x. \tag{2.32}$$

Proof. See Theorem 2.21. in [44] or Corollary 5.2.5 in [30]. □

We start by dividing the energy functional into two parts:

$$J(\Phi_\theta(\Omega_\alpha)) = \int_{\Phi_\theta(\Omega_\alpha)} f u_\alpha(\theta) \,\mathrm{d}x + \int_{\Phi_\theta(\Omega_\beta)} f u_\beta(\theta) \,\mathrm{d}x = A(\theta) + B(\theta)$$

where $u_\alpha(\theta)$ and $u_\beta(\theta)$ are defined as in (2.10) on the respective domains $\Phi_\theta(\Omega_\alpha)$ and

$\Phi_\theta(\Omega_\beta)$. From Proposition 2.2.25 we have

$$A'(0)[\theta] = \int_{\Omega_\alpha} f u'_\alpha(\theta)\,\mathrm{d}x + \int_{\Omega_\alpha} \operatorname{div}(f u_\alpha \theta)\,\mathrm{d}x$$
$$= \int_{\Omega_\alpha} f u'_\alpha(\theta)\,\mathrm{d}x + \int_{\Gamma} f u_\alpha \theta \cdot \boldsymbol{n}_\alpha\,\mathrm{d}S$$

Since $-\alpha\Delta u_\alpha = f$ in Ω_α we obtain

$$A'(0)[\theta] = -\int_{\Omega_\alpha} \alpha\Delta u_\alpha u'_\alpha(\theta)\,\mathrm{d}x + \int_{\Gamma} f u_\alpha \theta \cdot \boldsymbol{n}_\alpha\,\mathrm{d}S$$
$$= \int_{\Omega_\alpha} \alpha\nabla u_\alpha \cdot \nabla u'_\alpha(\theta)\,\mathrm{d}x - \int_{\Gamma} \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha u'_\alpha(\theta)\,\mathrm{d}S + \int_{\Gamma} f u_\alpha \theta \cdot \boldsymbol{n}_\alpha\,\mathrm{d}S$$
$$= \int_{\Gamma} \alpha u_\alpha \nabla u'_\alpha(\theta) \cdot \boldsymbol{n}_\alpha\,\mathrm{d}S - \int_{\Gamma} \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha u'_\alpha(\theta)\,\mathrm{d}S + \int_{\Gamma} f u_\alpha \theta \cdot \boldsymbol{n}_\alpha\,\mathrm{d}S,$$

where integration by parts is performed twice and the fact that $\Delta u'_\alpha(\theta) = 0$ in Ω_α is used. In the same way we conclude that

$$B'(0)[\theta] = \int_{\Gamma} \beta u_\beta \nabla u'_\beta(\theta) \cdot \boldsymbol{n}_\beta\,\mathrm{d}S - \int_{\Gamma} \beta\nabla u_\beta \cdot \boldsymbol{n}_\beta u'_\beta(\theta)\,\mathrm{d}S + \int_{\Gamma} f u_\beta \theta \cdot \boldsymbol{n}_\beta\,\mathrm{d}S.$$

$u = u_\alpha = u_\beta$ and $\alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha = \beta\nabla u_\beta \cdot \boldsymbol{n}_\alpha$ on Γ so we obtain

$$J'(\Omega_\alpha;\theta) = A'(0)[\theta] + B'(0)[\theta] = \int_{\Gamma} u(\alpha\nabla u'_\alpha(\theta) \cdot \boldsymbol{n}_\alpha - \beta\nabla u'_\beta(\theta) \cdot \boldsymbol{n}_\alpha)\,\mathrm{d}S$$
$$- \int_{\Gamma} \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha (u'_\alpha(\theta) - u'_\beta(\theta))\,\mathrm{d}S$$

From (2.28) we can conclude that

$$J'(\Omega_\alpha;\theta) = \int_{\Gamma} u(\alpha-\beta)\operatorname{div}_\Gamma(\nabla_\Gamma u(\theta \cdot \boldsymbol{n}_\alpha))\,\mathrm{d}S$$
$$- \int_{\Gamma} \alpha\nabla u_\alpha \cdot \boldsymbol{n}_\alpha \Big(\frac{\alpha-\beta}{\beta}\nabla u_\alpha \cdot \boldsymbol{n}_\alpha(\theta \cdot \boldsymbol{n}_\alpha)\Big)\,\mathrm{d}S$$
$$= -\int_{\Gamma} (\theta \cdot \boldsymbol{n}_\alpha)(\alpha-\beta)\nabla_\Gamma u \cdot \nabla_\Gamma u\,\mathrm{d}S - \int_{\Gamma} (\theta \cdot \boldsymbol{n}_\alpha)\frac{\alpha^2-\alpha\beta}{\beta}|\nabla u_\alpha \cdot \boldsymbol{n}_\alpha|^2\,\mathrm{d}S$$
$$= \int_{\Gamma} (\theta \cdot \boldsymbol{n}_\alpha)\left[\alpha\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - \beta\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 + (\beta-\alpha)|\nabla_\Gamma u|^2|\right]\,\mathrm{d}S,$$

which coincides with (2.23) since $|\nabla u|^2 = |\nabla_\Gamma u|^2 + \left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2$.

The previous method of calculating the shape derivative by using the local derivative is well known in the literature. The level set method usually uses shape derivatives written in boundary forms, so technical results as Proposition 2.2.25 were developed to simplify the calculation. This approach shall be later used to calculate the second order shape derivative in boundary form. Note that as before the shape derivative in the boundary representation always requires more regular interface Γ.

2.3 Second order derivative for transmission problem

2.3.1 Introduction

The second order derivatives of shape functional are much more complex to calculate then the first order shape derivatives. Before we start with calculations it is important to note that the aim is to find a bilinear map

$$(\theta, \psi) \mapsto J''(\omega, \theta, \psi)$$

such that the following Taylor expansion holds: for small enough θ in $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$

$$J(\Phi_\theta(\omega)) = J(\omega) + J'(\omega; \theta) + \frac{1}{2} J''(\omega; \theta, \theta) + o(\|\theta\|_k^2).$$

Although it is not obvious at the first glance, this cannot be done by taking a variation of the first order shape derivative since generally:

$$J''(\omega; \theta, \psi) \neq (J'(\omega; \theta))'(\omega; \psi) = \lim_{t \to 0} \frac{1}{t} \left(J'(\Phi_\psi(\omega); \theta) - J'(\omega; \theta) \right).$$

Indeed, as was remarked in [45] while the second variation with respect to a parameter is usually the variation of the first variation for the shape functional this is not true. Remember, the shape functional is defined on a family of regular open sets which does not have a structure of a vector space. In fact, if we take two successive variations by θ and ψ the result is not a variation by the sum $\theta + \psi$ since

$$(\mathrm{Id} + \psi) \circ (\mathrm{Id} + \theta) = \mathrm{Id} + (\theta + \psi \cdot (\mathrm{Id} + \theta))(\omega) \neq \mathrm{Id} + (\theta + \psi).$$

Recall the notation for the map $\mathcal{J}$ from Definition 2.1.10:

$$\mathcal{J}(\theta) = J((\mathrm{Id} + \theta)\omega).$$

Definition 2.3.1 (Second order shape differentiability). *Let $k \in \mathbb{N}$. A shape functional J is said to be twice shape differentiable at ω if the map*

$$\vartheta \mapsto \mathcal{J}'(\vartheta; \cdot) \in (\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d))'$$

is well defined in a zero-neighbourhood of $\mathrm{W}^{k,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ and Fréchet differentiable at zero. Directional derivative at zero in the first variation θ and the second variation ψ is denoted with $\mathcal{J}''(0; \theta, \psi)$, meaning

$$\mathcal{J}''(0; \theta, \psi) = \lim_{t \to 0} \frac{1}{t} \left(\mathcal{J}'(t\psi; \theta) - \mathcal{J}'(0; \theta) \right).$$

We shall also use the notation $J''(\omega;\theta,\psi) := \mathcal{J}''(0;\theta,\psi)$.

Notice that $\vartheta \mapsto \mathcal{J}'(\vartheta;\cdot) : \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d) \to (\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d))'$ is a mapping between Banach spaces, and $\mathcal{J}''(0;\cdot,\psi)$ is its directional derivative at zero in direction ψ Using classical results (e.g. see Proposition 3.2.28 in [22]) we can conclude that the mapping

$$(\theta,\psi) \mapsto \mathcal{J}''(0;\theta,\psi)$$

is symmetrical. One can even calculate expression $J''(\omega;\theta,\psi)$ using the first order shape derivative and the variation of the first order shape derivative:

$$J''(\omega;\theta,\psi) = (J'(\omega;\theta))'(\omega;\psi) - J'(\omega;\nabla\theta\psi). \tag{2.33}$$

This result can be found in [45] (this work was one of the first regarding second order derivative). See also [54] for an overview and relations to the speed method.

To demonstrate (2.33) let us suppose that J is twice differentiable. For a small t we have

$$\begin{aligned}
\mathcal{J}'(t\psi,\theta) &= \lim_{s\to 0}\frac{1}{s}\left(\mathcal{J}(t\psi+s\theta) - \mathcal{J}(t\psi)\right)\\
&= \lim_{s\to 0}\frac{1}{s}\left(J((\mathrm{Id}+s\theta+t\psi)\omega) - J((\mathrm{Id}+t\psi)\omega)\right)\\
&= \lim_{s\to 0}\frac{1}{s}\big(J((\mathrm{Id}+s\theta(\mathrm{Id}+t\psi)^{-1})\circ(\mathrm{Id}+t\psi)\omega) - J((\mathrm{Id}+t\psi)\omega)\big)\\
&= J'((\mathrm{Id}+t\psi)\omega\,;\,\theta\circ(\mathrm{Id}+t\psi)^{-1})
\end{aligned}$$

Again by definition, and using that the mapping $\mathcal{J}'(t\psi,\cdot)$ is linear and continuous

$$\begin{aligned}
J''(\omega;\theta,\psi) = \mathcal{J}''(0;\theta,\psi) &= \lim_{t\to 0}\frac{1}{t}\left(\mathcal{J}'(t\psi,\theta) - \mathcal{J}'(0,\theta)\right)\\
&= \lim_{t\to 0}\frac{1}{t}\big(J'((\mathrm{Id}+t\psi)\omega\,;\,\theta\circ(\mathrm{Id}+t\psi)^{-1}) - J'(\omega;\theta)\big)\\
&= \lim_{t\to 0}\frac{1}{t}\left(J'((\mathrm{Id}+t\psi)\omega;\theta) - J'(\omega;\theta)\right)\\
&\quad + \lim_{t\to 0}\frac{1}{t}\big(J'((\mathrm{Id}+t\psi)\omega;\theta\circ(\mathrm{Id}+t\psi)^{-1} - \theta)\big)\\
&= (J'(\omega;\theta))'(\omega;\psi) - J'(\omega;\nabla\theta\psi).
\end{aligned}$$

Remark 2.3.2. *It should be noted that the previous calculus could be also done for the local derivative $u'(\theta)$ in order to define the second variation of a state u. One can then define*

$$u''(\theta,\psi) = u'(\theta)'(\psi) - u'(\nabla\theta\psi)$$

and use it later for calculations of the second order derivative for various functionals *depending on u (see [3],[4]). Property*

$$u(\theta) = u(0) + u'(\theta) + \frac{1}{2}u''(\theta,\theta) + o(\|\theta\|_k^2)$$

still holds (see [45]). For our purposes this approach can be circumvented.

Remark 2.3.3. *With the previous expression we have also found a way to calculate the second order shape derivative directly. Observe that by definition*

$$J''(\omega;\theta,\psi) = \lim_{t\to 0}\frac{1}{t}\left(J'((\mathrm{Id}+t\psi)\omega\,;\,\theta\circ(\mathrm{Id}+t\psi)^{-1}) - J'(\omega;\theta)\right)$$

and if $J'(\omega;\theta)$ is known one only needs to provide appropriate Lagrange functional to directly calculate the second order shape derivative. Some authors even use this identity to define the symmetrical second order shape derivative and it offers a more direct way to calculate it (for details v. [49]).

Before we start with calculations let us give an analogous result to the Proposition 2.2.25 for calculating the shape derivative of functionals represented as boundary integrals:

Theorem 2.3.4. *Let ω be an open and bounded set of class C^1. Let $\theta \mapsto g(\theta) \in \mathrm{W}^{1,1}(\Phi_\theta(\omega))$ be well defined in a zero-neighbourhood of $\mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\theta \mapsto g(\theta)\circ\Phi_\theta$ is Fréchet differentiable at zero. Then the map*

$$\theta \mapsto \mathcal{G}(\theta) = \int\limits_{\Phi_\theta(\partial\omega)} g(\theta)\,\mathrm{d}S$$

is Fréchet differentiable at zero and for any $\theta \in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$:

$$\mathcal{G}'(0)[\theta] = \int\limits_{\partial\omega} \dot{g}(\theta) + g(0)\,\mathrm{div}_\Gamma\,\theta\,\mathrm{d}S$$

Moreover, if $\partial\omega$ is of class C^2 and $g(0)\in\mathrm{W}^{2,1}(\Omega)$, then

$$\mathcal{G}'(0)[\theta] = \int\limits_{\partial\omega} g'(\theta) + (\theta\cdot\boldsymbol{n})\left\{\frac{\partial g(0)}{\partial\boldsymbol{n}} + \mathrm{H}g(0)\right\}$$

Proof. The proof can be found in [30]. □

2.3.2 Calculation by virtue of local derivative

Now we have everything in order to calculate second order shape derivative of energy functional:

Theorem 2.3.5. *Let θ and ψ belongs to $\mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, the interface Γ of class $\mathcal{C}^3$ and the right-hand side f in $\mathrm{H}^1(\Omega)$. Then the mapping*

$$\theta \mapsto J(\Phi_\theta(\Omega_\alpha)) := \int\limits_{\Phi_\theta(\Omega)} f u(\theta)\,\mathrm{d}x, \theta \in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$$

is twice shape-differentiable at zero. Its directional derivative at zero in the direction $\theta \in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\operatorname{supp}\theta \subset\subset \Omega$ is given with:

$$\begin{aligned}
&J''(\Omega_\alpha;\theta,\psi) = \\
&\quad \alpha \int\limits_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right] + \frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\right\}\mathrm{d}S \\
&\quad - \beta \int\limits_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right] + \frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\right\}\mathrm{d}S \\
&\quad - \frac{2(\beta+\alpha)\alpha}{\beta-\alpha}\int\limits_{\Omega_\alpha}\nabla u'_\alpha(\theta)\cdot\nabla u'_\alpha(\psi)\,\mathrm{d}x + \frac{2(\beta+\alpha)\beta}{\beta-\alpha}\int\limits_{\Omega_\beta}\nabla u'_\beta(\theta)\cdot\nabla u'_\beta(\psi)\,\mathrm{d}x \\
&\quad + \frac{2\alpha\beta}{\beta-\alpha}\int\limits_\Gamma u'_\beta(\theta)\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\alpha(\psi)\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha} + u'_\alpha(\theta)\frac{\partial u'_\beta(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\beta(\psi)\frac{\partial u'_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S \\
&\quad + \alpha\int\limits_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S - \beta\int\limits_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\mathrm{d}S
\end{aligned}$$

where

$$Z(\theta,\psi) = \nabla\boldsymbol{n}_\alpha^{\mathcal{T}}\theta_\Gamma\cdot\psi_\Gamma - \nabla_\Gamma(\theta\cdot\boldsymbol{n}_\alpha)\cdot\psi_\Gamma - \nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\cdot\theta_\Gamma$$

and u is defined by (2.6) and $u'(\theta)$ by (2.28).

Proof. The equation (2.33) and Theorem 2.3.4 will play key role in calculation of shape derivative. By Theorem 2.2.16 the shape derivative of energy functional is given with (2.23):

$$J'(\Omega_\alpha;\theta) = \int_\Gamma \theta\cdot\boldsymbol{n}_\alpha\left[2\left\{\alpha\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - \beta\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2\right\} - \left\{\alpha|\nabla u_\alpha|^2 - \beta|\nabla u_\beta|^2\right\}\right]\mathrm{d}S.$$

We will divide functional in two parts:

$$J'(\Omega_\alpha;\theta) = J'_\alpha(\Omega;\theta) + J'_\beta(\Omega;\theta)$$

where

$$J'_\alpha(\Omega_\alpha;\theta) = \alpha\int\limits_\Gamma(\theta\cdot\boldsymbol{n}_\alpha)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S$$

and

$$J'_\beta(\Omega_\alpha;\theta) = -\beta \int\limits_\Gamma (\theta \cdot \boldsymbol{n}_\alpha) \left[2 \left| \frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] \mathrm{d}S.$$

By using Theorem 2.3.4 we can conclude that the shape derivative of $\Omega \mapsto J'_\alpha(\Omega_\alpha;\theta)$ is given with

$$\begin{aligned}
(J'_\alpha(\Omega_\alpha;\theta))'(\Omega_\alpha;\psi) = {} & \alpha \int\limits_\Gamma \theta \cdot \boldsymbol{n}'_\alpha(\psi) \left[2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \theta \cdot \boldsymbol{n}_\alpha \left\{ 4 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \left(\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + \nabla u_\alpha \cdot \boldsymbol{n}'_\alpha(\psi) \right) - 2 \nabla u_\alpha \cdot \nabla u'_\alpha(\psi) \right\} \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \psi \cdot \boldsymbol{n}_\alpha \left\{ (\theta \cdot \boldsymbol{n}_\alpha) \mathrm{H} \left[2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \right\} \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \psi \cdot \boldsymbol{n}_\alpha \left\{ \frac{\partial}{\partial \boldsymbol{n}_\alpha} \left[(\theta \cdot \boldsymbol{n}_\alpha) \left(2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right) \right] \right\} \mathrm{d}S
\end{aligned}$$

Since

$$\nabla u_\alpha \cdot \nabla u'_\alpha(\psi) = \nabla_\Gamma u_\alpha \cdot \nabla_\Gamma u'_\alpha(\psi) + \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha}$$

we can rewrite the second line in the following manner:

$$\alpha \int\limits_\Gamma \theta \cdot \boldsymbol{n}_\alpha \left\{ 2 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + 4 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \nabla u_\alpha \cdot \boldsymbol{n}'_\alpha(\psi) - 2 \nabla_\Gamma u_\alpha \cdot \nabla_\Gamma u'_\alpha(\psi) \right\} \mathrm{d}S$$

making

$$\begin{aligned}
(J'_\alpha(\Omega_\alpha;\theta))'(\Omega_\alpha;\psi) = {} & \alpha \int\limits_\Gamma \theta \cdot \boldsymbol{n}'_\alpha(\psi) \left[2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \theta \cdot \boldsymbol{n}_\alpha \left\{ 2 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + 4 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \nabla u_\alpha \cdot \boldsymbol{n}'_\alpha(\psi) - 2 \nabla_\Gamma u_\alpha \cdot \nabla_\Gamma u'_\alpha(\psi) \right\} \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \psi \cdot \boldsymbol{n}_\alpha \left\{ \mathrm{H}(\theta \cdot \boldsymbol{n}_\alpha) \left[2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \right\} \mathrm{d}S \\
& + \alpha \int\limits_\Gamma \psi \cdot \boldsymbol{n}_\alpha \left\{ \frac{\partial}{\partial \boldsymbol{n}_\alpha} \left[(\theta \cdot \boldsymbol{n}_\alpha) \left(2 \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right) \right] \right\} \mathrm{d}S.
\end{aligned}$$

Using identity (2.33):

$$J''_\alpha(\Omega;\theta) = (J'_\alpha(\Omega;\theta))'(\Omega;\psi) - J'_\alpha(\Omega;\nabla\theta\psi),$$

we obtain

$$
\begin{aligned}
J''_\alpha(\Omega_\alpha;\theta) &= (J'_\alpha(\Omega_\alpha;\theta))'(\Omega_\alpha;\psi) - J'_\alpha(\Omega_\alpha;\nabla\theta\psi),\\
&= \alpha\int_\Gamma \theta\cdot\boldsymbol{n}'_\alpha(\psi)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S\\
&\quad+\alpha\int_\Gamma \theta\cdot\boldsymbol{n}_\alpha\left\{2\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha}+4\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla u_\alpha\cdot\boldsymbol{n}'_\alpha(\psi)-2\nabla_\Gamma u_\alpha\cdot\nabla_\Gamma u'_\alpha(\psi)\right\}\mathrm{d}S\\
&\quad+\alpha\int_\Gamma \psi\cdot\boldsymbol{n}_\alpha\left\{\mathrm{H}(\theta\cdot\boldsymbol{n}_\alpha)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\right\}\mathrm{d}S\\
&\quad+\alpha\int_\Gamma \psi\cdot\boldsymbol{n}_\alpha\left\{\frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[(\theta\cdot\boldsymbol{n}_\alpha)\left(2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right)\right]\right\}\mathrm{d}S\\
&\quad-\alpha\int_\Gamma \nabla\theta\psi\cdot\boldsymbol{n}_\alpha\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S.
\end{aligned}
$$

Using that $\boldsymbol{n}'_\alpha(\psi) = -\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)$ the previous expression can be written as:

$$
J''_\alpha(\Omega_\alpha;\theta,\psi) = I_{\alpha,1}+I_{\alpha,2}+I_{\alpha,3}
$$

where

$$
\begin{aligned}
I_{\alpha,1} &= \alpha\int_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]+\frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\right\}\mathrm{d}S,\\
I_{\alpha,2} &= \alpha\int_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)\left\{2\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha}-4\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla u_\alpha\cdot\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)-2\nabla_\Gamma u_\alpha\cdot\nabla_\Gamma u'_\alpha(\psi)\right\}\mathrm{d}S,\\
I_{\alpha,3} &= \alpha\int_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S,
\end{aligned}
$$

and

$$
Z(\theta,\psi) = -\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\cdot\theta_\Gamma+\nabla(\theta\cdot\boldsymbol{n}_\alpha)\cdot\boldsymbol{n}_\alpha(\psi\cdot\boldsymbol{n}_\alpha)-\nabla\theta^{\mathcal{T}}\boldsymbol{n}_\alpha\cdot\psi.
$$

The function $Z(\theta,\psi)$ is actually symmetrical. If we write

$$
\nabla(\theta\cdot\boldsymbol{n}_\alpha)\cdot\psi = \nabla_\Gamma(\theta\cdot\boldsymbol{n}_\alpha)\cdot\psi_\Gamma+\nabla(\theta\cdot\boldsymbol{n}_\alpha)\cdot\boldsymbol{n}_\alpha(\psi\cdot\boldsymbol{n}_\alpha),
$$

we obtain using $\nabla(\theta\cdot\boldsymbol{n}_\alpha)\cdot\psi = \nabla\theta^{\mathcal{T}}\boldsymbol{n}_\alpha\cdot\psi+\nabla\boldsymbol{n}_\alpha^{\mathcal{T}}\theta\cdot\psi$ that

$$
\nabla\theta^{\mathcal{T}}\boldsymbol{n}_\alpha\cdot\psi+\nabla\boldsymbol{n}_\alpha^{\mathcal{T}}\theta\cdot\psi = \nabla_\Gamma(\theta\cdot\boldsymbol{n}_\alpha)\cdot\psi_\Gamma+\nabla(\theta\cdot\boldsymbol{n}_\alpha)\cdot\boldsymbol{n}_\alpha(\psi\cdot\boldsymbol{n}_\alpha).
$$

Using the fact that $|\boldsymbol{n}_\alpha|^2 = 1$ and consequently that $\nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \boldsymbol{n}_\alpha = 0$ we can see that

$$\nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta \cdot \psi = \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta_\Gamma \cdot \psi.$$

Since $\nabla \boldsymbol{n}_\alpha^{\mathcal{T}}$ is symmetric, the following holds

$$\nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta_\Gamma \cdot \psi = \theta_\Gamma \cdot \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \psi = \theta_\Gamma \cdot \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \psi_\Gamma = \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta_\Gamma \cdot \psi_\Gamma.$$

Combining all, we obtain

$$\nabla \theta^{\mathcal{T}} \boldsymbol{n}_\alpha \cdot \psi + \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta_\Gamma \cdot \psi_\Gamma = \nabla_\Gamma (\theta \cdot \boldsymbol{n}_\alpha) \cdot \psi_\Gamma + \nabla (\theta \cdot \boldsymbol{n}_\alpha) \cdot \boldsymbol{n}_\alpha (\psi \cdot \boldsymbol{n}_\alpha).$$

This implies that term $Z(\theta, \psi)$ can be written as:

$$Z(\theta, \psi) = \nabla \boldsymbol{n}_\alpha^{\mathcal{T}} \theta_\Gamma \cdot \psi_\Gamma - \nabla_\Gamma (\theta \cdot \boldsymbol{n}_\alpha) \cdot \psi_\Gamma - \nabla_\Gamma (\psi \cdot \boldsymbol{n}_\alpha) \cdot \theta_\Gamma,$$

thus showing that $I_{\alpha,1}$ and $I_{\alpha,3}$ are symmetrical as functions of θ and ψ. The term $I_{\alpha,2}$ is unfortunately more complex and we will only prove that in combination with $J''_\beta(\Omega; \theta, \psi)$ it becomes symmetrical. $I_{\alpha,2}$ is given with:

$$I_{\alpha,2} = \alpha \int_\Gamma (\theta \cdot \boldsymbol{n}_\alpha) \left\{ 2 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} - 4 \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \nabla u_\alpha \cdot \nabla_\Gamma (\psi \cdot \boldsymbol{n}_\alpha) - 2 \nabla_\Gamma u_\alpha \cdot \nabla_\Gamma u'_\alpha(\psi) \right\} \mathrm{d}S.$$

Using (2.28) we can recognize that

$$(\theta \cdot \boldsymbol{n}_\alpha) \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} = \frac{\beta}{\alpha - \beta} (u'_\alpha(\theta) - u'_\beta(\theta))$$

meaning that the first term in $I_{\alpha,2}$ can be written as:

$$\begin{aligned}
2\alpha \int_\Gamma (\theta \cdot \boldsymbol{n}_\alpha) \frac{\partial u_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha} \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} \mathrm{d}S &= \frac{2\alpha\beta}{\alpha - \beta} \int_\Gamma (u'_\alpha(\theta) - u'_\beta(\theta)) \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} \mathrm{d}S \\
&= \frac{2\alpha\beta}{\alpha - \beta} \left\{ \int_{\Omega_\alpha} \operatorname{div}(u'_\alpha(\theta) \nabla u'_\alpha(\psi)) \, \mathrm{d}x - \int_\Gamma u'_\beta(\theta) \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} \mathrm{d}S \right\} \\
&= \frac{2\alpha\beta}{\alpha - \beta} \left\{ \int_{\Omega_\alpha} \nabla u'_\alpha(\theta) \cdot \nabla u'_\alpha(\psi) \, \mathrm{d}x - \int_\Gamma u'_\beta(\theta) \frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} \mathrm{d}S \right\}
\end{aligned}$$

where we use partial integration and the equality $\Delta u'_\alpha(\theta)) = 0$ in Ω_α. Again, due to (2.28):

$$(\alpha - \beta) \operatorname{div}_\Gamma (\nabla_\Gamma u_\alpha (\theta \cdot \boldsymbol{n}_\alpha)) = (\alpha - \beta) \operatorname{div}_\Gamma (\nabla_\Gamma u (\theta \cdot \boldsymbol{n}_\alpha)) = \alpha \frac{\partial u'_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha} - \beta \frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha}.$$

Similarly, by partial integration the third term of $I_{\alpha,2}$ becomes

$$\begin{aligned}
-2\alpha \int_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)\nabla_\Gamma u_\alpha \cdot \nabla_\Gamma u'_\alpha(\psi)\,\mathrm{d}S &= 2\alpha \int_\Gamma u'_\alpha(\psi)\,\mathrm{div}_\Gamma(\nabla_\Gamma u_\alpha(\theta\cdot\boldsymbol{n}_\alpha))\,\mathrm{d}S \\
&= \frac{2\alpha}{\alpha-\beta}\int_\Gamma u'_\alpha(\psi)\left(\alpha\frac{\partial u'_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha} - \beta\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha}\right)\mathrm{d}S \\
&= \frac{2\alpha}{\alpha-\beta}\left\{\alpha\int_{\Omega_\alpha}\mathrm{div}(u'_\alpha(\psi)\nabla u'_\alpha(\theta))\,\mathrm{d}x - \beta\int_\Gamma u'_\alpha(\psi)\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S\right\} \\
&= \frac{2\alpha}{\alpha-\beta}\left\{\alpha\int_{\Omega_\alpha}\nabla u'_\alpha(\psi)\cdot\nabla u'_\alpha(\theta)\,\mathrm{d}x - \beta\int_\Gamma u'_\alpha(\psi)\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S\right\}.
\end{aligned}$$

Combining all, we get the following expression for $I_{\alpha,2}$:

$$\begin{aligned}
I_{\alpha,2} = &-\frac{2(\beta+\alpha)\alpha}{\beta-\alpha}\int_{\Omega_\alpha}\nabla u'_\alpha(\theta)\cdot\nabla u'_\alpha(\psi)\,\mathrm{d}x - 4\int_\Gamma \alpha\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla_\Gamma u\cdot\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\,\mathrm{d}S \\
&+ \frac{2\alpha\beta}{\beta-\alpha}\int_\Gamma u'_\beta(\theta)\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\alpha(\psi)\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S.
\end{aligned}$$

One can analogously calculate J''_β and obtain similar result:

$$J''_\beta(\Omega_\alpha;\theta,\psi) = I_{\beta,1} + I_{\beta,2} + I_{\beta,3},$$

where:

$$\begin{aligned}
I_{\beta,1} &= -\beta\int_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right] + \frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\right\}\mathrm{d}S, \\
I_{\beta,2} &= \frac{2(\beta+\alpha)\beta}{\beta-\alpha}\int_{\Omega_\beta}\nabla u'_\beta(\theta)\cdot\nabla u'_\beta(\psi)\,\mathrm{d}x + 4\int_\Gamma \beta\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla_\Gamma u\cdot\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\,\mathrm{d}S \\
&\quad + \frac{2\alpha\beta}{\beta-\alpha}\int_\Gamma u'_\alpha(\theta)\frac{\partial u'_\beta(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\beta(\psi)\frac{\partial u'_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S, \\
I_{\beta,3} &= -\beta\int_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\mathrm{d}S.
\end{aligned}$$

Since flux is continuous across the interface $\alpha\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} = \beta\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}$ we can see that:

$$-4\int_\Gamma \alpha\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla_\Gamma u\cdot\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\,\mathrm{d}S + 4\int_\Gamma \beta\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\nabla_\Gamma u\cdot\nabla_\Gamma(\psi\cdot\boldsymbol{n}_\alpha)\,\mathrm{d}S = 0.$$

Finally, the second order shape derivative is given with:

$$\begin{aligned}
J''(\Omega;\theta,\psi) &= J''_\alpha(\Omega;\theta,\psi) + J''_\beta(\Omega;\theta,\psi)\\
&= \alpha\int\limits_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right] + \frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\right\}\mathrm{d}S\\
&\quad - \beta\int\limits_\Gamma (\theta\cdot\boldsymbol{n}_\alpha)(\psi\cdot\boldsymbol{n}_\alpha)\left\{\mathrm{H}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right] + \frac{\partial}{\partial \boldsymbol{n}_\alpha}\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\right\}\mathrm{d}S\\
&\quad - \frac{2(\beta+\alpha)\alpha}{\beta-\alpha}\int\limits_{\Omega_\alpha}\nabla u'_\alpha(\theta)\cdot\nabla u'_\alpha(\psi)\,\mathrm{d}x + \frac{2(\beta+\alpha)\beta}{\beta-\alpha}\int\limits_{\Omega_\beta}\nabla u'_\beta(\theta)\cdot\nabla u'_\beta(\psi)\,\mathrm{d}x\\
&\quad + \frac{2\alpha\beta}{\beta-\alpha}\int\limits_\Gamma u'_\beta(\theta)\frac{\partial u'_\alpha(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\alpha(\psi)\frac{\partial u'_\beta(\theta)}{\partial \boldsymbol{n}_\alpha} + u'_\alpha(\theta)\frac{\partial u'_\beta(\psi)}{\partial \boldsymbol{n}_\alpha} + u'_\beta(\psi)\frac{\partial u'_\alpha(\theta)}{\partial \boldsymbol{n}_\alpha}\,\mathrm{d}S\\
&\quad + \alpha\int\limits_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\alpha|^2\right]\mathrm{d}S - \beta\int\limits_\Gamma Z(\theta,\psi)\left[2\left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 - |\nabla u_\beta|^2\right]\mathrm{d}S.
\end{aligned}$$

□

2.3.3 Direct calculation

In the previous section two different ways of calculating the first order shape derivative were demonstrated. We continue in this fashion to obtain similar result for the second order shape derivative. In (2.33) we have also found the following useful identity:

$$J''(\Omega;\theta,\psi) = \lim_{t\to 0^+}\frac{1}{t}\left[J'((\mathrm{Id}+t\psi)\Omega;\theta\circ(\mathrm{Id}+t\psi)^{-1}) - J'(\Omega;\psi)\right]. \tag{2.34}$$

The advantage of using (2.34) lies in the fact that one may offer a direct proof by the method presented in the proof of Theorem 2.2.17. Throughout the proof we shall use the following notation for a given $\theta\in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$:

$$\begin{aligned}
\Phi_{t\theta} &= \mathrm{Id}+t\theta,\\
p_\theta(t) &= \det|\nabla\Phi_{t\theta}|,\\
P_\theta(t) &= p_\theta(t)\nabla\Phi_{t\theta}^{-1}\nabla\Phi_{t\theta}^{-\mathcal{T}}.
\end{aligned}$$

Theorem 2.3.6. *The second order shape derivative of the energy functional in the trans-*

mission problem is given with:

$$
\begin{aligned}
J''(\Omega;\theta,\psi) = &\int\limits_{\Omega} \mathbf{a}\left[-\operatorname{div}\theta\operatorname{div}\psi\,\mathbf{I}+\nabla\theta:\nabla\psi^{\mathcal{T}}\,\mathbf{I}-\nabla\theta\nabla\psi^{\mathcal{T}}-\nabla\psi\nabla\theta^{\mathcal{T}}\right]\nabla u\cdot\nabla u\,\mathrm{d}x\\
&+\int\limits_{\Omega} \mathbf{a}\left[-\nabla\theta\nabla\psi-\nabla\psi\nabla\theta-\nabla\theta^{\mathcal{T}}\nabla\psi^{\mathcal{T}}-\nabla\psi^{\mathcal{T}}\nabla\theta^{\mathcal{T}}\right]\nabla u\cdot\nabla u\,\mathrm{d}x\\
&+\int\limits_{\Omega} \mathbf{a}\left[\operatorname{div}\theta(\nabla\psi+\nabla\psi^{\mathcal{T}})+\operatorname{div}\psi(\nabla\theta+\nabla\theta^{\mathcal{T}})\right]\nabla u\cdot\nabla u\,\mathrm{d}x\\
&+2\int\limits_{\Omega}\left[f\operatorname{div}\theta\operatorname{div}\psi+\theta\cdot\nabla f\operatorname{div}\psi+\psi\cdot\nabla f\operatorname{div}\theta+Hf\psi\cdot\theta\right]u\,\mathrm{d}x\\
&-2\int\limits_{\Omega}\nabla\theta:\nabla\psi^{\mathcal{T}}fu\,\mathrm{d}x+\frac{1}{2}\int\limits_{\Omega}\mathbf{a}\nabla v(\theta)\cdot\nabla v(\psi)\,\mathrm{d}x
\end{aligned}
\tag{2.35}
$$

where u is a solution of (2.6) and $v(\theta)\in \mathrm{H}_0^1(\Omega)$ satisfies the following equality for any $\varphi\in\mathrm{H}_0^1(\Omega)$:

$$
\int\limits_{\Omega}\mathbf{a}\nabla v(\theta)\cdot\nabla\varphi\,\mathrm{d}x = 2\int\limits_{\Omega}\operatorname{div}(f\theta)\varphi\,\mathrm{d}x+2\int\limits_{\Omega}\mathbf{a}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u\cdot\nabla\varphi\,\mathrm{d}x. \tag{2.36}
$$

Proof. We have divided the proof in several steps:

1. *Notation and creation of functional G_2:*
   Similarly, like in the proof of Theorem 2.2.17 we begin by defining Lagrange functional

$$
\begin{aligned}
\mathcal{L}_2(\Omega_\alpha,\theta;u,v) &= J'(\Omega_\alpha;\theta)-\int\limits_{\Omega}\mathbf{a}\nabla u\cdot\nabla v\,\mathrm{d}x+\int\limits_{\Omega}fv\,\mathrm{d}x\\
&=\alpha\int\limits_{\Omega_\alpha}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u\cdot\nabla u\,\mathrm{d}x\\
&\quad+\beta\int\limits_{\Omega_\beta}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u\cdot\nabla u\,\mathrm{d}x\\
&\quad+2\int\limits_{\Omega}\operatorname{div}(f\theta)u\,\mathrm{d}x-\alpha\int\limits_{\Omega_\alpha}\nabla u\cdot\nabla v\,\mathrm{d}x-\beta\int\limits_{\Omega_\beta}\nabla u\cdot\nabla v\,\mathrm{d}x+\int\limits_{\Omega}fv\,\mathrm{d}x.
\end{aligned}
$$

   Observe that we need to take into account both the set Ω_α and the direction θ. We now proceed by writing $\mathcal{L}_2(\Phi_{t\psi}(\Omega_\alpha),\theta\circ\Phi_{t\psi}^{-1};u,v)$ into four separate terms:

$$
\mathcal{L}_2(\Phi_{t\psi}(\Omega_\alpha),\theta\circ\Phi_{t\psi}^{-1};u,v) = I_\alpha+I_\beta+I_0+I_S
$$

where

$$I_\alpha = \alpha \int\limits_{\Phi_{t\psi}(\Omega_\alpha)} \left[-\operatorname{div}(\theta \circ \Phi_{t\psi}^{-1})\,\mathbf{I} + \nabla(\theta \circ \Phi_{t\psi}^{-1}) + \nabla(\theta \circ \Phi_{t\psi}^{-1})^{\mathcal{T}}\right] \nabla u \cdot \nabla u \,\mathrm{d}x,$$

$$I_\beta = \beta \int\limits_{\Phi_{t\psi}(\Omega_\beta)} \left[-\operatorname{div}(\theta \circ \Phi_{t\psi}^{-1})\,\mathbf{I} + \nabla(\theta \circ \Phi_{t\psi}^{-1}) + \nabla(\theta \circ \Phi_{t\psi}^{-1})^{\mathcal{T}}\right] \nabla u \cdot \nabla u \,\mathrm{d}x,$$

$$I_0 = 2 \int\limits_{\Phi_{t\psi}(\Omega)} \operatorname{div}(f\theta \circ \Phi_{t\psi}^{-1}) u \,\mathrm{d}x,$$

and

$$I_S = -\alpha \int\limits_{\Phi_{t\psi}(\Omega_\alpha)} \nabla u \cdot \nabla v \,\mathrm{d}x - \beta \int\limits_{\Phi_{t\psi}(\Omega_\beta)} \nabla u \cdot \nabla v \,\mathrm{d}x + \int\limits_{\Phi_{t\psi}(\Omega)} f v \,\mathrm{d}x.$$

By change of variables to original Ω_α, we obtain that

$$\begin{aligned} I_\alpha = {} & \alpha \int\limits_{\Omega_\alpha} \left[-\operatorname{div}(\theta \circ \Phi_{t\psi}^{-1}) \circ \Phi_{t\psi}\,\mathbf{I}\right] \nabla u \circ \Phi_{t\psi} \cdot \nabla u \circ \Phi_{t\psi}\, p_\psi(t) \,\mathrm{d}x \\ & + \alpha \int\limits_{\Omega_\alpha} \left[\nabla(\theta \circ \Phi_{t\psi}^{-1}) \circ \Phi_{t\psi} + \nabla(\theta \circ \Phi_{t\psi}^{-1})^{\mathcal{T}} \circ \Phi_{t\psi}\right] \nabla u \circ \Phi_{t\psi} \cdot \nabla u \circ \Phi_{t\psi}\, p_\psi(t) \,\mathrm{d}x. \end{aligned}$$

Using simple calculus one can easily check that following holds

$$\nabla(\theta \circ \Phi_{t\psi}^{-1}) \circ \Phi_{t\psi} = (\nabla\theta \circ \Phi_{t\psi}^{-1} \nabla \Phi_{t\psi}^{-1}) \circ \Phi_{t\psi} = \nabla\theta\, \nabla(\Phi_{t\psi}^{-1} \circ \Phi_{t\psi}).$$

Since $\operatorname{div}(\cdot) = \operatorname{tr}(\nabla \cdot)$ we can conclude

$$\operatorname{div}(\theta \circ \Phi_{t\psi}^{-1}) \circ \Phi_{t\psi} = \operatorname{tr}(\nabla\theta\, \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi}) = \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi}$$

meaning

$$\begin{aligned} I_\alpha = {} & \alpha \int\limits_{\Omega_\alpha} -(\nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi}) P_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) \,\mathrm{d}x \\ & + \alpha \int\limits_{\Omega_\alpha} \nabla\Phi_{t\psi}^{-1} (\nabla\theta\, \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi}) \nabla\Phi_{t\psi}^{-\mathcal{T}} \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) p_\psi(t) \,\mathrm{d}x \\ & + \alpha \int\limits_{\Omega_\alpha} \nabla\Phi_{t\psi}^{-1} (\nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi}\, \nabla\theta^{\mathcal{T}}) \nabla\Phi_{t\psi}^{-\mathcal{T}} \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) p_\psi(t) \,\mathrm{d}x. \end{aligned}$$

An application of similar arguments to the cases of I_β, I_0 and I_S gives

$$
\begin{aligned}
I_\beta = \beta \int_{\Omega_\beta} &-(\nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi}) P_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) \, \mathrm{d}x \\
&+ \beta \int_{\Omega_\beta} \nabla\Phi_{t\psi}^{-1} (\nabla\theta \, \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi}) \nabla\Phi_{t\psi}^{-\mathcal{T}} p_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) \, \mathrm{d}x \\
&+ \beta \int_{\Omega_\beta} \nabla\Phi_{t\psi}^{-1} (\nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} \, \nabla\theta^{\mathcal{T}}) \nabla\Phi_{t\psi}^{-\mathcal{T}} p_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(u \circ \Phi_{t\psi}) \, \mathrm{d}x,
\end{aligned}
$$

$$
I_0 = 2 \int_\Omega \left[f \circ \Phi_{t\psi} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} + \theta \cdot \nabla f \circ \Phi_{t\psi} \right] u \circ \Phi_{t\psi} p_\psi(t) \, \mathrm{d}x,
$$

and

$$
\begin{aligned}
I_S = &-\alpha \int_{\Omega_\alpha} P_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(v \circ \Phi_{t\psi}) \, \mathrm{d}x - \beta \int_{\Omega_\beta} P_\psi(t) \nabla(u \circ \Phi_{t\psi}) \cdot \nabla(v \circ \Phi_{t\psi}) \, \mathrm{d}x \\
&+ \int_\Omega f \circ \Phi_{t\psi} \, v \circ \Phi_{t\psi} p_\psi(t) \, \mathrm{d}x.
\end{aligned}
$$

Combining all this we can define functional G_2 (for small t):

$$
\begin{aligned}
G_2(t; u, v) &= \mathcal{L}_2(\Phi_{t\psi}(\Omega_\alpha), \theta \circ \Phi_{t\psi}^{-1}; u \circ \Phi_{t\psi}^{-1}, v \circ \Phi_{t\psi}^{-1}) \\
&= \int_\Omega \mathbf{a} \nabla\Phi_{t\psi}^{-1} \left[\nabla\theta \, \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi} + \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} \, \nabla\theta^{\mathcal{T}} \right] \nabla\Phi_{t\psi}^{-\mathcal{T}} \nabla u \cdot \nabla u \, p_\psi(t) \, \mathrm{d}x \\
&\quad - \int_\Omega \mathbf{a} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} P_\psi(t) \nabla u \cdot \nabla u \, \mathrm{d}x \\
&\quad + 2 \int_\Omega \left[f \circ \Phi_{t\psi} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} + \theta \cdot \nabla f \circ \Phi_{t\psi} \right] u \, p_\psi(t) \, \mathrm{d}x \\
&\quad - \int_{\Omega_\alpha} \mathbf{a} P_\psi(t) \nabla u \cdot \nabla v \, \mathrm{d}x + \int_\Omega f \circ \Phi_{t\psi} \, v \, p_\psi(t) \, \mathrm{d}x.
\end{aligned}
$$

2. *Connecting J' and G:*
   By choosing u^t to be a solution of the boundary value problem:

$$
\left\{
\begin{aligned}
&\text{find } u^t \in \mathrm{H}_0^1(\Omega) \text{ such that } \forall \varphi \in \mathrm{H}_0^1 \\
&\int_\Omega \mathbf{a} P_\psi(t) \nabla u^t \cdot \nabla\varphi \, \mathrm{d}x = \int_\Omega p_\psi(t) f \circ \Phi_{t\psi} \, \varphi \, \mathrm{d}x,
\end{aligned}
\right.
\tag{2.37}
$$

we can write

$$\begin{aligned} J'(\Phi_{t\psi}(\Omega);\theta\circ\Phi_{t\psi}^{-1}) - J'(\Omega;\theta) &= G_2(t;u^t,v^t) - G_2(0;u^0,v^t) \\ &= G_2(t;u^t,v^t) - G_2(t;u^0,v^t) + G_2(t;u^0,v^t) - G_2(0;u^0,v^t) \end{aligned}$$

where v^t is chosen such that the following holds

$$G_2(t;u^t,v^t) - G_2(t;u^0,v^t) = 0 \tag{2.38}$$

making

$$J'(\Phi_t(\Omega);\theta\circ\Phi_t^{-1}) - J'(\Omega;\theta) = G_2(t;u^0,v^t) - G_2(0;u^0,v^t).$$

3. *Averaged adjoint method (justification of* (2.35)*):*
Observe that the mapping $(t,u,v)\mapsto G_2(t;u,v) : \langle -\delta,\delta\rangle \times \mathrm{H}_0^1(\Omega)\times \mathrm{H}_0^1(\Omega)\to\mathbb{R}$ is well defined for $\delta>0$ small enough. For the beginning we only require that (2.37) defines uniquely u^t, which is obtained if $\mathbf{a}P(t)$ is coercive for $t\in\langle -\delta,\delta\rangle$. One can show that for fixed t and $v\in \mathrm{H}_0^1(\Omega)$

$$u\mapsto G_2(t;u,v) : \mathrm{H}_0^1(\Omega)\to\mathbb{R}$$

is Fréchet differentiable and its directional derivative at u in direction w is given with

$$\begin{aligned} D_uG(t;u,v)[w] = &-\int_\Omega \mathbf{a}P_\psi(t)\nabla v\cdot\nabla w\,\mathrm{d}x \\ &+2\int_\Omega \left[f\circ\Phi_{t\psi}\nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi} + \theta\cdot\nabla f\circ\Phi_{t\psi}\right]\, w\,p_\psi(t)\,\mathrm{d}x \\ &-2\int_\Omega \mathbf{a}\nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}P_\psi(t)\nabla u\cdot\nabla w\,\mathrm{d}x \\ &+2\int_\Omega \mathbf{a}\nabla\Phi_{t\psi}^{-1}\left[\nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi} + \nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}\,\nabla\theta^{\mathcal{T}}\right]\nabla\Phi_{t\psi}^{-\mathcal{T}}\nabla u\cdot\nabla w\,p_\psi(t)\,\mathrm{d}x. \end{aligned}$$

Then (2.35) can be written as

$$0 = G_2(t;u^t,v^t) - G_2(t;u^0,v^t) = \int_0^1 D_uG(t;u^*(s),v)[u^t-u^0]\,\mathrm{d}s$$

where $u^*(s) = u^0 + s(u^t - u^0)$. Let us define a linear operator $B_t : \mathrm{H}_0^1(\Omega) \to \mathbb{R}$

$$\begin{aligned}
B_t(\varphi) = 2 \int_\Omega & \left[f \circ \Phi_{t\psi} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} + \theta \cdot \nabla f \circ \Phi_{t\psi} \right] \varphi \, p_\psi(t) \, \mathrm{d}x \\
& - 2 \int_0^1 \int_\Omega \mathbf{a} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} P_\psi(t) \nabla u^*(s) \cdot \nabla\varphi \, \mathrm{d}x\mathrm{d}s \\
& + 2 \int_0^1 \int_\Omega \mathbf{a} \nabla\Phi_{t\psi}^{-1} (\nabla\theta \, \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi}) \nabla\Phi_{t\psi}^{-\mathcal{T}} \nabla u^*(s) \cdot \nabla\varphi \, p_\psi(t) \, \mathrm{d}x\mathrm{d}s \\
& + 2 \int_0^1 \int_\Omega \mathbf{a} \nabla\Phi_{t\psi}^{-1} (\nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} \, \nabla\theta^{\mathcal{T}}) \nabla\Phi_{t\psi}^{-\mathcal{T}} \nabla u^*(s) \cdot \nabla\varphi \, p_\psi(t) \, \mathrm{d}x\mathrm{d}s
\end{aligned}$$

Since family (u^t) is bounded for small t (arguments are similar to those presented in the proof Theorem 2.2.17), and for fixed $\theta, \psi \in \mathrm{W}^{2,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ we can easily conclude that operator B_t is continuous. Observe that a solution $v^t \in \mathrm{H}_0^1(\Omega)$ of

$$\left\{ \begin{array}{l} \text{find } v^t \in \mathrm{H}_0^1(\Omega) \text{ such that } \forall \varphi \in \mathrm{H}_0^1(\Omega) \\ \displaystyle\int_\Omega \mathbf{a} P_\psi(t) \nabla v^t \cdot \nabla\varphi \, \mathrm{d}x = B_t(\varphi), \end{array} \right. \tag{2.39}$$

satisfies (2.35) if we replace φ by $u^t - u^0$.

4. v^t *converges weakly in* $\mathrm{H}_0^1(\Omega)$
   Since B_t is continuous by the Lax-Milgram lemma we can conclude that the family $(v^t)_t$ is bounded for $t \in \langle -\delta, \delta \rangle$. This implies that for a sequence (t_n) such that $t_n \to 0$ as $n \to +\infty$ the following holds (up to a subsequence):

$$v^{t_n} \to \overline{v} \text{ weakly in } \mathrm{H}^1 .$$

For $\varphi \in \mathrm{H}_0^1(\Omega)$:

$$\begin{aligned}
\lim_{n\to+\infty} \int_\Omega \mathbf{a} P(t_n) \nabla v^{t_n} \cdot \nabla\varphi \, \mathrm{d}x &= \lim_{n\to+\infty} \int_\Omega \mathbf{a} P(t_n) \nabla\varphi \cdot \nabla v^{t_n} \, \mathrm{d}x \\
&= \int_\Omega \mathbf{a} \nabla\varphi \cdot \nabla\overline{v} \, \mathrm{d}x
\end{aligned}$$

because $P(t_n) \to \mathbf{I}$ strongly in $\mathrm{L}^\infty(\Omega)$, thus $\mathbf{a} P(t_n) \nabla\varphi \to \mathbf{a} \nabla\varphi$ in $\mathrm{L}^2(\Omega)$, meaning that we have product of strong and weak sequences. One can also put $B_t(\varphi)$ to the limit obtaining

$$\lim_{n\to\infty} B_t(\varphi) = 2\int\limits_\Omega \operatorname{div}(f\theta)\varphi\,\mathrm{d}x + 2\int\limits_\Omega \mathbf{a}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla\varphi\,\mathrm{d}x.$$

Therefore, $\overline{v}$ satisfies variational equality

$$\int\limits_\Omega \mathbf{a}\nabla\overline{v}\cdot\nabla\varphi\,\mathrm{d}x = 2\int\limits_\Omega \operatorname{div}(f\theta)\varphi\,\mathrm{d}x + 2\int\limits_\Omega \mathbf{a}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla\varphi\,\mathrm{d}x,$$

for any $\varphi\in \mathrm{H}_0^1(\Omega)$. One can conclude that the weak limit $\overline{v}$ is uniquely determined and coincides with v^0, the solution of (2.37) for $t=0$. Moreover, since it is the only accumulation point of the sequence (v_n^t), it is the limit of the whole sequence. The same holds for every sequence (t_n) converging to zero.

5. *Calculation of the shape derivative:*
   Now we have everything to finish the proof.

$$\begin{aligned}
\frac{G_2(t;u^0,v^t)-G_2(0;u^0,v^t)}{t} = &-\int\limits_\Omega \mathbf{a}\frac{\nabla\theta:\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}P_\psi(t)-\operatorname{div}\theta\,\mathbf{I}}{t}\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\
&+\int\limits_\Omega \mathbf{a}\frac{\nabla\Phi_{t\psi}^{-1}\nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi}\nabla\Phi_{t\psi}^{-\mathcal{T}}p_\psi(t)-\nabla\theta}{t}\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\
&+\int\limits_\Omega \mathbf{a}\frac{\nabla\Phi_{t\psi}^{-1}\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}\,\nabla\theta^{\mathcal{T}}\nabla\Phi_{t\psi}^{-\mathcal{T}}p_\psi(t)-\nabla\theta^{\mathcal{T}}}{t}\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\
&+2\int\limits_\Omega \mathbf{a}\frac{f\circ\Phi_{t\psi}\nabla\theta:\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}p_\psi(t)-f\operatorname{div}(\theta)}{t}u^0\,\mathrm{d}x\\
&+2\int\limits_\Omega \mathbf{a}\frac{\theta\cdot\nabla f\circ\Phi_{t\psi}p_\psi(t)-\theta\cdot\nabla f}{t}u^0\,\mathrm{d}x\\
&-\int\limits_\Omega \mathbf{a}\frac{P_\psi(t)-\mathbf{I}}{t}\nabla u^0\cdot\nabla v^t\,\mathrm{d}x+\int\limits_\Omega \frac{f\circ\Phi_{t\psi}p_\psi(t)-f}{t}v^t\,\mathrm{d}x.
\end{aligned}$$

With some work the following results can be verified:

$$\begin{aligned}\nabla\theta:\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}P_\psi(t)-\operatorname{div}\theta\,\mathbf{I} = t(&-\nabla\theta:\nabla\psi^{\mathcal{T}}\,\mathbf{I}+\operatorname{div}\theta\operatorname{div}\psi\,\mathbf{I}-\operatorname{div}\theta\nabla\psi\\
&-\operatorname{div}\theta\nabla\psi^{\mathcal{T}})+o(t),\end{aligned}\tag{2.40}$$

$$\begin{aligned}\nabla\Phi_{t\psi}^{-1}\nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi}\nabla\Phi_{t\psi}^{-\mathcal{T}}p_\psi(t)-\nabla\theta = t(&-\nabla\psi\nabla\theta-\nabla\theta\nabla\psi-\nabla\theta\nabla\psi^{\mathcal{T}}\\
&+\operatorname{div}(\psi)\nabla\theta)+o(t),\end{aligned}\tag{2.41}$$

(2.42)
$$\nabla\Phi_{t\psi}^{-1}\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}\,\nabla\theta^{\mathcal{T}}\nabla\Phi_{t\psi}^{-\mathcal{T}}p_\psi(t)-\nabla\theta^{\mathcal{T}}=t(-\nabla\psi\nabla\theta^{\mathcal{T}}-\nabla\psi^{\mathcal{T}}\nabla\theta^{\mathcal{T}}\\ -\nabla\theta^{\mathcal{T}}\nabla\psi^{\mathcal{T}}+\operatorname{div}\psi\nabla\theta^{\mathcal{T}})+o(t),$$

$$f\circ\Phi_{t\psi}\nabla\theta:\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}p_\psi(t)-f\operatorname{div}(\theta)=t(\nabla f\cdot\psi\operatorname{div}(\theta)-f\nabla\theta:\nabla\psi^{\mathcal{T}}\\ +\operatorname{div}\theta\operatorname{div}\psi)+o(t), \tag{2.43}$$

$$\theta\cdot\nabla f\circ\Phi_{t\psi}p_\psi(t)-\theta\cdot\nabla f=t(Hf\psi\cdot\theta+\nabla f\cdot\theta\operatorname{div}\psi)+o(t), \tag{2.44}$$

with respect to L^∞ norm. Since the following holds

$$\begin{aligned}J''(\Omega;\theta,\psi)&=\lim_{t\to0}\frac{1}{t}\left\{J'(\Phi_t(\Omega);\theta\circ\Phi_t^{-1})-J'(\Omega;\theta)\right\}\\&=\lim_{t\to0}\frac{1}{t}\left\{G_2(t;u^0,v^t)-G_2(0;u^0,v^t)\right\}\end{aligned}$$

one can obtain

$$\begin{aligned}J''(\Omega;\theta,\psi)=&\int_\Omega\mathbf{a}\left[-\operatorname{div}\theta\operatorname{div}\psi\,\mathbf{I}+\nabla\theta:\nabla\psi^{\mathcal{T}}\,\mathbf{I}-\nabla\theta\nabla\psi^{\mathcal{T}}-\nabla\psi\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\&+\int_\Omega\mathbf{a}\left[-\nabla\theta\nabla\psi-\nabla\psi\nabla\theta-\nabla\theta^{\mathcal{T}}\nabla\psi^{\mathcal{T}}-\nabla\psi^{\mathcal{T}}\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\&+\int_\Omega\mathbf{a}\left[\operatorname{div}\theta(\nabla\psi+\nabla\psi^{\mathcal{T}})+\operatorname{div}\psi(\nabla\theta+\nabla\theta^{\mathcal{T}})\right]\nabla u^0\cdot\nabla u^0\,\mathrm{d}x\\&+2\int_\Omega\left[f\operatorname{div}\theta\operatorname{div}\psi+\theta\cdot\nabla f\operatorname{div}\psi+\psi\cdot\nabla f\operatorname{div}\theta+Hf\psi\cdot\theta\right]u^0\,\mathrm{d}x\\&-2\int_\Omega\nabla\theta:\nabla\psi^{\mathcal{T}}fu^0\,\mathrm{d}x\\&+\int_\Omega\mathbf{a}[-\operatorname{div}(\psi)\,\mathbf{I}+\nabla\psi+\nabla\psi^{\mathcal{T}}]\nabla u^0\cdot\nabla v^0\,\mathrm{d}x+\int_\Omega\operatorname{div}(f\psi)v^0\,\mathrm{d}x\end{aligned}$$

By taking $v^0(\theta)\in\mathrm{H}_0^1(\Omega)$ which satisfies the following equality for any $\varphi\in\mathrm{H}_0^1(\Omega)$:

$$\int_\Omega\mathbf{a}\nabla v^0(\theta)\cdot\nabla\varphi\,\mathrm{d}x=2\int_\Omega\operatorname{div}(f\theta)\varphi\,\mathrm{d}x+2\int_\Omega\mathbf{a}\left[-\operatorname{div}(\theta)\,\mathbf{I}+\nabla\theta+\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla\varphi\,\mathrm{d}x.$$

we can rewrite the previous result

$$J''(\Omega;\theta,\psi)=\int_\Omega\mathbf{a}\left[-\operatorname{div}\theta\operatorname{div}\psi\,\mathbf{I}+\nabla\theta:\nabla\psi^{\mathcal{T}}\,\mathbf{I}-\nabla\theta\nabla\psi^{\mathcal{T}}-\nabla\psi\nabla\theta^{\mathcal{T}}\right]\nabla u^0\cdot\nabla u^0\,\mathrm{d}x$$

$$
\begin{aligned}
&+ \int\limits_{\Omega} \mathbf{a} \left[-\nabla\theta\nabla\psi - \nabla\psi\nabla\theta - \nabla\theta^{\mathcal{T}}\nabla\psi^{\mathcal{T}} - \nabla\psi^{\mathcal{T}}\nabla\theta^{\mathcal{T}}\right] \nabla u^0 \cdot \nabla u^0 \,\mathrm{d}x \\
&+ \int\limits_{\Omega} \mathbf{a} \left[\operatorname{div}\theta(\nabla\psi + \nabla\psi^{\mathcal{T}}) + \operatorname{div}\psi(\nabla\theta + \nabla\theta^{\mathcal{T}})\right] \nabla u^0 \cdot \nabla u^0 \,\mathrm{d}x \\
&+ 2\int\limits_{\Omega} \left[f \operatorname{div}\theta \operatorname{div}\psi + \theta\cdot\nabla f \operatorname{div}\psi + \psi\cdot\nabla f \operatorname{div}\theta + H f \psi\cdot\theta\right] u^0 \,\mathrm{d}x \\
&- 2\int\limits_{\Omega} \nabla\theta : \nabla\psi^{\mathcal{T}} f u^0 \,\mathrm{d}x + \frac{1}{2}\int\limits_{\Omega} \mathbf{a}\nabla v^0(\theta)\cdot\nabla v^0(\psi)\,\mathrm{d}x.
\end{aligned}
$$

□

Remark 2.3.7. *Expression (2.35) can be obtained in the manner of the proof of Theorem 2.2.16. From*

$$
\begin{aligned}
J'(\Phi_{t\psi}(\Omega_\alpha), \theta\circ\Phi_{t\psi}^{-1}) = &\int\limits_{\Phi_{t\psi}(\Omega)} \mathbf{a}\circ\Phi_{t\psi}^{-1}\left(-\operatorname{div}(\theta\circ\Phi_{t\psi}^{-1})\mathbf{I}\right)\nabla u(t\psi)\cdot\nabla u(t\psi)\,\mathrm{d}x \\
&+ \int\limits_{\Phi_{t\psi}(\Omega)} \mathbf{a}\circ\Phi_{t\psi}^{-1}\left(\nabla(\theta\circ\Phi_{t\psi}^{-1})\right)\nabla u(t\psi)\cdot\nabla u(t\psi)\,\mathrm{d}x \\
&+ \int\limits_{\Phi_{t\psi}(\Omega)} \mathbf{a}\circ\Phi_{t\psi}^{-1}\left(\nabla(\theta\circ\Phi_{t\psi}^{-1})^{\mathcal{T}}\right)\nabla u(t\psi)\cdot\nabla u(t\psi)\,\mathrm{d}x \\
&+ 2\int\limits_{\Phi_{t\psi}(\Omega)} \operatorname{div}(f\theta\circ\Phi_{t\psi}^{-1})u(t\psi)\,\mathrm{d}x
\end{aligned}
$$

by changing of variables to Ω, writing $\nabla u(t\psi)\circ\Phi_{t\psi} = \nabla\Phi_{t\psi}^{-\mathcal{T}}\nabla(u(t\psi)\circ\Phi_{t\psi})$, using identities

$$
\nabla(\theta\circ\Phi_{t\psi}^{-1})\circ\Phi_{t\psi} = \nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi}
$$

and

$$
\operatorname{div}(\theta\circ\Phi_{t\psi}^{-1})\circ\Phi_{t\psi} = \operatorname{tr}(\nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi}) = \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}
$$

we obtain

$$
\begin{aligned}
J'(\Phi_{t\psi}(\Omega_\alpha), \theta\circ\Phi_{t\psi}^{-1}) = &\int\limits_{\Omega} \mathbf{a}\nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi} P_\psi(t)\nabla(u(t\psi)\circ\Phi_{t\psi})\cdot\nabla(u(t\psi)\circ\Phi_{t\psi})\,\mathrm{d}x \\
&+ \int\limits_{\Omega} \mathbf{a}\nabla\Phi_{t\psi}^{-1}\nabla\theta\,\nabla\Phi_{t\psi}^{-1}\circ\Phi_{t\psi}\nabla\Phi_{t\psi}^{-\mathcal{T}} p_\psi(t)\nabla(u(t\psi)\circ\Phi_{t\psi})\cdot\nabla(u(t\psi)\circ\Phi_{t\psi})\,\mathrm{d}x \\
&+ \int\limits_{\Omega} \mathbf{a}\nabla\Phi_{t\psi}^{-1}\nabla\Phi_{t\psi}^{-\mathcal{T}}\circ\Phi_{t\psi}\,\nabla\theta^{\mathcal{T}}\nabla\Phi_{t\psi}^{-\mathcal{T}} p_\psi(t)\nabla(u(t\psi)\circ\Phi_{t\psi})\cdot\nabla(u(t\psi)\circ\Phi_{t\psi})\,\mathrm{d}x
\end{aligned}
$$

$$+ 2\int_\Omega f \circ \Phi_{t\psi} \nabla\theta : \nabla\Phi_{t\psi}^{-\mathcal{T}} \circ \Phi_{t\psi} p_\psi(t) u(t\psi) \circ \Phi_{t\psi} \,\mathrm{d}x$$
$$+ 2\int_\Omega \theta \cdot \nabla f \circ \Phi_{t\psi} p_\psi(t) u(t\psi) \circ \Phi_{t\psi} \,\mathrm{d}x.$$

The material derivative $\dot{u}(\psi)$ satisfies

$$u(t\psi) \circ \Phi_{t\psi} = u + t\dot{u}(\psi) + o(t)$$

Observing (2.40)-(2.44) *and using Leibniz rule (which holds for multiplication of Fréchet differentiable function) we can write*

$$J'(\Phi_{t\psi}(\Omega_\alpha); \theta \circ \Phi_{t\psi}^{-1}) = J'(\Omega_\alpha; \theta) + tJ''(\Omega_\alpha; \theta, \psi) + o(t)$$

thus easily identifying expression $J''(\Omega_\alpha; \theta, \psi)$:

$$\begin{aligned}
J''(\Omega_\alpha; \theta, \psi) = & \int_\Omega \mathbf{a} \left[- \operatorname{div}\theta \operatorname{div}\psi \,\mathbf{I} + \nabla\theta : \nabla\psi^{\mathcal{T}} \,\mathbf{I} - \nabla\theta\nabla\psi^{\mathcal{T}} - \nabla\psi\nabla\theta^{\mathcal{T}}\right] \nabla u \cdot \nabla u \,\mathrm{d}x \\
& + \int_\Omega \mathbf{a} \left[-\nabla\theta\nabla\psi - \nabla\psi\nabla\theta - \nabla\theta^{\mathcal{T}}\nabla\psi^{\mathcal{T}} - \nabla\psi^{\mathcal{T}}\nabla\theta^{\mathcal{T}}\right] \nabla u \cdot \nabla u \,\mathrm{d}x \\
& + \int_\Omega \mathbf{a} \left[\operatorname{div}\theta(\nabla\psi + \nabla\psi^{\mathcal{T}}) + \operatorname{div}\psi(\nabla\theta + \nabla\theta^{\mathcal{T}})\right] \nabla u \cdot \nabla u \,\mathrm{d}x \\
& + 2\int_\Omega \left[f \operatorname{div}\theta \operatorname{div}\psi + \theta \cdot \nabla f \operatorname{div}\psi + \psi \cdot \nabla f \operatorname{div}\theta + Hf\psi \cdot \theta\right] u \,\mathrm{d}x \\
& - 2\int_\Omega \nabla\theta : \nabla\psi^{\mathcal{T}} f u \,\mathrm{d}x + 2\int_\Omega \mathbf{a}\nabla\dot{u}(\theta) \cdot \nabla\dot{u}(\psi) \,\mathrm{d}x.
\end{aligned}$$

This allows us to easily obtain expression for a volume representation of the second shape derivative (observe that the most calculations remain the same as in the proof of Theorem 2.3.6)

Example 2.3.8 (Second order shape derivative of the volume)**.** *Let us consider the shape functional* $\mathrm{vol}(\omega) = \int_\omega \mathrm{d}x$*. The volume (distributed) representation of the shape derivative is given by*

$$\mathrm{vol}'(\omega; \theta) = \int_\omega \operatorname{div}(\theta) \,\mathrm{d}x.$$

By applying (2.34) *we find that*

$$\mathrm{vol}''(\omega; \theta, \psi) = \lim_{t\to 0} \frac{1}{t} \left[\mathrm{vol}'(\Phi_{t\psi}(\omega); \theta \circ \Phi_{t\psi}^{-1}) - \mathrm{vol}'(\omega; \theta)\right]$$

$$= \lim_{t\to 0} \frac{1}{t}\Bigg[\int\limits_{\Phi_{t\psi}(\omega)} \operatorname{div}(\theta \circ \Phi_{t\psi}^{-1})\,\mathrm{d}x - \int\limits_{\omega} \operatorname{div}(\theta)\,\mathrm{d}x \Bigg].$$

Since

$$\begin{aligned}
\int\limits_{\Phi_{t\psi}(\omega)} \operatorname{div}(\theta \circ \Phi_{t\psi}^{-1})\,\mathrm{d}x &= \int\limits_{\omega} \nabla\theta : \nabla\Phi_{t\psi}^{-1} \circ \Phi_{t\psi} p_{\psi}(t)\,\mathrm{d}x \\
&= \int\limits_{\omega} \operatorname{div}(\theta)\,\mathrm{d}x + t \int\limits_{\omega} -\nabla\theta : \nabla\psi^{\mathcal{T}} + \operatorname{div}(\theta)\operatorname{div}(\psi)\,\mathrm{d}x + o(t)
\end{aligned}$$

we conclude that

$$\operatorname{vol}''(\omega;\theta,\psi) = \int\limits_{\omega} -\nabla\theta : \nabla\psi^{\mathcal{T}} + \operatorname{div}(\theta)\operatorname{div}(\psi)\,\mathrm{d}x. \tag{2.45}$$

Therefore we have shown that $\theta \mapsto \operatorname{vol}(\omega;\theta)$ *is twice shape differentiable at zero from* $\mathrm{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ *to* $\mathbb{R}$. *No additional restriction on the regularity of the open set* ω *is needed in this calculation.*

Note that the second order shape derivative can be expressed in the boundary representations if ω *is domain with* C^2 *boundary and* $\theta,\psi \in \mathrm{W}^{2,\infty}(\mathbb{R}^d;\mathbb{R}^d)$*:*

$$\operatorname{vol}''(\omega;\theta,\psi) = \int\limits_{\partial\omega} \mathrm{H}(\theta\cdot\boldsymbol{n})(\psi\cdot\boldsymbol{n})\,\mathrm{d}S.$$

Remark 2.3.9. *For numerical purposes it is convenient to write the second order shape derivative of the energy functional as two sums*

$$J''(\Omega_\alpha;\theta,\psi) = J''_{design}(\Omega_\alpha;\theta,\psi) + J''_u(\Omega_\alpha;\theta,\psi)$$

where

$$J''_u(\Omega_\alpha;\theta,\psi) := 2\int\limits_{\Omega} \mathbf{a}\nabla\dot{u}(\theta)\cdot\nabla\dot{u}(\psi)\,\mathrm{d}x.$$

This play a key role in numerical implementations since $J''_u(\Omega_\alpha;\theta,\psi)$ *after a discretization in FEM leads to a full matrix (see [54]). Generally, this means that creation of a full Hessian for the Newton method may not be feasible (especially for higher dimensions) due to limiting computing power.*

Chapter 3

Numerical approximation

3.1 Shape derivative based algorithms

3.1.1 Introduction

Let us recall, in optimization problem (2.9) the aim is to maximize the energy functional $J(\Omega_\alpha) = \int_\Omega f u \, \mathrm{d}x$ for $\Omega_\alpha \in \mathcal{D}$ such that $\mathrm{vol}(\Omega_\alpha) = q_\alpha$, where

$$\mathcal{D} := \{\Omega_\alpha \subset \Omega \text{ is a Lipschitz domain s.t. } \Omega_\alpha \subset\subset \Omega \text{ or } \Omega \setminus \Omega_\alpha \subset\subset \Omega\}.$$

This means that the problem (2.9) is a problem of constrained maximization:

$$\max_{\Omega_\alpha \in \mathcal{D} : \, \mathrm{vol}(\Omega_\alpha) = q_\alpha} J(\Omega_\alpha). \tag{3.1}$$

A constrained optimization problems with only equality constraints are often solved by a method of Lagrange multipliers. By introducing Lagrangian functional

$$L(\lambda, \Omega_\alpha) := J(\Omega_\alpha) - \lambda \mathrm{vol}(\Omega_\alpha), \tag{3.2}$$

where $\lambda \in \mathbb{R}$, we can introduce an unconstrained maximization problem:

$$\max_{\Omega_\alpha \in \mathcal{D}} L(\lambda, \Omega_\alpha). \tag{3.3}$$

Ideally, we would like that for any volume constraint q_α there exists $\lambda(q_\alpha) \in \mathbb{R}$ such that (3.1) is equivalent to (3.3). Although, the actual proof that (3.1) is equivalent to (3.3) for some $\lambda \in \mathbb{R}$ is still lacking, in numerics such replacement of problems is one possible heuristics for solving constrained problems. Henceforth, for simplicity we shall assume that we were given fixed $\lambda = \lambda(q_\alpha) \in \mathbb{R}$ corresponding to the volume constraint q_α and focus on a finding a numerical solution to (3.3). An alternative is to introduce an update strategy for a multiplier λ e.g. the one given by the augmented Lagrangian method (see [37],[12]).

The next step is to define an ascent vector for the shape functional through the frame-

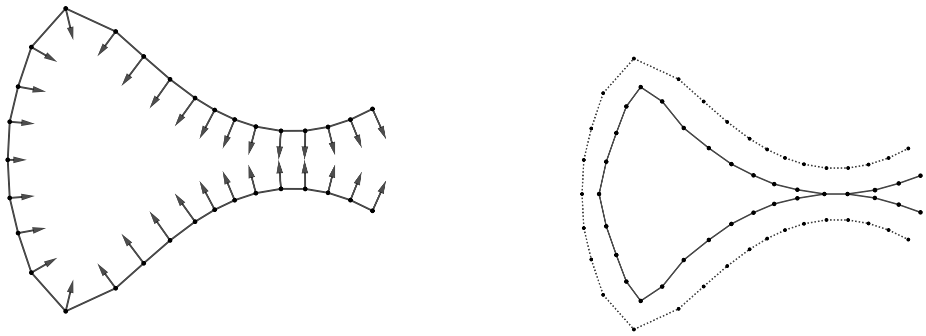


Figure 3.1: Left: The original (Lipschitz) boundary. Right: The boundary after an update is not Lipschitz and the shape changes topology.

work of the shape derivative. For any $\theta \in \mathrm{W}_0^{k,\infty}(\Omega, \mathbb{R}^d),\ k \in \mathbb{N}$ the following holds

$$L((\mathrm{Id} + \theta)\Omega_\alpha) = L(\Omega_\alpha) + L'(\Omega_\alpha; \theta) + o(\|\theta\|_k)$$

so we define an ascent vector for L in the following manner:

Definition 3.1.1. *We say that $\theta \in \mathrm{W}_0^{k,\infty}(\Omega, \mathbb{R}^d)$ is an ascent vector for the shape functional L if there exists $\delta > 0$ such that for any $t \in \langle 0, \delta \rangle$*

$$L((\mathrm{Id} + t\theta)\Omega_\alpha) > L(\Omega_\alpha).$$

Observe that $\theta \in \mathrm{W}_0^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ implies that the outer boundary $\partial\Omega$ remains fixed during perturbations $\mathrm{Id} + t\theta$. This is standard for transmission models since we are only interested in changes to the interface Γ. After finding the ascent vector one then needs to define a step size t_0 and apply $\Phi_{t_0\theta} = \mathrm{Id} + t_0\theta$ to generate the next approximation of the interface Γ. In summary, every considered algorithm will follow the same procedure:

Algorithm 3.1.2.

1. *Input: approximation of interface Γ: $\mathcal{T}_k$*
2. *Construction of ascent vector θ*
3. *Determining step size t_0*
4. *Output: new approximation of interface Γ: $\mathcal{T}_{k+1}$*

3.1.2 Representation of shapes

The first step in numerical implementations is to determine a representation of shapes, particularly their boundaries. An explicit (Lagrange) approach represents boundary by the union of convex polygons (lines in 2D, triangles in 3D) arranged so that the intersection

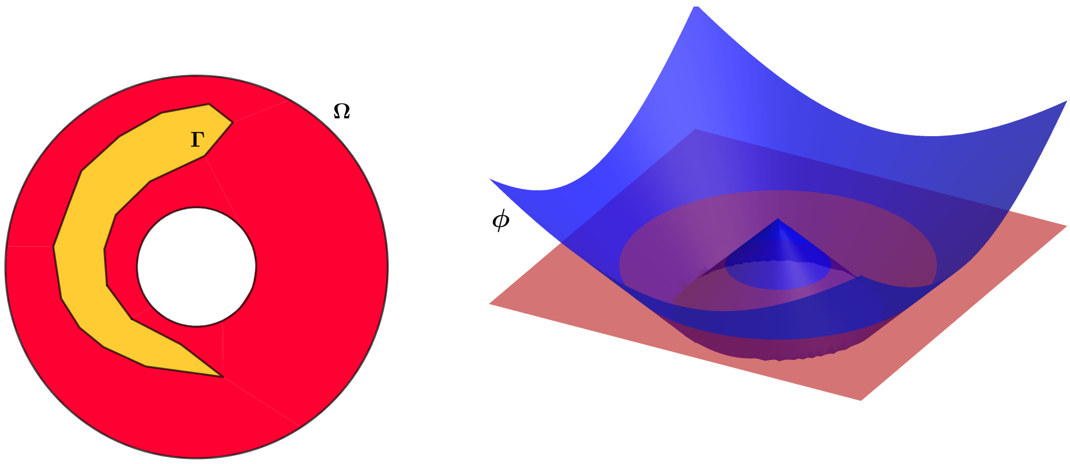


Figure 3.2: Left: Lagrange method in 2D. Right: Level set function ϕ in 2D.

of any two polygons is either a shared vertex or an edge or the empty set. This explicit way of approximating boundary simplifies any movement, e.g. by a perturbation of identity $\Phi_{t\theta} = \mathrm{Id} + t\theta$ we only have to update a position of each vertex. Unfortunately, this approach requires special care when dealing with changes in topologies which may occur because we do not require for the map $\Phi_{t\theta}$ to be a bijection (observe Figures 3.1).

Another implicit approach is by a level set function which can be used to represent a shape. A level set function $\phi : \Omega \to \mathbb{R}$ is usually constructed by the following property:

$$\begin{cases} \Omega_\beta = \phi^{-1}(\langle 0, \infty\rangle), \\ \Gamma = \phi^{-1}(\{0\}) \\ \Omega_\alpha = \phi^{-1}(\langle -\infty, 0\rangle \end{cases} \tag{3.4}$$

meaning that the boundary Γ is implicitly given as the preimage of $\{0\}$ under ϕ. The method can handle topological changes of shapes in a more elegant way, e.g. by replacing ϕ by $\phi \pm \varepsilon$ for a small constant ε. Both representations of shapes shall be used in our numerical implementations.

3.1.3 Calculations of ascent vector for first order shape derivative

The second step in the algorithm is a construction of an ascent vector. There are many ways how this can be accomplished, but we will focus on one particular approach which is technically easier to implement. We say that a distribution $T : C_c^\infty(D; \mathbb{C})$ is continuous if the following condition is satisfied:

$$\forall K \subset\subset D,\ \exists n \in \mathbb{N},\ \exists C_k > 0\ :\ |T(\varphi)| \leq \|\varphi\|_{\mathrm{W}^{n,\infty}(K)}.$$

The order of distribution T is the smallest integer $k \in \mathbb{N}$ for which the following holds:

$$\forall K \subset\subset D,\ \exists C_k > 0 \ :\ |T(\varphi)| \leq \|\varphi\|_{\mathrm{W}^{k,\infty}(K)}$$

If this integer does not exist, the order of the distribution is defined as infinity.

Let us recall the Hadamard structure theorem for the first order shape derivative:

Theorem 3.1.3. *Assume that $\partial\omega \subset\subset D$ is of class C^k and shape functional J such that $\theta \mapsto J((\mathrm{Id}+\theta)\omega)$ is well defined in a neighbourhood of $\mathrm{W}^{k+1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ and differentiable at zero. Then*

$$C_c^\infty(D, \mathbb{R}^d) \to \mathbb{R} : \theta \mapsto J'(\omega;\theta)$$

defines a distribution of order less than or equal to $k \geq 0$. Moreover, if $\partial\omega$ is of class C^{k+1} then there exists a continuous functional $l_1 : C^k(\partial\omega) \to \mathbb{R}$ such that

$$J'(\omega,\theta) = l_1(\theta_\Gamma \cdot \boldsymbol{n}).$$

Proof. See Chapter 9, Section 3.4 of [21], Theorem 3.6. and Corollary 1. See also Section 5.9 of [30]. $\square$

It means that the support of $J'(\omega;\theta)$ is on the boundary $\partial\omega$. For example, in Theorem 2.2.16 the shape derivative of the energy functional in our transmission problem is given by the expression (2.23):

$$J'(\Omega_\alpha;\theta) = \int_\Gamma \theta \cdot \boldsymbol{n}_\alpha \left[2\left\{ \alpha \left|\frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha}\right|^2 - \beta \left|\frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha}\right|^2 \right\} - \left\{ \alpha|\nabla u_\alpha|^2 - \beta|\nabla u_\beta|^2 \right\} \right] \mathrm{d}S. \tag{3.5}$$

Usually, we have an existence of $g_0 \in \mathrm{L}^2(\partial\omega)$ such that

$$J'(\omega;\theta) = \int_{\partial\omega} g_0\, \theta \cdot \boldsymbol{n} \,\mathrm{d}S.$$

Proposition 2.1.12 states that for all ”free PDE” shape functional $G(\omega) = \int_\omega f(x)\,\mathrm{d}x$ if ω is Lipschitz domain and $f \in \mathrm{W}^{1,1}(\mathbb{R}^d)$ then its shape derivative at ω in direction $\theta \in \mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ is in the following form:

$$G'(\omega;\theta) = \int_{\partial\omega} f\,\theta \cdot \boldsymbol{n},$$

Furthermore, one works with $g_0 \in C(\partial\omega)$ whenever it is possible. For the shape derivative of the volume this is satisfied since for any $\theta \in \mathrm{W}_0^{k,\infty}(\Omega;\mathbb{R}^d)$:

$$\mathrm{vol}'(\Omega_\alpha;\theta) = \int\limits_\Gamma 1(\theta\cdot\boldsymbol{n})\,\mathrm{d}S$$

if the Assumption 2.1.16 holds. For the expression (3.5) this is also true under higher regularity assumptions to the interface and the right-hand side. For example in both dimension two and three for the right hand side $f \in \mathrm{H}^1(\Omega)$ and the interface Γ being of class C^3 we have that $u_\alpha \in \mathrm{H}^3(\Omega_\alpha)$ and $u_\beta \in \mathrm{H}^3(\Omega_\beta)$. The classical Sobolev Embedding Theorem then states that $u_\alpha \in C^1(\overline{\Omega}_\alpha)$ and $u_\beta \in C^1(\overline{\Omega}_\beta)$ (see Theorem 6.3 in [2]) meaning that integrand in (3.5) consists of a continuous function multiplied with the term $(\theta\cdot\boldsymbol{n})$. Therefore Lagrangian functional (3.2) for $\lambda > 0$ admits the form

$$L'(\Omega_\alpha;\theta) = J'(\Omega_\alpha;\theta) - \lambda\,\mathrm{vol}'(\Omega_\alpha;\theta) = \int\limits_\Gamma g_0\,\theta\cdot\boldsymbol{n}\,\mathrm{d}S$$

where $g_0 \in C(\Gamma)$ under suitable regularity assumptions.

Let $\theta \in \mathrm{W}_0^{k,\infty}(\mathbb{R}^d,\mathbb{R}^d)$, $k\in\mathbb{N}$ be such that

$$\theta = g_0\boldsymbol{n}, \qquad \text{on } \Gamma. \tag{3.6}$$

Since the following holds

$$\begin{aligned} L((\mathrm{Id}+t\theta)\Omega_\alpha) - L(\Omega_\alpha) &= tL'(\Omega_\alpha;\theta) + o(t) \\ &= t\int\limits_\Gamma g_0^2\,\mathrm{d}S + o(t) \end{aligned}$$

there exists $\delta > 0$ such that for any $t \in \langle 0,\delta\rangle$

$$L((\mathrm{Id}+t\theta)\Omega_\alpha) - L(\Omega_\alpha) > 0,$$

meaning that θ is an ascent vector for L. Unfortunately, possible lack of regularity of g_0 can make this reasoning ambiguous, e.g. for the interface Γ of C^2 we have existence of (3.5) but g_0 may fail to be continuous. One way to mitigate this problem is by a classical regularization technique by virtue of the Poisson equation:

$$\begin{cases} -\Delta\theta = 0, & \text{in } \Omega \\ \nabla\theta\boldsymbol{n} = g_0\boldsymbol{n}, & \text{on } \Gamma \\ \theta = 0, & \text{on } \partial\Omega,+. \end{cases} \tag{3.7}$$

By the Lax-Milgram lemma we have a unique solution of (3.7) denoted by $\theta_0 \in \mathrm{H}_0^1(\Omega)$

which satisfies the following:

$$0 < \int_\Omega \nabla\theta_0 : \nabla\theta_0 \,\mathrm{d}x = \int_\Gamma g_0\theta_0 \cdot \boldsymbol{n} \,\mathrm{d}S, \text{ for } g_0 \neq 0,$$

making it an ascent vector for L. Moreover, (3.6) is replaced by the following condition (in terms of traces):

$$\nabla\theta_0\boldsymbol{n} = g_0\boldsymbol{n}, \qquad \text{on } \Gamma.$$

Remark 3.1.4. *The previous extensions is motivated by the Neumann-to-Dirichlet map. If $\theta \in \mathrm{H}^1(\omega)$ solves the following problem:*

$$\begin{cases} -\Delta\theta = 0, & \text{in } \omega \\ \nabla\theta\boldsymbol{n} = g\boldsymbol{n}, & \text{on } \partial\omega, \end{cases}$$

then the map $g\boldsymbol{n} \mapsto \theta_{|\partial\omega} : \mathrm{H}^{-1/2}(\partial\omega;\mathbb{R}^d) \to \mathrm{H}^{1/2}(\partial\omega;\mathbb{R}^d)$ is well defined and gives an ascent vector θ for the functional $G(\theta) = \int_{\partial\omega} g\theta \cdot \boldsymbol{n} \,\mathrm{d}S$ whenever the velocity field is not regular enough. One can also smooth boundary data g directly by applying Laplace-Beltrami operator on the boundary $\partial\omega$. For details see [8].

In the same manner one can use a scalar product for $\mathrm{H}^1(\Omega)$ to obtain a vector function $\theta \in \mathrm{H}^1_0(\Omega)$ such that

$$\int_\Omega \eta\nabla\theta : \nabla\varphi + \theta\cdot\varphi \,\mathrm{d}x = \int_\Gamma g_0\varphi \cdot \boldsymbol{n} \,\mathrm{d}S, \quad \varphi \in \mathrm{H}^1_0(\Omega)$$

for some fixed $\eta > 0$. Note that such θ also doesn't satisfy condition (3.6) but it is an ascent vector for the functional L since

$$0 < \int_\Omega \eta\nabla\theta : \nabla\theta + \theta\cdot\theta \,\mathrm{d}x = \int_\Gamma g_0\theta \cdot \boldsymbol{n} \,\mathrm{d}S, \text{ for } g_0 \neq 0.$$

Thus one can construct an ascent vector by solving the following boundary value problem:

$$\begin{cases} \text{find } \theta \in \mathrm{H}^1_0(\Omega)^d \text{ such that} \\ \int_\Omega \eta\nabla\theta : \nabla\varphi + \theta\cdot\varphi \,\mathrm{d}x = L'(\Omega_\alpha;\varphi), \quad \varphi \in \mathrm{H}^1_0(\Omega). \end{cases} \tag{3.8}$$

where $\eta > 0$. The problem (3.8) is considered in [9],[34],[35] and it seems appropriate for transmission problems, as well for problems arising in the electrical impedance tomography. The right-hand side $L'(\Omega_\alpha;\cdot)$ is usually left in the distributional (volume) form. From the numerical aspect, this is reasonable, since it requires less regularity then boundary representations. Recent results have also shown that a distributed shape derivative is more accurate than a boundary representation from a numerical point of view (see [42]).

Remark 3.1.5. *Let us emphasize the fact that the space* $\mathrm{W}_0^{k,\infty}(\Omega,\mathbb{R}^d), k \in \mathbb{N}$ *is not a Hilbert space, since the scalar product*

$$\langle\theta,\varphi\rangle = \int_{\Omega} \eta\nabla\theta : \nabla\varphi + \theta\cdot\varphi \,\mathrm{d}x$$

is not complete for the norm induced by the preceding inner product. Note that the completion of the space $\mathrm{W}_0^{k,\infty}(\Omega,\mathbb{R}^d)$ *with respect to the scalar product is* $\mathrm{H}_0^1(\Omega)$*, for which the notion of shape differentiability is not defined. Indeed, as we can see in Definitions 2.1.9 and 2.1.10 the perturbations of identity* $\mathrm{Id}+\theta$ *are not even continuous for* $\theta \in \mathrm{H}_0^1(\Omega)$*. Furthermore, in [35] a scalar product for* $\mathrm{H}^k(\Omega)$ *is used but we are not going to implement it because it may lead to excessive numerical regularization. Also we shall be using only distributed representations of the shape derivative so there is no need for a scalar product involving derivatives of the order higher then 1.*

Therefore, we propose the following numerical method for solving problem (2.9):

Method 3.1.6 (Gradient method)**.** *In the second part of Algorithm 3.1.2 we construct an ascent vector using the first order shape derivative of* L *by solving: find* $\theta \in \mathrm{H}_0^1(\Omega)$ *such that*

$$\int_{\Omega} \eta\nabla\theta : \nabla\psi + \theta\cdot\psi \,\mathrm{d}x = L'(\Omega_\alpha;\psi), \quad \psi \in \mathrm{H}_0^1(\Omega)$$

where $\eta = \eta(\mathcal{T}_k) > 0$ *depends on the average diameter of simplices in triangulation.*

One can understand solution of (3.8) as an “extension” of $L'(\Omega_\alpha;\theta)$ from interface Γ to the domain Ω, so we shall be calling it a gradient method. Strictly speaking we are dealing with an ascent method which uses an approximative extension in H^1 obtained from the first order shape derivative.

Remark 3.1.7. *The constant* η *is a small positive parameter, typically of the order of mesh cell diameters. The motivation behind this approach can be found indirectly in [54],[23] and will play key role later for implementation of the second order shape derivative. For an ascent vector based only on the first order shape derivative standard scalar product with* $\eta = 1$ *can be used. Numerically, an ascent vector calculated with smaller* η *has the support smaller compared to the ascent vector corresponding to a larger* η*.*

3.1.4 Level set function and applications

By using an explicit (Lagrange) representation of shapes we can apply any perturbation $\Phi_{t\theta}$ in a straightforward manner. In Section 3.1.6 an example of such implementation of gradient method in 2D is written in `Freefem++`. While the simulation is quite stable one can easily observe that implemented explicit representations of shape does not change the topology of the shape. Essentially, in order to achieve convergence one has to offer an initial shape approximation which is topologically equivalent to the optimal solution (notice that the existence of optimal solution is not a trivial questions for problems which are not spherically symmetric).

Implementations based on level set functions, also known as the level set methods, for a given shape Ω_α introduce a scalar function ϕ which satisfy (3.4). There are several ways how one can create such level set function. One canonical way to create it is by an interface distance function (see Definition 2.2.7):

$$\phi(x) := d_{\Gamma|\Omega}(x) = \begin{cases} \operatorname{dist}(x,\Gamma), & x \in \Omega_\beta \\ 0, & x \in \Gamma \\ -\operatorname{dist}(x,\Gamma), & x \in \Omega_\alpha. \end{cases} \tag{3.9}$$

Numerically, one can obtain it as a steady state solution of the unsteady Eikonal equation, also known as the redistancing equation:

$$\begin{cases} \partial_t \phi + \operatorname{sgn}(\phi_0)(\|\nabla\phi\| - 1) = 0, & \text{in } \langle 0,\infty\rangle \times \Omega \\ \phi(0,\cdot) = \phi_0(x), & \text{on } \Omega, \end{cases} \tag{3.10}$$

where ϕ_0 is any continuous function that satisfies (3.4). For details see [20].

Hamilton-Jacobi equation

Assume that the interface Γ evolves under fictitious time, meaning $\Gamma(t) = \Phi_{t\theta}(\Gamma)$ where θ is a given ascent/descent vector for L. Then, there exists a mapping $t \mapsto \phi(t,\cdot)$ with the following property

$$\phi(t, x(t)) = 0 \iff x(t) \in \Gamma(t).$$

Taking the derivative of the above expression with respect to t gives

$$\partial_t \phi + \dot{x} \cdot \nabla\phi = 0.$$

Since the ascent/descent vector θ is already calculated and $\Gamma(t) = (\mathrm{Id} + t\theta)\Gamma$ then $\dot{x}(t) = \theta$ giving us a simple Hamilton-Jacobi equation:

$$\partial_t \phi + \theta \cdot \nabla\phi = 0. \tag{3.11}$$

Observe that the previous equation is posed in the whole domain Ω and not only on the interface Γ.

Numerically, we are dealing with a sequence of level set function ϕ_k, $k = 0, 1, \ldots$. For the current function ϕ_k we calculate the respective ascent/descent vector θ_k and define step size $t_k > 0$. From (3.11) we know how to propagate ϕ_k by the following level set advection equation:

$$\begin{cases} \partial_t \phi + \theta^k \cdot \nabla \phi = 0, & \text{in } \langle 0, t_k \rangle \times \Omega, \\ \phi(0, \cdot) = \phi_k, & \text{in } \Omega. \end{cases} \tag{3.12}$$

We can see that transporting ϕ_k with (3.12) is equivalent to moving the interface Γ along direction θ. Then we use the solution ϕ of (3.12) to define the next level set function by $\phi_{k+1} := \phi(t_k, \cdot)$. Even if we start with $\phi_k = b_{\Gamma_k}$ solution of advection equation (3.12) will fail to be an interface distance function. Therefore, it is recommended to reinitialize the level set function after several iterations.

Remark 3.1.8. *Periodic reinitialization of the level set function by* (3.9) *is standard in shape optimization, see [8]. The reinitialization is sometimes done after every step of level set advection as in [6], meaning that* b_{Γ_k} *is used instead of* ϕ_k *for initial condition in* (3.12).

To illustrate why this is needed, one can imagine a level set function ϕ_k *with two distinct disjunct areas: in area around* $\Gamma_1 \subset \Gamma$, $\|\nabla \phi_k\| \approx 50\|\boldsymbol{n}\|$ *and in area around* $\Gamma_2 \subset \Gamma$ $\|\nabla \phi_k\| \approx 0.5\|\boldsymbol{n}\|$. *Let's say that ascent vector* θ_k *for* L *on* Γ_k *satisfies locally in an area around* Γ_1 *and* Γ_2 *that* $\theta_k \approx \boldsymbol{n}$, *meaning that homeomorphism* $\mathrm{Id} + t\theta_k$ *should move boundaries* Γ_1 *and* Γ_2 *approximately the same amount in the direction of the normal of* Γ. *By solving* (3.12) *this is not satisfied since "moving" of boundary* Γ_1 *results in drastically smaller change then that of boundary* Γ_2. *This means that an advection* (3.12) *could lead to an incorrect applications of the homeomorphism* $\Phi_{t\theta} = \mathrm{Id} + t\theta_k$, *making periodic reinitialization of level set function a necessary step.*

How often should one reinitialize a level set function? This depends on the concrete optimization problem, particularly on regularity of state equations, functional, choice of initial approximation, etc. Heuristically, one needs to find balance between the computational cost (speed) and the stability of numerical scheme. In [34] where the distributed (volume) shape gradient was used it was observed experimentally that the level set functions ϕ_k *remained a good approximations of the corresponding oriented distance functions during simulations. They hypothesized this is due to better regularity of the velocity vector.*

Scalar approach

To complete this section let us also describe another popular approach for constructing ascent/descent vectors. As we mentioned before when the shape derivative is given with

$$L'(\Omega_\alpha; \theta) = \int_\Gamma g_0\, \theta \cdot \boldsymbol{n} \,\mathrm{d}S$$

for some $g_0 \in \mathrm{L}^2(\Gamma)$, the main idea is to construct an ascent vector $\theta \in \mathrm{W}_0^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$

with the following property:

$$\theta = g_0 \boldsymbol{n}, \quad \text{on } \Gamma.$$

Then Hamilton-Jacobi equation (3.11) on Γ satisfies

$$\partial_t \phi + g_0 \boldsymbol{n} \cdot \nabla \phi = 0.$$

Since the normal on Γ can be recovered from the level set function by $\boldsymbol{n} = \frac{\nabla\phi}{\|\nabla\phi\|}$ we get:

$$\partial_t \phi + g_0 \boldsymbol{n} \cdot \nabla \phi = \partial_t \phi + g_0 \frac{\nabla \phi}{\|\nabla \phi\|} \cdot \nabla \phi = \partial_t \phi + g_0 \|\nabla \theta\| = 0, \quad \text{on } \Gamma.$$

If we were given an extension g of g_0, we have well defined Hamilton-Jacobi equation on Ω:

$$\partial_t \phi + g\|\nabla \phi\| = 0. \tag{3.13}$$

Then, we only have to solve a level set advection equation in order to move the interface. Extension $g \in \mathrm{H}_0^1(\Omega)$ of g_0 can be constructed by means of the following scalar elliptic equation:

$$\int\limits_{\Omega} \nabla g \cdot \nabla \varphi + g\varphi \, \mathrm{d}x = \int\limits_{\Gamma} g_0 \varphi \, \mathrm{d}S, \quad \varphi \in \mathrm{H}_0^1(\Omega) \tag{3.14}$$

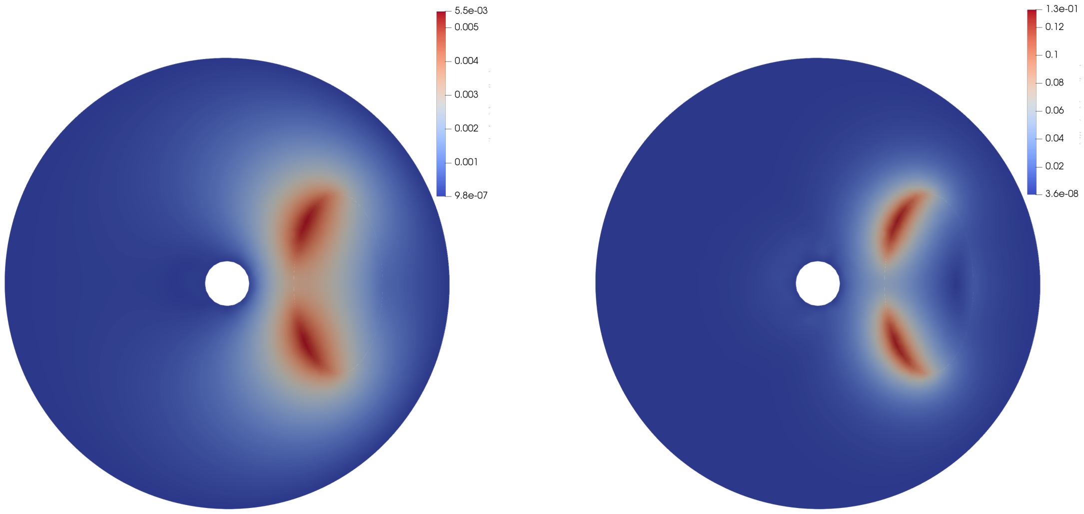
provided $g_0 \in \mathrm{H}^{1/2}(\Gamma)$.

There are several advantages for using scalar this approach. Main advantage is that everything is done with less variables, e.g. in the vector case in order to define a vector θ, one need to solve the system of partial differential equations, while in the scalar case extensions g can be found with only one partial differential equation. The other advantage of the scalar version is the fact that an ascent/descent vector is never fully constructed since in (3.13) advection for ϕ only requires scalar function g. When dealing with contact problems, i.e. connection of two disjunct parts of interfaces, there are also numerical advantages regarding regularity of the vector field θ. If seen as distribution over Ω, the normal velocity is more regular than the vector velocity (see Figure 3.1 where $\theta \cdot \boldsymbol{n}$ is of constant sign unlike θ which changes orientation). For more details, see [23].

Remark 3.1.9. *While the scalar approach offers several advantages, it always highly depends on the background problem. Finding g_0 numerically may be ill-posed, especially for transmission problems where discontinuous jumps are present. Observe that for energy functional respective boundary shape derivative is:*

$$J'(\Omega_\alpha; \theta) = \int_\Gamma \theta \cdot \boldsymbol{n}_\alpha \left[2 \left\{ \alpha \left| \frac{\partial u_\alpha}{\partial \boldsymbol{n}_\alpha} \right|^2 - \beta \left| \frac{\partial u_\beta}{\partial \boldsymbol{n}_\alpha} \right|^2 \right\} - \left\{ \alpha |\nabla u_\alpha|^2 - \beta |\nabla u_\beta|^2 \right\} \right] \mathrm{d}S.$$

making g_0 a difference of two functions in $\mathrm{L}^2(\Gamma)$. Generally, just evaluation of boundary integrals is hard task and should be taken with special care making distributed shape derivative much easier to implement as described in Method 3.1.6. Furthermore, support of distributed $L'(\Omega_\alpha;\theta)$ is again present in the vicinity of the interface as one can see in Figure 3.3 where θ is well defined in a neighbourhood of the interface.



(a) $\eta = 1$ (b) $\eta = 0.015 \approx$ mesh size

Figure 3.3: Ascent vector θ obtained by Method 3.1.6.

By taking a smaller η and a finer mesh, the support of the distributed (volume) shape derivative shrinks as demonstrated on Figure 3.3. While there is no difference for Method 3.1.6, with appropriate scaling of the step size smaller η will play key role for the second order shape derivative. This also means that the distributed shape derivative can only be computed in a neighbourhood of the interface as it was done in [1].

3.1.5 Newton-like methods

If $L''(\Omega_\alpha;\theta,\psi)$ and $L'(\Omega_\alpha;\theta)$ are known, ideally one would like to find $\theta \in \mathrm{W}_0^{k,\infty}(\mathbb{R}^d,\mathbb{R}^d)$ such that

$$L''(\Omega_\alpha;\theta,\psi) = -L'(\Omega_\alpha,\psi), \quad \psi \in \mathrm{W}_0^{k,\infty}(\mathbb{R}^d,\mathbb{R}^d), \tag{3.15}$$

or equivalently an extreme point of

$$\theta \mapsto L'(\Omega_\alpha,\theta) + \frac{1}{2}L''(\Omega_\alpha;\theta,\theta)$$

since locally we want to maximize (or minimize) Lagrange function L.

There are many approaches for implementation of Newton's like methods for the previous problem. For Newton methods based on the second order shape derivatives in a boundary form we refer the interested reader to the doctoral dissertation by Vie [54], where an extensive overview of several numerical implementations is given (see also Remark 3.1.11). Naturally, we would like to find a solution to (3.15) directly, again by replacing space $\mathrm{W}_0^{k,\infty}(\mathbb{R}^d,\mathbb{R}^d)$ by $H_0^k(\Omega;\mathbb{R}^d)$ but this trick does not work particularly well for the second order methods. One can show that the map $(\theta,\psi)\mapsto L''(\Omega_\alpha;\theta,\psi)$ is a bilinear continuous functional which is not coercive on $H_0^k(\Omega;\mathbb{R}^d)$, i.e. there are no guaranties that there exists $\theta\in \mathrm{H}_0^1(\Omega)$ such that

$$L''(\Omega_\alpha;\theta,\psi) = -L'(\Omega_\alpha,\psi), \quad \psi\in \mathrm{H}_0^1(\Omega)$$

This is quite standard since differentiability is usually expressed in terms of the norm of space $\mathrm{W}^{k,\infty}(\mathbb{R}^d;\mathbb{R}^d)$, but even if the coercivity holds, it holds only for a (weaker) norm of spaces like $C(\Gamma)$ or $\mathrm{H}^{1/2}(\Gamma)$. One way to treat this deficiency is by solving (3.15) directly on the interface Γ.

Let us recall the structure theorem regarding the first and the second order shape derivative:

Theorem 3.1.10. *Assume that $\partial\omega$ is compact, $J = J(\omega)$ is a given shape functional and $k\in\mathbb{N}$.*

1) If $\partial\omega$ is of class C^{k+1} and J is differentiable at ω then there exists a continuous linear map $l_1 : C^1(\partial\omega)\to\mathbb{R}$ such that for all $\theta\in W^{k+1,\infty}(\mathbb{R}^d,\mathbb{R}^d)$:

$$J'(\omega;\theta) = l_1(\theta\cdot\boldsymbol{n}).$$

2) If $\partial\omega$ is of class C^{k+2} and J is twice differentiable at ω then there exists a continuous bilinear map $l_2 : C^2(\partial\omega)\to\mathbb{R}$ such that for all $\theta,\psi\in W^{k+2,\infty}(\mathbb{R}^d,\mathbb{R}^d)$:

$$J''(\omega;\theta,\psi) = l_2(\theta\cdot\boldsymbol{n},\psi\cdot\boldsymbol{n}) + l_1(\nabla\boldsymbol{n}^{\mathcal{T}}\theta_{\partial\omega}\cdot\psi_{\partial\omega} - \nabla_{\partial\omega}(\theta\cdot\boldsymbol{n})\cdot\psi_{\partial\omega} - \nabla_{\partial\omega}(\psi\cdot\boldsymbol{n})\cdot\theta_{\partial\omega})$$

Remark 3.1.11. *The structure theorem depends highly on the choice of a family of homeomorphism by which the shape ω, or rather the boundary of the shape, is propagated. A shape derivation with respect to a normal evolution is considered, particularly we refer to Theorem 10.1.4. in [54]:*

Theorem 3.1.12. *Let $k\in\mathbb{N}$, $J = J(\omega)$ be a shape functional, twice differentiable at domain ω_0 with C^{k+2} boundary and $v(t,x)$ be a C^k real function defined on $R^+\times R^d$. Let ϕ_0 be the signed distance function associated to ω_0. For some time $\tau>0$, let $\phi\in C^{k+2}([0,\tau]\times\mathbb{R}^d)$ be a smooth solution of*

$$\begin{cases} \partial_t\phi(t,x) + v(t,x)|\nabla\phi(t,x)| = 0, \\ \phi(0,x) = \phi_0(x). \end{cases} \tag{3.16}$$

Define $\omega_t = \{x \in \mathbb{R}^d : \phi(t,x) < 0\}$ *and* $k(t) = J(\omega_t)$. *Then* k *is twice differentiable at* 0 *and it holds*

$$k'(0) = l_1(v(0,\cdot)) \quad and \quad k''(0) = l_2(v(0,\cdot), v(0,\cdot)) + l_1(z_v(0,\cdot)),$$

where linear form l_1 *and bilinear form* l_2 *are defined as in Theorem 3.1.10, and where* $z_v = \partial_t v + v\nabla v \cdot \boldsymbol{n}$.

Then

$$\begin{aligned} J(\omega_t) &= J(\omega_0) + tk'(0) + \frac{t^2}{2}k''(0) + o(t^2) \\ &= J(\omega_0) + tl_1(v_\gamma) + \frac{t^2}{2}(l_2(v_\gamma, v_\gamma) + l_1(\partial_t v_\gamma + v_\gamma \nabla v_\gamma \cdot \boldsymbol{n})) + o(t^2) \end{aligned}$$

where v_γ *is chosen as an function from* $\partial\omega$ *to* $\mathbb{R}$*, which for simplicity is time-independent, i.e.* $\partial_t v_\gamma = 0$. *By choosing* v_γ *such that*

$$l_2(v_\gamma, w) = -l_1(w), \quad w \in C^k(\partial\omega) \tag{3.17}$$

one can construct an extensions of v_γ *such that* $l_1(v_\gamma \nabla v_\gamma \cdot \boldsymbol{n}) \leq 0$ *by adapting Eikonal equation* (3.10). *Problem* (3.17) *is solved numerically on the* $\partial\omega$*, offering scalar version of a descent vector.*

As we can see the support of the second order shape derivative is again present in Γ, e.g. see result of the Theorem 2.3.5, therefore it is natural to try to solve a problem (3.15) on the interface Γ. Notice that $u'_\alpha(\theta)$ and $u'_\beta(\theta)$ can be understood as functions of $(\theta \cdot \boldsymbol{n})$ from (2.28) which justifies the expression in Theorem 3.1.10.

Now we have everything to present a modified Newton method for searching an ascent vector for the Lagrange functional L. The main idea is to solve (3.15) using distributed volume representation:

$$L''(\Omega_\alpha; \theta, \psi) = -L'(\Omega_\alpha, \psi), \quad \psi \in \mathrm{H}^1_0(\Omega).$$

First due to Remark 2.3.9 instead of using the full second order shape derivative

$$J''(\Omega_\alpha; \theta, \psi) = J''_{\text{design}}(\Omega_\alpha; \theta, \psi) + J''_{\text{u}}(\Omega_\alpha; \theta, \psi)$$

we replace it with only $J''_{\text{design}}(\Omega_\alpha; \theta, \psi)$ since $J''_{\text{u}}(\Omega_\alpha; \theta, \psi)$ always leads to a full matrix. Now we need to solve

$$L''_{\text{design}}(\Omega_\alpha; \theta, \psi) = -L'(\Omega_\alpha, \psi), \quad \psi \in \mathrm{H}^1_0(\Omega),$$

where $L''_{\text{design}}(\Omega_\alpha; \theta, \psi) = J''_{\text{design}}(\Omega_\alpha; \theta, \psi) - \lambda \text{vol}''(\Omega_\alpha; \theta, \psi)$. Due to the obvious lack of coercivity and since we are searching for the maximum we introduce $L''_{\text{design}}(\Omega_\alpha;\theta,\psi) - \langle\theta,\psi\rangle$ instead of $L''_{\text{design}}(\Omega_\alpha;\theta,\psi)$ on the left-hand side of the equation, thus giving us

$$-\langle\theta,\psi\rangle + L''_{\text{design}}(\Omega_\alpha;\theta,\psi) = -L'(\Omega_\alpha,\psi), \quad \psi \in \mathrm{H}^1_0(\Omega).$$

Since we want to solve $L''_{\text{design}}(\Omega_\alpha;\theta,\psi) = -L'(\Omega_\alpha,\psi)$ on the interface Γ for scalar product we choose

$$\langle\theta,\psi\rangle = \int_\Omega \eta\nabla\theta : \nabla\psi + \theta\cdot\psi \,\mathrm{d}x$$

where η is small positive parameter, typically of the order of mesh cell diameters. We propose the following heuristic for finding the ascent vector:

Method 3.1.13 (Newton-like method)**.** *In the second part of Algorithm 3.1.2 construct an ascent vector using the first and the second order shape derivative of L: find $\theta \in \mathrm{H}^1_0(\Omega)$ such that*

$$\int_\Omega \eta\nabla\theta : \nabla\psi + \theta\cdot\psi\,\mathrm{d}x = L'(\Omega_\alpha;\psi) + J''_{\text{design}}(\Omega_\alpha;\theta,\psi) - \lambda\mathrm{vol}''(\Omega_\alpha;\theta,\psi),\ \psi \in \mathrm{H}^1_0(\Omega),$$

where $\eta = \eta(\mathcal{T}_k) > 0$ depends on the size of average diameter of simplices in triangulation.

Remark 3.1.14. *The idea behind this Newton-like method is rather simple. Let $\mathcal{T}_h$ be a uniform conforming triangulation of Ω of size h. We introduce $\mathcal{V}_h \subset \mathrm{H}^1_0(\Omega)$ the Lagrange finite elements space of continuous scalar function that are piecewise linear functions on each simplex of the triangulation. For each vertex q_i, $i = 1, 2, ..., N_h$ the basis function ϕ_i in $\mathcal{V}_h$ is given with the following properties:*

$$\phi_j(q_i) = \delta_{ij} \quad i = 1, ..., N_h, j = 1, ..., N_h$$

and for every $v \in V_h$

$$v(x) = \sum_{i=1}^{N_h} v(q_i)\phi_i(x).$$

Ideally, we would like to solve the following variational equation:

$$\begin{cases} \text{find } u_h \in V_h, \text{ such that} \\ L''_{\text{design}}(\Omega_\alpha; u_h, v_h) = -L'(\Omega_\alpha; v_h), \quad v_h \in V_h. \end{cases} \tag{3.18}$$

but this leads to severely ill-posed problem since the support of the $L''(\Omega_\alpha; u_h, v_h)$ is present only on the interface Γ. If we write $u_h = \sum_{i=1}^{N_h} u_i\phi_i(x)$ and test with $v = \phi_j$ for $j = 1, 2, ..., N_j$ we obtain stiffness matrix of problem (3.18) $A_{i,j} = L''_{\text{design}}(\Omega_\alpha; \phi_i, \phi_j)$ and the *right hand side* $F_i = -L'(\Omega_\alpha;\phi_i)$ *giving us the following linear system*

$$AU = F, \tag{3.19}$$

where $U_i = (u_1, ..., u_{N_h})^\tau$. *After testing with initial distribution of phases (see Figure 3.4)*

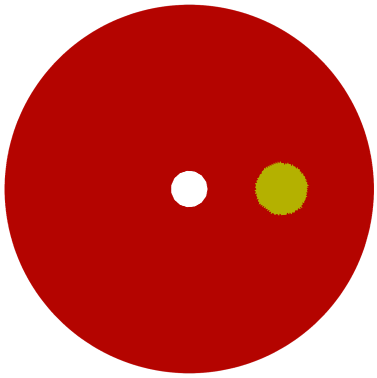


Figure 3.4: Initial approximation

with the best ascent method we have found the following: the stiffness matrix A *from* (3.19) *is indefinite matrix. In particular as can be seen in Figure 3.5 minimal eigenvalues are always less the* -0.5. *Furthermore, in several iteration if one takes ascent vector* $\theta_k \in \mathrm{H}^1_0(\Omega)$ *from Method 3.1.6 for* Ω^k_α *then both values* $L''_{\text{design}}(\Omega^k_\alpha;\theta^k,\theta^k)$ *and* $L''(\Omega^k_\alpha;\theta^k,\theta^k)$ *change signs. This limits possible numerical approaches but Method 3.1.13 shows rather nice behaviour.*

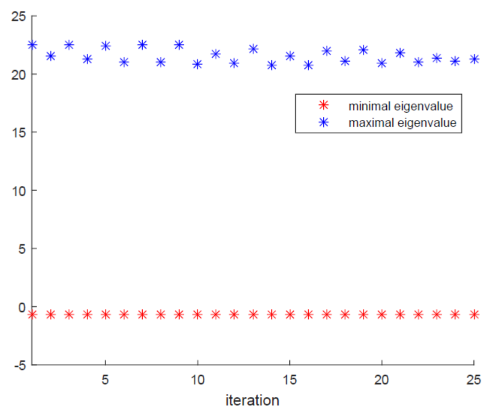


Figure 3.5: Minimal and maximal eigenvalue of stiffness matrix for each iteration of the best ascent method.

3.1.6 Code in Freefem++

```
real alpha = 0.5;     // conductivity
real beta = 1.0;
real r0=0.1;          // radii of annulus
real r1=1.0;
real lambda = .05;    // lagrange multiplier (fixed, for simplicity)
real coef=1;          // size of the step for shape gradient method
real sizeT=0.06;      // for mesh size
real eta=0.1; // for ascent vector
int maxIterat=200;    // number of iterations
func truncate=(((x*x+y*y)<0.999*r1^2 && (x*x+y*y) >1.001*r0^2)? 1:0);
// borders:
border OuterBorder (t=0,2*pi) { x=r1*cos(t); y=r1*sin(t); }        // outer border
border InnerBorder (t=0,2*pi) { x=r0*cos(t); y=r0*sin(t); }        // inner border
border Interface(t=0,2*pi) { x=0.4+0.2*cos(t); y=0.0+0.4*sin(t);}  // interface
// areas:
mesh Omega = buildmesh (OuterBorder(50)+Interface(30)+InnerBorder(-20));
Omega = adaptmesh (Omega,sizeT,IsMetric=1);
//    iteration of the method
for ( int k=0 ; k<maxIterat ; ++k) {
  // for creating conductivity
  fespace Ph(Omega,P0);
  Ph reg=region;
  int nBeta=reg(.45,.0);
  int nAlpha=reg(-r1+0.1,.0);
  Ph AA = alpha*(region==nAlpha) + beta*(region==nBeta);
  // for visual, could be turn off
  plot (AA, fill=1,ShowMeshes=1,wait=0);
  // creating space for vector function
  fespace VO(Omega,P1);
  VO u,theta1,theta2,v1,v2;
  problem StateEquation (u,v1) =
    int2d (Omega) (AA*(dx(u)*dx(v1)+dy(u)*dy(v1)))- int2d (Omega) (v1)
    + on (OuterBorder , u=0 ) + on (InnerBorder, u=0 );
  //  creation of ascent/descent vector function theta
  problem Main ( [theta1,theta2], [v1,v2] ) =
     int2d (Omega) (eta*(dx(theta1)*dx(v1)+dy(theta1)*dy(v1)+dx(theta2)*dx(v2)+dy(theta2)*dy(v2))+ theta1*v1+theta2*v2)
       - int2d (Omega) (2*AA*( dx(u)*dx(u)*dx(v1)+dy(u)*dy(u)*dy(v2) + dx(u)*dy(u)*(dx(v2)+dy(v1)))+ (dx(v1)+dy(v2))*(2*u-AA*(dx(u)*dx(u)+dy(u)*dy(u))))
     - int2d (Omega) (lambda*reg*(dx(v1)+dy(v2)))
    + on (OuterBorder , theta1=0 , theta2=0 )  + on (InnerBorder, theta1=0, theta2=0 );
  StateEquation;  Main;
  coef=2.0; // for determining if movemesh could be applied
  real minT0 = checkmovemesh (Omega,[x,y])/5.0;
  while(1) {
    real minT = checkmovemesh (Omega,[x+coef*truncate*psi1,y+coef*truncate*psi2]);
    if (minT > minT0) break ;
    coef/=2;
  }
  // moving mesh
  Omega = movemesh (Omega,[x+coef*truncate*psi1,y+coef*truncate*psi2]);
  Omega = adaptmesh (Omega,sizeT,IsMetric=1);
}
```

The implementation of the algorithm in `Freefem++` is particularly simple and results by a code no longer then 100 lines as we can see above. Applying the map $\Phi_{t\theta} = \mathrm{Id} + t\theta$ is done using `movemesh`. The procedure `checkmovemesh` was used to generate the step size which ensures that moving of mesh doesn't create wrong ordering of elements, i.e. volume of triangle should not be negative. In 2D for `Freefem++` we used `adaptmesh` which plays a key role for creating uniform regular mesh. Surprisingly, the previous code works very well in finding the optimal shape of the problem (2.9) considering that Lagrange (direct) representation is not best suited for changing the topology of a shape. For details about used procedures and short overview we recommend [29]. See also [9] for using `Freefem++` with shape derivatives. The most recent manual and software can be find on the webpage: `https://freefem.org/`.

Several versions of the algorithm using level set function approach were created. In current implementations we have used two algorithms `mshdist` and `advect` which do not come with `Freefem++`. The latter is a program for solving linear advection problems in two and three dimensions and `mshdist` is a simple algorithm to generate the signed distance function to given objects in two and three space dimensions (see [20]). They can be find on webpage: `https://github.com/ISCDtoolbox`. We would like to thank C. Dapogny for his advices and help on this topic.

3.2 Numerical results

3.2.1 Test of gradient based methods

In Figure 3.6 several iterations of the Algorithm 3.1.2 with 3.1.6 applied to (2.9) with a constant right-hand side $f \equiv 1$ on the annulus Ω are presented. White circles with radii r_+, r_- are calculated from system (1.40a)-(1.40c) with the prescribed amount q_0 of the first phase and represent interface between phases for the optimal shape given by Theorem 1.3.5.

Notice that we can guess the optimal radii r_+, r_- after few iterations: in all iterations the shape which represents phase β is a subset of the corresponding optimal shape. This phenomena is observed for different q_α but with small constant step size of the algorithm.

Figure 3.7 compares the optimal radii calculated from (1.40a)-(1.40c) and numerical approximations of radii obtained by the shape gradient method. While resulting differences are expected since domain is not a perfect annulus, with finer mesh one obtains more accurate approximation.

In Figure 3.8 the comparison of numerical and exact solution for multiple state optimal design problem is presented in terms of radii r_* and r^*, where annulus Ω was approximated with 2100 triangles. Here, the calculation of the shape derivative is straightforward: $J'(\Omega_\alpha, \psi) = \mu_1 J_1'(\Omega_\alpha, \psi) + \mu_2 J_2'(\Omega_\alpha, \psi)$ where $J_1'(\Omega, \psi)$ and $J_2'(\Omega, \psi)$ are the shape derivatives of energy functionals which are expressed by the formula (2.22).

Level set function was utilized in several manners. Particularly, we combined it with

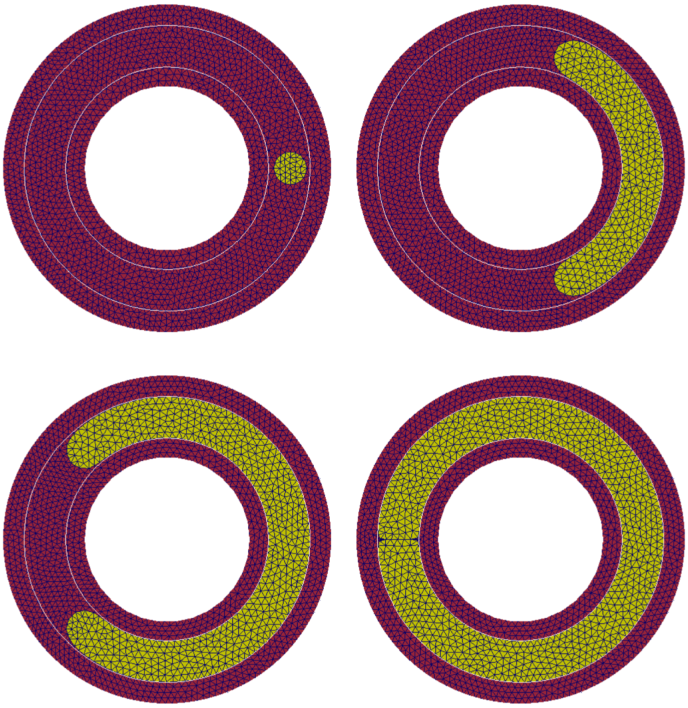


Figure 3.6: Numerical results for the single-state problem ($d = 2$) obtained with `Freefem++`; the white circles represent interface between phases in the optimal shape.

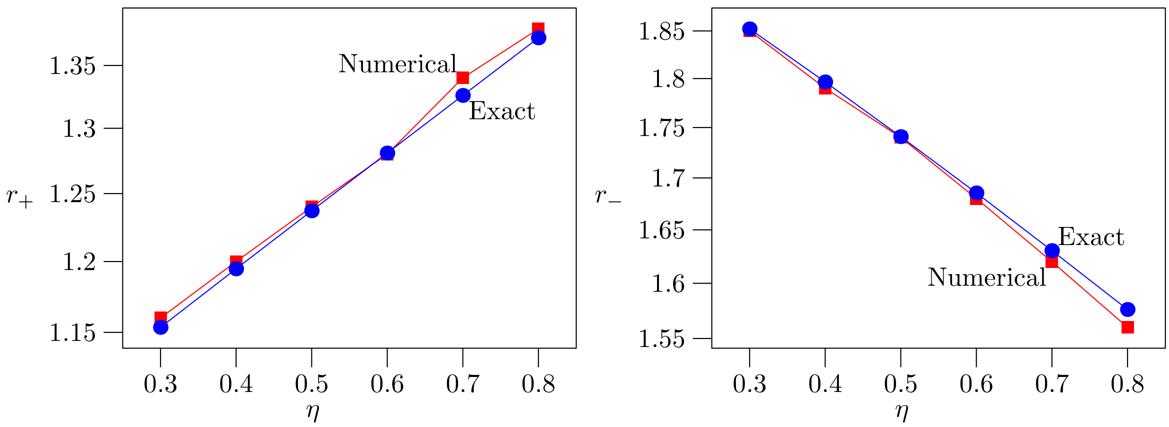


Figure 3.7: The comparison of the exact and numerical radii on a mesh with approximately 5300 triangles (the example from Section 2, $d = 2$).

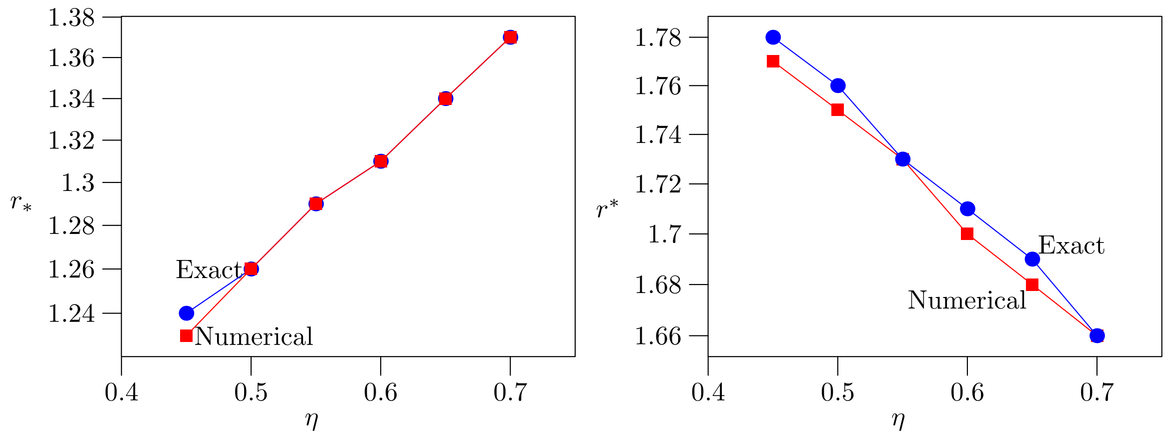


Figure 3.8: The comparison of the exact and numerical radii for the multiple state problem for $\alpha = 1$, $\beta = 2$, $r_1 = 1$, $r_2 = 2$, $\mu_1 = \mu_2 = 0.5$, and $b = 2.5$.

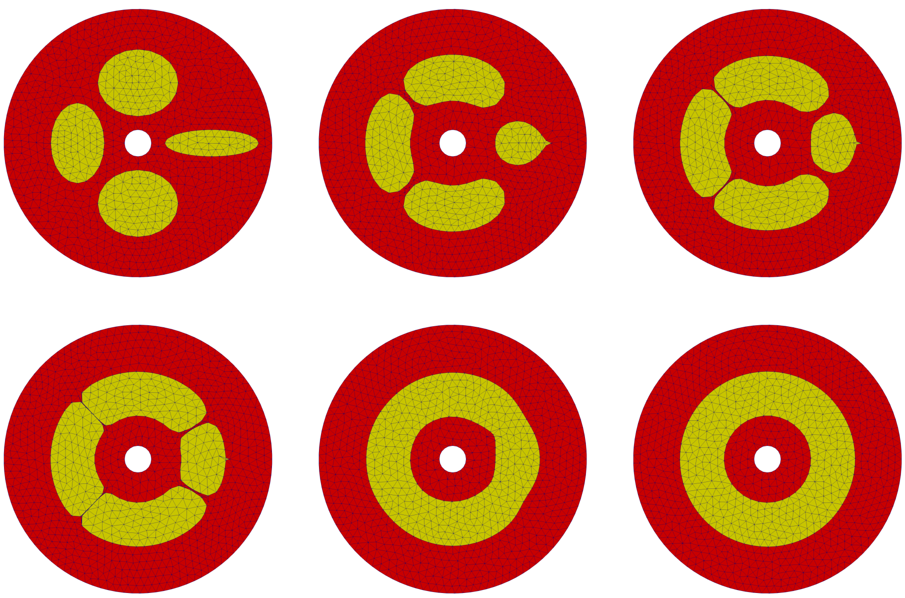


Figure 3.9: Topological changes by using level set functions.

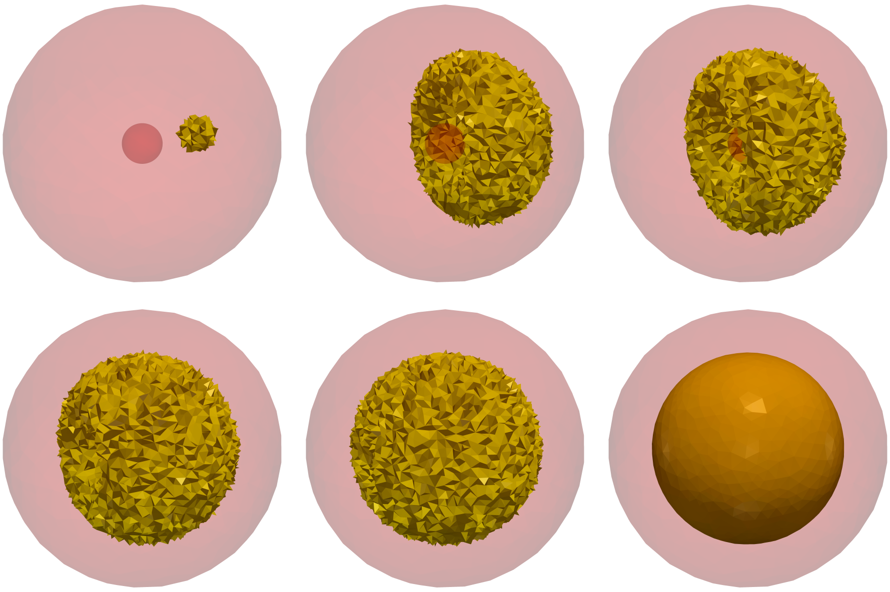


Figure 3.10: 3D case with level set method.

Lagrange (direct) representation to handle topological changes (see Figure 3.9). There are several issues with three-dimensional problems for Lagrange (direct) representation. On the other hand adapting level set function as the representations of shapes seems rather easy. Results for 3D case can be seen in Figure 3.10.

3.2.2 Comparison of gradient and Newton-like methods

In Figures 3.11 and 3.12 a comparison of two different strategies for construction of an ascent vector described by Methods 3.1.6 and 3.1.13 We follow the same example as in the last subsection. Convergence history of Lagrange functional $L = J - \lambda \text{vol}$ is shown in Figure 3.13. We have implemented the optimal step size, meaning that at any iteration we solve numerically the following problem.

$$\min_{t \geq 0} L((\mathrm{Id} + t\theta)\Omega_\alpha)$$

for given ascent vector θ. Note that for the small step size there is no significant differences between methods. We would like to point out that Newton-like method achieves convergence in a small number of only 13 iterations which is half the number of iterations needed for gradient method. Furthermore, the second order method may offer fast way of calculating the optimal step size making it significantly faster then gradient method.

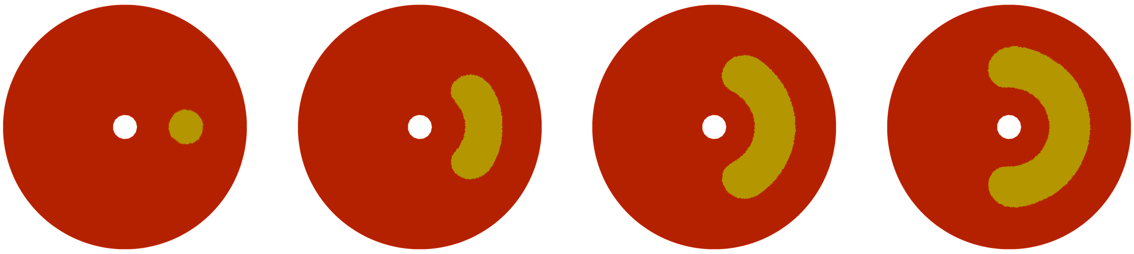


Figure 3.11: Gradient method

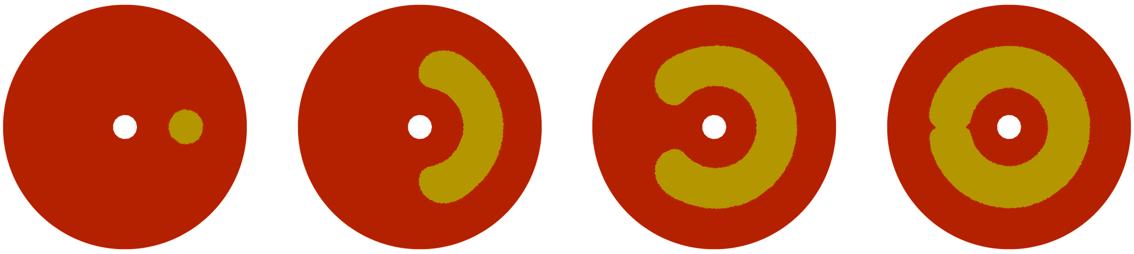


Figure 3.12: Newton-like method

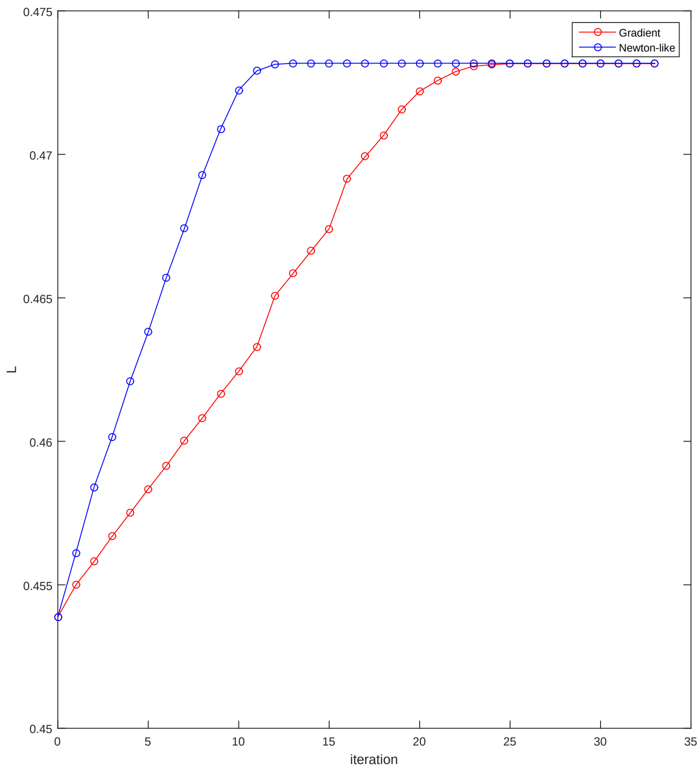


Figure 3.13: Convergence history of L for gradient and Newton-like method

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Curriculum Vitae

Petar Kunštek was born on April 18, 1991 in Zagreb, Croatia. After graduating from XV gymnasium in Zagreb, he enrolled in the undergraduate program in Mathematics at Department of Mathematics, Faculty of Science, University of Zagreb and obtained his Bachelor degree in July 2013. The same year he enrolled in the graduate program of Applied Mathematics at the same faculty. During his studies he performs the duty of student tutor for 8 different courses (2 of them being graduate courses). He defended his master thesis: "Metoda nivo skupa u optimizaciji oblika (Level set method in optimal design)" under the supervision of Assoc. Prof. Marko Vrdoljak in July 13, 2015. obtaining his master's degree.

In academic year 2015/2016 he enrolled in the Croatian doctoral program at Department of Mathematics, Faculty of Science, University of Zagreb where he has been employed as a teaching assistant. He participated in more then 15 international conferences and workshops, giving talk on seven of them and poster presentation on two. During summer 2015 he spent five weeks at Scuola Matematica Interuniversitaria in Perugia, Italy where he successfully completed two graduate courses "Functional analysis" and "Game theory" with the highest grade. In the workshop: VII Partial differential equations, optimal design and numerics in Benasque, Spain, 20 Aug. – 1 Sep. 2017; he was organizer of the thematic session: "Homogenization and application in optimal design".

He is one of the collaborators in two research project: "Analysis of fluid-structure interaction problems and applications" (2018–2022, Croatian Science Fondation, leader: Boris Muha) and "Anisotropic distributions and H-distributions" (2018–2019, bilateral project with Austria, leader: Nenad Antonić) and has participated in the work of Seminar on Differential Equations and Numerical Analysis.

Journal publication:

P. Kunštek, M. Vrdoljak. *Classical optimal designs on annulus and numerical approximations.* Journal of Differential Equations, in press.
`doi:10.1016/j.jde.2019.11.077`

Izjava o izvornosti rada

Ja, Petar Kunštek student Prirodoslovnog-matematičkog fakulteta Sveučilišta u Zagrebu, s prebivalištem na adresi Vijenac Frane Gotovca 14, Zagreb, JMBAG 1191219518, ovim putem izjavljujem pod materijalnom i kaznenom odgovornošću da je moj doktorski rad pod naslovom

Shape derivative techniques in optimal design
(Tehnike derivacije oblika u optimalnom dizajnu)

isključivo moje autorsko djelo, koje je u potpunosti samostalno napisano uz naznaku izvora drugih autora i dokumenata korištenih u radu.

U Zagrebu, 7.1.2019.

P Kunt

Potpis