Shape Optimization
for Time-dependent Domains

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Chapter I

Introduction

Shape optimization appears naturally in a wide range of applications in engineering, especially for designing and constructing industrial components or in non-destructive testing. A classical application is for example the planning of components of aircrafts, where the geometry of the airfoil should be designed to minimize the drag while prescribing a "cruise Mach number and a target lift coefficient" [Huy01]. The general idea is to find the optimal geometric shape under certain constraints, especially constraints given by partial differential equations. This is due to the fact that many practical problems from engineering amount to partial differential equations for an unknown function u defined on a domain Q. This function enters into the quantity of interest, which is usually a functional $J(Q, u)$. Shape optimization is then concerned with the minimization of this quantity of interest over an appropriate set of admissible domains $Q \in \mathcal{U}_{\mathrm{ad}}$. The usual way, which is also pursued in this thesis, is to apply a gradient based minimization method such as steepest descent or a quasi-Newton method for finding this minimum. There exist two approaches for computing the required *shape derivative* of the functional J with respect to the shape Q, namely *first optimize, then discretize* and *first discretize, then optimize*. The latter approach does not compute a derivative analytically but approximates the derivative by a numerical method as for example finite differences. In contrast, we pursue the first approach and analytically compute the derivative of the functional.

Shape optimization is a well studied topic in literature in the case of *elliptic partial differential equations*. It has been established for the perturbation of identity (Murat and Simon) and the speed method (Sokolowski and Zolésio), see [DZ11, HM03, HP06, MS75, Sim80, SZ92, Zol79] and the references therein. However, not so much is known about shape optimization in case of *parabolic partial differential equations*. The simplest case, which is also studied in this thesis, is the *heat equation*

$$\partial_t u - \Delta u = 0 \quad \text{in } Q.$$

Theoretical results for parabolic shape optimization problems with *time-independent shapes* can be found in [Sok88, SZ92, YS96], while practical computational results are found for example in [CKY98, CKY99, HT11, HT13]. This is in contrast to results for parabolic shape optimization problems with *time-dependent shapes*, in which the spatial domain varies within time. Theoretical results are for example available in [DZ99b, DZ01, MZ06], but to the best of the author's knowledge, very few results about efficient computations of such time-dependent shape optimization problems exist. This is possibly caused by the fact that time-dependent shapes lead to several complications compared to time-independent shapes. Firstly, one has to elaborate how shape derivatives are computed on time-dependent domains. Secondly, the existence and uniqueness of the solution u of the partial differential equation on the time-dependent domain has to be established. Thirdly, one needs to be able to numerically compute a solution of such a differential equation. Let us discuss these difficulties in more detail.

For parabolic problems with time-dependent domains, the seemingly only available literature for shape optimization goes back to the above mentioned references [DZ99b, DZ01, MZ06] from Zolésio et al. They consider a spatial domain $\Omega_t \subset \mathbb{R}^d$, $d \in \mathbb{N}$, for every point of time t, where the index t emphasizes that the spatial domain may vary with time t. This then yields a *time-dependent* or so-called *non-cylindrical* domain, or simply, *tube*, by setting

$$Q_T = \bigcup_{0<t<T} \big(\{t\} \times \Omega_t\big).$$

As in the case of elliptic partial differential equations, there exist the *speed method* and the *perturbation of identity* for computing the shape derivative of the functional. In the case of the speed method, the sought tube is described implicitly by the evolution of a known initial domain prescribed by a time-dependent vector field $\mathbf{V}$. The shape of the tube can then be obtained by solving an ordinary differential equation. In contrast, for the perturbation of identity, the shape of the tube is explicitly available via a parametrization. As we are interested in the shape in the numerical computations, the more promising approach is to use a parametrization of the tube with the perturbation of identity. The parametrization can then be discretized by applying a suitable selection of basis functions. Notice that the speed method is preferable in an Eulerian setting, while the perturbation of identity is more suited for the Lagrangian setting. They are different descriptions of the same matter.

We are then interested in computing the directional derivative of the functional under consideration given by

$$\lim_{s \searrow 0} \frac{J(Q_T^s, u_s) - J(Q_T, u)}{s},$$

as this gradient is used for the minimization process. In here, Q_T^s denotes a perturbed tube and u_s is the solution of the partial differential equation solved on this perturbed tube. In the speed method, this perturbed tube is generated by considering a second time-dependent vector field $\mathbf{W}$ and studying the evolution induced by $\mathbf{V} + s\mathbf{W}$. In the case of the perturbation of identity, we perturb the tube for each point of time by applying $\mathrm{id} + s\mathbf{Z}$ for a time-dependent vector field $\mathbf{Z}$, where id denotes the spatial identity map.

The structure of the directional derivative is described by the Hadamard structure theorem, which can be applied to the time-dependent setting as we will remark in this thesis. This implies that the derivative is a boundary integral containing the perturbation field in spatial normal direction. In our case, it will also involve the solution of the partial differential equation and of an *adjoint problem*, which is introduced to alleviate the computational cost. Therefore, we need to compute the solution of the partial differential equation on a time-dependent domain for every time of interest.

Depending on the application, the solution theory of the heat equation on *time-independent domains*, also called *cylindrical domains*, has been discussed for various anisotropic Sobolev spaces, see for example [Cos90, LSU68, Wlo87]. In particular, boundary integral equations are a well-known technique to analyse elliptic partial differential equations, see for example [SS10a, Ste08]. For parabolic equations on time-independent domains anisotropic Sobolev spaces and the mapping properties of the layer operators for the heat equation are introduced in [Cos90, Noo88]. On the other hand, to the best of the author's knowledge, no such existence and uniqueness theory for parabolic equations exists for time-dependent domains and the theory of boundary integral operators is not rigorously available.

Once a suitable functional analytic setting with existence and uniqueness results on time-dependent domains is found, the next step towards computational shape optimization is the numerical solution of the underlying partial differential equation on time-dependent domains. One of the most established tool to numerically solve elliptic partial differential equations are finite element methods. A standard approach to extend them to the parabolic setting in cylindrical domains is the method of lines, see [Sch91]. It solves the partial differential equation by using finite elements in space and a Runge-Kutta scheme in time. In a non-cylindrical domain, this scheme cannot be applied directly, because we cannot consider straight lines in time. One idea to overcome this problem is to map the differential equation back to a cylindrical domain, when assuming that the tube is built by mapping a cylindrical domain onto a tube. This procedure complicates the differential equation significantly as also terms of lower order appear, but one could apply standard tools to solve it. Instead of mapping the problem back to a cylindrical domain, one can apply deforming-mesh methods or fixed-mesh methods to solve problems with time-dependent boundaries. Deforming-mesh methods contort the mesh according to the deformation of the domain, while fixed-mesh methods use a stationary background mesh on which the domain evolves. For an illustration, see for example [Gaw15]. While deforming-mesh methods have problems with large deformations, fixed-mesh methods cannot represent the geometry accurately. To overcome this, in [GL14, Gaw15], the so-called universal mesh is introduced, which uses a background mesh with a small number of perturbed nodes to match the geometry. In [DE07], a method of solving a partial differential equation on an evolving hypersurface is presented. The idea of the method is to approximate the hypersurface.

Solving a partial differential equation can also be done with a boundary element method as mentioned above. The advantage over the finite element method is that only a time-space boundary mesh rather than a full time-space volume mesh is required as for finite elements. Moreover, a boundary element method naturally fits with the Hadamard structure theorem. This reduces complexity, but also has some limitations. The functional analytic framework is more complicated, boundary element methods are only suitable if there exists a known fundamental solution, the system matrices are dense and implementation requires a serious amount of expert knowledge, see also [Cos04].

The difficulties outlined above make the analysis and implementation of parabolic shape optimization problems on time-dependent domains significantly more involved than for time-independent domains. To the best of the author's knowledge, there seems to be only few literature available for numerical computations for time-dependent domains in more than one dimension.

We would like to mention [DBH+13], where the authors monitor the formation of solid deposits inside a container for nuclear waste. This is a so-called *inverse geometric problem*. They use the method of fundamental solutions to solve a two-dimensional heat equation and reconstruct the internal moving boundary by measuring the Dirichlet and the Neumann data at the exterior. Similar to the boundary element method, the advantage of the method of fundamental solutions is that no meshing of the domain or the boundary is required. The drawback is that the method generates ill conditioned matrices, see [AA18]. Another problem, that falls into this class of inverse geometric problems, is considered in [HT98]. They reconstructed a time-dependent boundary in two dimensions using a conjugate gradient method and a boundary element method.

Time-dependent boundaries also appear in the class of the *moving boundary problems*, which could be interesting to solve with the tools of shape optimization. In general, such problems contain time-dependent boundaries which are unknown and depend on time and spatial variables. Moving boundary problems are also called *Stefan problems*, going back to J. Stefan in 1889, who studied the formation of ice in the polar sea, see [Ste89]. They find their application, for example, in the modelling of phase transitions, chemical reactions, fluid flow in porous medium or melting of ice, compare [Cra84]. There exists a wide variety of literature on Stefan problems, see for example [FK75, Gup03, Mei92, Rub71, Tar88] and the references therein. This literature mostly treats the analysis of the Stefan problem. [LT21] solves the one-dimensional Stefan problem with the tools of shape optimization and served as an inspiration to treat the multi-dimensional Stefan problem with shape optimization in this thesis. Other possibilities to solve Stefan problem numerically are explained in [Cra84]: there exist front-tracking methods, front-fixing methods and fixed-domain methods. Notice that moving boundary problems are also studied in optimal control, see for example [BH11, HZ07, PL08].

In view of the above mentioned status of the literature, the contributions of this thesis are as follows:

1. We develop a suitable functional analytic framework in anisotropic Sobolev spaces on time-dependent domains for the heat equation with Dirichlet or Neumann data. Using the framework of boundary integral equations then allows us to show existence and uniquenes of solutions for the Dirichlet and the Neumann problem with zero initial condition within these Sobolev spaces. These results are available in [BHT20] and are a generalization to the parabolic time-space boundary element theory as in [Cos90].

2. We summarize the theoretical results for shape calculus on time-dependent domains from [MZ06], evaluate their usability for numerical computations and expand the results for general functionals serving as a reference for further research. For the convenience of the reader, we provide proofs of the statements when they seem to be missing in the literature. Moreover, using the correct anisotropic Sobolev spaces from the first part, we rigorously derive the local shape derivative of the Dirichlet problem, which is published in slightly less general form in [BHT21] based on the cylindrical setting treated in [CKY98].

3. We provide numerical examples which serve as a proof of concept for the theoretical findings. On the one hand, we consider an inverse geometric problem and, on the other hand, as a forward problem, a Stefan problem. Both types of problems are rewritten such that they can be solved using shape optimization techniques. These examples are also in [BHT21, BH21].

The remainder of this thesis is now structured as follows.

Chapter II covers the notion of classical function spaces such as Sobolev spaces and some basic terms of differential geometry such as tangential differential operators and the necessary divergence theorems from the literature. We would like to point out, that we especially introduce the so-called tangential Stokes formula, which serves as an integration by parts formula on boundaries.

Chapter III recalls the notion of parabolic partial differential equations on tubes and the corresponding traces. It moreover states uniqueness and solvability of such problems based on boundary integral operators in the appropriate anisotropic Sobolev spaces. To the best of the author's knowledge, no such theory exists for tubes. Therefore, we aim to extend the theory from cylindrical domains to non-cylindrical domains.

Given sufficient regularity of the tube, several possibilities on how to establish analogous integral equations and properties of integral operators as on cylindrical domains came to our mind. In the following, we briefly discuss these possibilities and explain why the chosen approach seems to be the most promising one.

A first approach could be to exploit the fact that the fundamental solution does not use boundary data and is thus defined on the free space $\mathbb{R} \times \mathbb{R}^d$. Therefore, it is the same for a cylindrical and a non-cylindrical domain and allows to state the integral operators in cylindrical and non-cylindrical domains. To derive the mapping properties of the integral operators, one could make use of the equivalence of norms on the tube and on the cylindrical domain by establishing equivalence results of the fundamental solution, evaluated on the tube and on the cylindrical domain. The problem is that the Neumann trace, which will be considered here, contains an additional term involving the normal velocity of the tube, which needs to be dealt with.

A second approach could be to map back the partial differential equation from the non-cylindrical domain onto the cylindrical domain. The advantage is that one now considers a cylindrical domain, for which more theory is available. The drawback is that the differential equation in the reference domain is more complicated because of time and space dependent coefficients. Finding a fundamental solution is more difficult and one could for example pursue the parametrix ansatz, taken in [Fri83], and then find the according mapping properties of the respective layer operators. Summarizing, it seems that a heavy theoretical machinery is required for this approach.

The third approach considers the partial differential equation on the non-cylindrical domain. Here, the partial differential equation is simple, but the domain is more involved in contrast to the second approach. This approach was used in [Tau19], but without the corresponding Sobolev spaces and mapping properties of the integral operators. Since we already did computations in [BHT21] based on [Tau19], and since [Cos90] provides a self-contained analysis of the mapping properties of the layer operators for the heat equation in a cylindrical domain, we follow this approach and generalize the theory of [Cos90] to tubes.

Chapter IV gives an introduction to shape optimization for tubes. More precisely, we first recall how a tube is generated and perturbed in the setting of the speed method as well as in the setting of the perturbation of identity. This mostly follows the literature available, but we intend to provide and clarify the proofs where needed. Since we outlined above that it is easier to use the perturbation of identity for our numerical computations, the focus is placed on this. We then compute shape derivatives for general functionals, in particular a domain functional and a boundary functional. Although the proofs are similar to the proofs for the time-independent shape calculus, we state them because they seem not to be carried out in the literature and we notice that some of the technical details are crucial for formulating the correct boundary functional. Moreover, we rigorously compute the local shape derivative for a Dirichlet problem and then give formulae for general functionals dependent on a Dirichlet problem, both of which cannot be found to this extent in the literature to the best of the author's knowledge.

In Chapter V, we then apply shape optimization techniques to an inverse problem. It is the time-dependent analogue of the problem stated in [HT13], where a parabolic shape optimization problem is considered for a time-independent shape. The goal therein is to detect a fixed inclusion or void of zero temperature inside a solid or liquid body by measurements of the temperature and the transient heat flux at the accessible outer boundary. In contrast, in this chapter, we now consider an inclusion which changes its shape during time.

The problem under consideration is reformulated as a shape optimization problem by means of a tracking-type functional for the Neumann data. Therefore, for a given temperature at the exterior boundary, the mismatch of the Neumann data is minimized in a least-squares sense. Since we intend to apply a gradient-based optimization algorithm, we compute the shape gradient of this functional by means of the adjoint approach, which is known to reduce the computational effort. Then, we make a parametric ansatz for the inclusion and use a boundary element method to solve the heat equations for the primal state and the adjoint state. As only the boundary has to be discretized, the dimensionality of the problem is reduced by one, which allows for efficient computation of the solution. Numerical results in two spatial dimensions validate that the present approach is feasible, leading to meaningful reconstructions.

In Chapter VI, we treat the one-phase Stefan problem with the developed tools of shape optimization as a second example and as a forward problem. The one-dimensional case was covered in [LT21]. In here, we treat the multi-dimensional case, which requires an adequate reformulation of the so-called Stefan condition in order to obtain a functional whose shape derivative is analytically computable.

Our objective functional is chosen such that it is minimal if the Stefan condition is satisfied. Therefore, the goal is to minimize this objective functional over all admissible surfaces and as in Chapter V, we would like to apply a gradient based method. Hence, we compute the shape derivative of the functional and introduce the adjoint problem to alleviate again the computational cost. We present a numerical example, which serves as a proof of concept for the theoretical findings by making once more a parametric ansatz of the boundary. The appearing differential equations are solved by a finite element method and the method of lines after mapping the problem back to a cylindrical reference domain.

Finally, Chapter VII contains final remarks and an outlook for possible future work.

Chapter II

Preliminaries

II.1 Function spaces and derivatives

In this section, we fix the notion of the standard function spaces needed throughout the thesis, which include the spaces of smooth functions, L^p spaces and Sobolev spaces. We also recall the notion of a Gâteaux and Fréchet derivative.

Let us denote by $\langle \cdot, \cdot \rangle$ the standard scalar product in $\mathbb{R}^d$, $d \in \mathbb{N}$, and $\| \cdot \|$ its associated norm.

II.1.1 Smooth functions

The following definitions, unless indicated otherwise, are given along the lines of [Alt12, Sections 1.2–1.7].

Definition II.1.1. *Let $\Omega \subset \mathbb{R}^d$ be open and bounded, and Y a Banach space over $\mathbb{R}$ with the norm $\| \cdot \|_Y$. Let $k \in \mathbb{N}_0$. The space of* k-times differentiable functions *is defined as*

$$\begin{aligned} C^k(\overline{\Omega}; Y) := \{ & f \colon \Omega \to Y \colon f \text{ is } k\text{-times continuously differentiable in } \Omega \\ & \text{and } \partial^{\boldsymbol{\alpha}} f \text{ is continuously extendable to } \overline{\Omega} \text{ for } |\boldsymbol{\alpha}| \leq k \} . \end{aligned}$$

The spaces $C^k(\overline{\Omega}; Y)$ are Banach spaces with the norm

$$\|f\|_{C^k(\overline{\Omega};Y)} := \sum_{|\boldsymbol{\alpha}| \leq k} \|\partial^{\boldsymbol{\alpha}} f\|_{C^0(\overline{\Omega};Y)},$$

where

$$\|f\|_{C^0(\overline{\Omega};Y)} := \sup_{\mathbf{x} \in \Omega} \|f(\mathbf{x})\|_Y .$$

Let us set $C^k(\overline{\Omega}) := C^k(\overline{\Omega}; \mathbb{R})$.

We have the following definition, see also [Alt12, Section 2.26].

Definition II.1.2. *Let Ω, $\widetilde{\Omega} \subset \mathbb{R}^d$. We call $f \colon \Omega \to \widetilde{\Omega}$ a C^k-*diffeomorphism*, if f is bijective, $f \in C^k(\Omega; \mathbb{R}^d)$ and $f^{-1} \in C^k(\widetilde{\Omega}; \mathbb{R}^d)$.*

To measure regularity on a finer scale, we recall the subsequent definition of Hölder spaces.

Definition II.1.3. *Let $\Omega \subset \mathbb{R}^d$ be open and bounded and Y a Banach space with the norm $\|\cdot\|_Y$. Let $k \in \mathbb{N}_0$ and $\kappa \in (0,1]$. We define the* Hölder spaces *as*

$$C^{k,\kappa}(\overline{\Omega};Y) := \left\{f \in C^k(\overline{\Omega};Y)\colon\ \mathrm{H\ddot{o}l}_\kappa(\partial^{\boldsymbol{\alpha}} f, \overline{\Omega}) < \infty \text{ for } |\boldsymbol{\alpha}| = k\right\},$$

where

$$\mathrm{H\ddot{o}l}_\kappa(f,\Omega) := \sup\left\{\frac{|f(\mathbf{x}) - f(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^\kappa}\colon\ \mathbf{x},\mathbf{y} \in \Omega,\ \mathbf{x} \neq \mathbf{y}\right\}.$$

These spaces are Banach spaces with norm

$$\|f\|_{C^{k,\kappa}(\overline{\Omega};Y)} := \sum_{|\boldsymbol{\alpha}| \le k} \|\partial^{\boldsymbol{\alpha}} f\|_{C^0(\overline{\Omega};Y)} + \sum_{|\boldsymbol{\alpha}|=k} \mathrm{H\ddot{o}l}_\kappa(\partial^{\boldsymbol{\alpha}} f, \overline{\Omega}).$$

Functions in $C^{0,1}(\overline{\Omega};Y)$ are called *Lipschitz continuous.*

If $\overline{\Omega}$ is not a compact set, we can nevertheless define the above function spaces by considering $\Omega \subset \mathbb{R}^d$, such that there exists an exhaustion $(K_i)_{i\in\mathbb{N}}$ with compact sets $K_i \subset \mathbb{R}^d$ fulfilling

$$\begin{aligned} &\Omega = \bigcup_{i\in\mathbb{N}} K_i \text{ and } \emptyset \neq K_i \subset K_{i+1} \subset \Omega \text{ for } i \in \mathbb{N}, \\ &\mathbf{x} \in \Omega \Rightarrow B_\delta(\mathbf{x}) \cap \Omega \subset K_i \text{ for a } \delta > 0 \text{ and } i \in \mathbb{N}. \end{aligned} \tag{II.1.1}$$

Moreover, let Y be a Banach space over $\mathbb{R}$. The set

$$C^0(\Omega;Y) := \{f\colon \Omega \to Y\colon f \text{ is continuous on } \Omega\}$$

is again a vector space and with the Fréchet metric

$$\rho(f) := \sum_{i\in\mathbb{N}} 2^{-i} \frac{\|f\|_{C^0(K_i)}}{1 + \|f\|_{C^0(K_i)}} \text{ for } f \in C^0(\Omega;Y)$$

also a complete metric space. The topology is independent of the choice of the exhaustion. In complete analogy, we can introduce the spaces $C^k(\Omega;Y)$ and $C^{k,\kappa}(\Omega;Y)$.

Definition II.1.4. *Let $\Omega \subset \mathbb{R}^d$ and Y a Banach space. For functions $f\colon \Omega \to Y$, the* support *of f is defined as*

$$\operatorname{supp} f := \overline{\{\mathbf{x} \in \Omega\colon\ f(\mathbf{x}) \neq 0\}}.$$

We say that f has compact support *in Ω, if* $\operatorname{supp} f \Subset \Omega$*. In here, the notation $G \Subset \Omega$ means that the closure $\overline{G} \subset \Omega$ and $\overline{G}$ is a compact subset of $\mathbb{R}^d$, see [AF03, Section 1.3].*

With this definition at hand, we can introduce the functions with *compact support* as

$$C_0^0(\Omega;Y) := \{f \in C^0(\Omega;Y)\colon\ \operatorname{supp}(f) \Subset \Omega\},$$

see [AF03, Section 1.26] and [Alt12, Section 1.4], and analogously $C_0^k(\Omega;Y)$.

Along the lines of [Alt12, Section 1.8] or [AF03, Section 1.26], we recall the space of smooth functions.

Definition II.1.5. *Let $\Omega \subset \mathbb{R}^d$ be an open domain and Y a Banach space. The space of* smooth functions *is defined as*

$$C^\infty(\Omega; Y) := \bigcap_{k \in \mathbb{N}} C^k(\Omega; Y).$$

Analogously, one can define the smooth functions with compact support *as*

$$C_0^\infty(\Omega; Y) := \{f \in C^\infty(\Omega; Y) \colon \operatorname{supp}(f) \Subset \Omega\}.$$

Notice that $C_0^\infty(\Omega; Y)$ can be equipped with a topology and then becomes a topological vector space also denoted by $\mathcal{D}(\Omega)$, see e.g. [AF03, Section 1.56] or [Alt12, Section 3.20 and 3.21]. This vector space is called the space of *test functions*, which is used in the following to introduce distributions.

II.1.2 Linear operators and dual spaces

We give the notion of linear operators and dual spaces along the lines of [Alt12, p. 148ff.].

Definition II.1.6. *Let X and Y be general topological vector spaces. The* space of linear operators *is defined as*

$$\mathcal{L}(X; Y) := \{T \colon X \to Y : T \textit{ is linear and continuous}\}.$$

If X and Y are normed spaces, we speak of bounded operators and, for every $T \in \mathcal{L}(X; Y)$, we can associate its operator norm by

$$\|T\|_{\mathcal{L}(X;Y)} := \sup_{\|x\|_X \leq 1} \|Tx\|_Y < \infty.$$

Note that $T \in \mathcal{L}(X; Y)$ if and only if $\|T\|_{\mathcal{L}(X;Y)}$ is finite. Using linear operators, we can introduce the dual space.

Definition II.1.7. *For a topological vector space X over $\mathbb{R}$, we denote by*

$$X' := \mathcal{L}(X; \mathbb{R})$$

its dual space.

Let X be a Banach space. Writing $\langle x, x' \rangle_{X \times X'} := x'(x)$ for $x \in X$, we define an isometric map $J_X \in \mathcal{L}(X; X'')$ via

$$\langle x', J_X x \rangle_{X' \times X''} := \langle x, x' \rangle_{X \times X'} \quad \text{for } x \in X, x' \in X',$$

where X'' denotes the dual space of X'. X is called *reflexive* if the map J_X is surjective, see [Alt12, Chapter 6]. Thus, a reflexive space X is isometric isomorph to its bidual space X'' with respect to the isometry J_X. Moreover, a topological space X is called *separable* if it contains a dense, countable subset [Alt12, Definition 0.13].

We introduce the notion of a distribution along the lines of [Gra14, Section 2.3].

Definition II.1.8. *Elements of the dual space $\mathcal{D}'(\mathbb{R}^d) = \big(C_0^\infty(\mathbb{R}^d)\big)'$ are called* distributions *and $\mathcal{D}'(\mathbb{R}^d)$ is called the* space of distributions.

By the definition of the dual space, we have that $T_k \to T$ in $\mathcal{D}'(\mathbb{R}^d)$ if and only if $T_k, T \in \mathcal{D}'(\mathbb{R}^d)$ and $T_k(f) \to T(f)$ for all $f \in C_0^\infty(\mathbb{R}^d)$.

Following [McL00, p. 72], we define rapidly decreasing smooth functions, which we will use in Section II.1.4 to introduce the notion of Sobolev spaces.

Definition II.1.9. *The* Schwartz space $\boldsymbol{\mathcal{S}}(\mathbb{R}^d)$ *is defined as*

$$\boldsymbol{\mathcal{S}}(\mathbb{R}^d) := \Big\{ \psi \in C^\infty(\mathbb{R}^d) \colon \sup_{\mathbf{x}\in\mathbb{R}^d} \left| \mathbf{x}^{\boldsymbol{\alpha}} \partial^{\boldsymbol{\beta}} \psi(\mathbf{x}) \right| < \infty \text{ for all multi-indices } \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^d \Big\}.$$

Remark II.1.10. *Clearly, the Schwartz space contains the space $C_0^\infty(\mathbb{R}^d)$. We call $\boldsymbol{\mathcal{S}}'(\mathbb{R}^d)$ the space of* tempered distributions*, see also [Bon11, Definition 9.3.1].*

II.1.3 L^p spaces

In the sequel, we introduce the Lebesgue spaces L^p along the lines of [Alt12, Section 1.15]. The used generality corresponds to the case of Bochner spaces, compare [Boc33].

We first state the notion of a measure space.

Definition II.1.11. *Let X be a set and $\mathcal{B}$ a non-empty system of subsets of X. We call $(X, \mathcal{B}, \mu)$ a* complete measure space *and μ a measure on $\mathcal{B}$ if*

- *$\mathcal{B}$ is a σ-algebra,*
- *$\mu \colon \mathcal{B} \to [0, \infty]$ with $\mu(\emptyset) = 0$ is σ-additive, i.e. if for $E_i \in \mathcal{B}$ for $i \in \mathbb{N}$ pairwise disjoint it follows $\mu\left(\cup_{i\in\mathbb{N}} E_i\right) = \sum_{i\in\mathbb{N}} \mu(E_i)$,*
- *if $N \in \mathcal{B}$ with $\mu(N) = 0$ and $E \subset N$, then also $E \in \mathcal{B}$.*

Definition II.1.12. *Let $(X, \mathcal{B}, \mu)$ be a measure space and Y a Banach space over $\mathbb{R}$ with norm $\|\cdot\|_Y$. For $f \colon X \to Y$ a μ-measurable function, we define the norms*

$$\|f\|_{L^p_\mu(X;Y)} := \begin{cases} \left(\int_X \|f\|_Y^p \,\mathrm{d}\mu \right)^{\frac{1}{p}} & \text{for } 1 \le p < \infty, \\ \operatorname{ess\,sup} \|f\|_Y & \text{for } p = \infty. \end{cases}$$

We define the $L^p_\mu(X;Y)$-spaces for $1 \le p \le \infty$ as

$$L^p_\mu(X;Y) := \{ f \colon X \to Y \colon f \ \mu\text{-measurable and } \|f\|_{L^p_\mu(X;Y)} < \infty \}$$

under the equivalence relation

$$f = g \text{ in } L^p_\mu(X;Y) \Leftrightarrow f = g \ \mu\text{-almost everywhere.}$$

If μ is the Lebesgue measure, we write $L^p(X;Y) = L^p_\mu(X;Y)$ and, if $(Y, \|\cdot\|_Y) = (\mathbb{R}, |\cdot|)$, we set $L^p(X) = L^p(X;Y)$ for ease of notation. These standard L^p spaces are for example also defined in [For09, Paragraph 12, Definition p. 133]. We will use the Bochner spaces to classify the function spaces required for the heat equation in Chapter III.

The space $L^p_\mu(X;Y)$ is a Banach space for all $1 \le p \le \infty$, see also [AF03, Theorem 2.16]. Moreover, for $p = 2$ and Y a Hilbert space with scalar product $(\cdot,\cdot)_Y$, the space $L^2_\mu(X;Y)$ is a Hilbert space with

$$(f, g)_{L^2_\mu(X;Y)} := \int_X \big(f(\mathbf{x}), g(\mathbf{x}) \big)_Y \,\mathrm{d}\mu. \tag{II.1.2}$$

We define locally integrable functions according to [AF03, Section 1.58].

Definition II.1.13. *Let $\Omega \subset \mathbb{R}^d$ be a non-empty open set. A function f is called* locally integrable *on Ω, if $f \in L^1(S)$ for all $S \Subset \Omega$. We write $f \in L^1_{\mathrm{loc}}(\Omega)$.*

The following is in accordance with [AF03, Theorem 2.19, Corollary 2.30].

Lemma II.1.14. *Let $\Omega \subset \mathbb{R}^d$ be a non-empty open set. Then, $C_0(\Omega)$ and $C_0^\infty(\Omega)$ are dense in $L^p(\Omega)$ for all $1 \leq p < \infty$.*

II.1.4 Sobolev spaces

We define the weak derivative as in [AF03, Section 1.62].

Definition II.1.15. *Let $\Omega \subset \mathbb{R}^d$ be a non-empty open set. Let $f \in L^1_{\mathrm{loc}}(\Omega)$ and $\boldsymbol{\alpha} \in \mathbb{N}_0^d$. If there exists a $g_{\boldsymbol{\alpha}} \in L^1_{\mathrm{loc}}(\Omega)$ such that*

$$\int_\Omega f(\mathbf{x}) \partial^{\boldsymbol{\alpha}} \varphi(\mathbf{x}) \,\mathrm{d}\mathbf{x} = (-1)^{|\boldsymbol{\alpha}|} \int_\Omega g_{\boldsymbol{\alpha}}(\mathbf{x}) \varphi(\mathbf{x}) \,\mathrm{d}\mathbf{x}$$

for all $\varphi \in \mathcal{D}(\Omega)$, we call $g_{\boldsymbol{\alpha}} =: \partial^{\boldsymbol{\alpha}} f$ the weak derivative *of f.*

Notice that the weak derivative is unique up to a set of measure zero. Moreover, the classical strong derivative coincides with the weak derivative if f is smooth enough such that it exists. On the other hand, the weak derivative might exist for functions which have no classical derivative.

We now have all the ingredients to define Sobolev norms and spaces as in [AF03, Chapter 3].

Definition II.1.16. *Let $k \in \mathbb{N}_0$ and $1 \leq p \leq \infty$. We define the* Sobolev norms

$$\|u\|_{W^{k,p}(\Omega)} = \begin{cases} \left(\sum\limits_{0 \leq |\boldsymbol{\alpha}| \leq k} \|\partial^{\boldsymbol{\alpha}} u\|_{L^p(\Omega)}^p \right)^{\frac{1}{p}}, & \text{if } 1 \leq p < \infty, \\ \max\limits_{0 \leq |\boldsymbol{\alpha}| \leq k} \|\partial^{\boldsymbol{\alpha}} u\|_{L^\infty(\Omega)}, & \text{if } p = \infty. \end{cases}$$

As before, we consider equivalence classes.

We define two vector spaces, for which $\|\cdot\|_{W^{m,p}(\Omega)}$ is a norm:

- *$W^{k,p}(\Omega)$ is defined as the set $\{u \in L^p(\Omega) \colon \partial^{\boldsymbol{\alpha}} u \in L^p(\Omega) \text{ for } 0 \leq |\boldsymbol{\alpha}| \leq k\}$.*
- *$W_0^{k,p}(\Omega)$ is defined as $\overline{C_0^\infty(\Omega)}^{\|\cdot\|_{W^{k,p}(\Omega)}}$.*

These spaces are called Sobolev spaces *when equipped with the norm $\|\cdot\|_{W^{m,p}(\Omega)}$.*

In [MS64] it is proven that for $k \in \mathbb{N}$, $1 \leq p < \infty$, the space $W^{k,p}(\Omega)$ coincides with the space defined as the completion of the set $\{u \in C^k(\Omega) \colon \|u\|_{W^{k,p}(\Omega)} < \infty\}$ with respect to the norm $\|\cdot\|_{W^{k,p}(\Omega)}$ (see also [AF03, Theorem 3.17]). According to [Alt12, Theorem 2.24], we then have that $W^{k,p}(\Omega) \cap C^\infty(\Omega)$ is dense in $W^{k,p}(\Omega)$ for all $1 \leq p < \infty$.

It holds $W^{0,p}(\Omega) = L^p(\Omega)$ and, since $C_0^\infty(\Omega)$ is dense in $L^p(\Omega)$ (see Lemma II.1.14), also $W_0^{0,p}(\Omega) = L^p(\Omega)$ for $1 \leq p < \infty$. Moreover, for any $k \in \mathbb{N}$, we have the chain of embeddings $W_0^{k,p}(\Omega) \hookrightarrow W^{k,p}(\Omega) \hookrightarrow L^p(\Omega)$. The spaces $W^{k,p}(\Omega)$ are Banach spaces (see [AF03, Theorem 3.3]) and separable if $1 \leq p < \infty$ (see [AF03, Theorem 3.6]). Especially, $W^{k,2}(\Omega)$ is a separable Hilbert space with inner product

$$(u, v)_{W^{k,2}(\Omega)} = \sum_{0 \leq |\boldsymbol{\alpha}| \leq m} (\partial^{\boldsymbol{\alpha}} u, \partial^{\boldsymbol{\alpha}} v)_{L^2(\Omega)}, \tag{II.1.3}$$

where the L^2 inner product is defined in (II.1.2).

We now introduce fractional Sobolev spaces, that is, instead of $k \in \mathbb{N}$, we consider $s \in \mathbb{R}$. This can be done in different ways, see for example the survey paper [DNPV12]. Here, we follow [McL00, Chapter 3] to introduce the Sobolev-Slobodeckii norm.

Definition II.1.17. *Let $s \in \mathbb{R}_{>0}$ with $s = k + \kappa$, where $k \in \mathbb{N}_0$ and $\kappa \in (0, 1)$. Let $\Omega \subset \mathbb{R}^d$ be an open subset. The Sobolev-Slobodeckii norm is defined as*

$$\|u\|_{W^{s,p}(\Omega)} := \left(\|u\|^p_{W^{k,p}(\Omega)} + |u|^p_{W^{s,p}(\Omega)} \right)^{\frac{1}{p}},$$

where

$$|u|^p_{W^{s,p}(\Omega)} = \sum_{|\boldsymbol{\alpha}| = k} \int_\Omega \int_\Omega \frac{|\partial^{\boldsymbol{\alpha}} u(\mathbf{x}) - \partial^{\boldsymbol{\alpha}} u(\mathbf{y})|^p}{\|\mathbf{x} - \mathbf{y}\|^{d+p\kappa}} \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}.$$

In complete analogy to the above, we can define, see [McL00, p. 74],

$$W^{s,p}(\Omega) := \left\{ u \in W^{k,p}(\Omega) \colon |u|_{W^{s,p}(\Omega)} < \infty \right\}$$

and, see [DNPV12, p. 527],

$$W^{s,p}_0(\Omega) := \overline{C^\infty_0(\Omega)}^{\|\cdot\|_{W^{s,p}(\Omega)}}.$$

For $p = 2$ and real $s \geq 0$, we have that $W^{s,2}(\Omega)$ is a Hilbert space with the inner product

$$\begin{aligned}(u, v)_{W^{s,2}(\Omega)} :=& (u, v)_{W^{k,2}(\Omega)} \\ &+ \sum_{|\boldsymbol{\alpha}| = k} \int_\Omega \int_\Omega \frac{\left(\partial^{\boldsymbol{\alpha}} u(\mathbf{x}) - \partial^{\boldsymbol{\alpha}} u(\mathbf{y})\right)\left(\partial^{\boldsymbol{\alpha}} v(\mathbf{x}) - \partial^{\boldsymbol{\alpha}} v(\mathbf{y})\right)}{\|\mathbf{x} - \mathbf{y}\|^{d+2\kappa}} \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y},\end{aligned}$$

where the inner product $(\cdot, \cdot)_{W^{k,2}(\Omega)}$ is introduced in (II.1.3).

For $s < 0$ and $1 < p < \infty$, the Sobolev space $W^{s,p}(\Omega)$ is defined as the dual space of $W^{-s,q}_0(\Omega)$, where q satisfies $\frac{1}{p} + \frac{1}{q} = 1$. The norm is the usual dual norm given by

$$\|u\|_{W^{s,p}(\Omega)} := \sup_{0 \neq v \in W^{-s,q}_0(\Omega)} \frac{|(u, v)_{L^2(\Omega)}|}{\|v\|_{W^{-s,q}_0(\Omega)}},$$

where the following remark justifies the use of the L^2 inner product notation instead of the duality pairing.

Remark II.1.18. *For a reflexive Banach space V and a Hilbert space H with $\iota \colon V \hookrightarrow H$ a continuous, injective, dense embedding, we have the so-called* Gelfand triple

$$V \hookrightarrow H \hookrightarrow V'.$$

The embedding $\iota' \colon H \hookrightarrow V'$ is again continuous, injective and dense (compare [Wlo87, Definition 17.1]). We can then continuously extend the inner product $(\cdot, \cdot)_H$ to $V' \times V$. Therefore, the dual norm introduced above makes sense.

In the following, we introduce a second notion of Sobolev spaces along the lines of [McL00, p. 75ff.].

Definition II.1.19. *For $s \in \mathbb{R}$, we define the continuous linear operator $\mathcal{J}^s\colon \boldsymbol{\mathcal{S}}(\mathbb{R}^d) \to \boldsymbol{\mathcal{S}}(\mathbb{R}^d)$, called the* Bessel potential *of order s, by*

$$\mathcal{J}^s u(\mathbf{x}) = \int_{\mathbb{R}^d} \left(1 + \|\boldsymbol{\xi}\|^2\right)^{\frac{s}{2}} \hat{u}(\boldsymbol{\xi}) e^{i2\pi\langle \mathbf{x}, \boldsymbol{\xi}\rangle} \,\mathrm{d}\boldsymbol{\xi} \quad \text{for } \mathbf{x} \in \mathbb{R}^d.$$

In here, $\hat{u} = \mathcal{F}u$ denotes the Fourier transform defined by

$$\hat{u}(\boldsymbol{\xi}) = \int_{\mathbb{R}^d} e^{-i2\pi\langle \boldsymbol{\xi}, \mathbf{x}\rangle} u(\mathbf{x}) \,\mathrm{d}\mathbf{x} \quad \text{for } \boldsymbol{\xi} \in \mathbb{R}^d,$$

which is a continuous linear operator $\mathcal{F}\colon \boldsymbol{\mathcal{S}}(\mathbb{R}^d) \to \boldsymbol{\mathcal{S}}(\mathbb{R}^d)$ with continuous inverse, see [McL00, p. 69ff.].

Definition II.1.20. *For $s \in \mathbb{R}$, we define the Sobolev space $H^s(\mathbb{R}^d)$ of order s on $\mathbb{R}^d$ by*

$$H^s(\mathbb{R}^d) = \left\{u \in \boldsymbol{\mathcal{S}}'(\mathbb{R}^d)\colon \mathcal{J}^s u \in L^2(\mathbb{R}^d)\right\}.$$

We have the inner product

$$(u, v)_{H^s(\mathbb{R}^d)} = (\mathcal{J}^s u, \mathcal{J}^s v)_{L^2(\mathbb{R}^d)}$$

and the induced norm

$$\|u\|_{H^s(\mathbb{R}^d)} = \sqrt{(u, u)_{H^s(\mathbb{R}^d)}} = \|\mathcal{J}^s u\|_{L^2(\mathbb{R}^d)}.$$

For a non-empty domain $\Omega \subset \mathbb{R}^d$, we can introduce the Sobolev spaces $H^s(\Omega)$ as restrictions of $H^s(\mathbb{R}^d)$, see [McL00, p. 77]:

Definition II.1.21. *Let $\Omega \subset \mathbb{R}^d$ be a non-empty domain and $s \in \mathbb{R}$. We define*

$$H^s(\Omega) := \left\{u = U|_\Omega \colon U \in H^s(\mathbb{R}^d)\right\}$$

with the norm

$$\|u\|_{H^s(\Omega)} = \inf_{\substack{U \in H^s(\mathbb{R}^d) \\ U|_\Omega = u}} \|U\|_{H^s(\mathbb{R}^d)}.$$

Moreover, we define

$$\begin{aligned} \widetilde{H}^s(\Omega) &:= \overline{\mathcal{D}(\Omega)}^{\|\cdot\|_{H^s(\mathbb{R}^d)}}, \\ H_0^s(\Omega) &:= \overline{\mathcal{D}(\Omega)}^{\|\cdot\|_{H^s(\Omega)}}. \end{aligned} \tag{II.1.4}$$

The equivalence of $W^{s,2}(\Omega)$ spaces and $H^s(\Omega)$ spaces depends on the smoothness of the domain Ω. Therefore, we introduce the notion of $C^{k,\kappa}$-domains along the lines of [McL00, Chapter 3 and Definition 3.28], where $k \in \mathbb{N}_0$ and $\kappa \in (0, 1]$. To this end, let $\Omega \subset \mathbb{R}^d$ be an open set with boundary

$$\Gamma = \partial\Omega = \overline{\Omega} \cap (\mathbb{R}^d \backslash \Omega).$$

Then, we say that Ω is a $C^{k,\kappa}$*-hypograph* if there is a function $\xi\colon C^{k,\kappa}(\mathbb{R}^{d-1}) \to \mathbb{R}$ such that

$$\Omega = \{\mathbf{x} \in \mathbb{R}^d \colon x_d < \xi(x_1, \ldots, x_{d-1}) \text{ for all } (x_1, \ldots, x_{d-1}) \in \mathbb{R}^{d-1}\}. \tag{II.1.5}$$

Definition II.1.22. *Let $k \in \mathbb{N}_0$ and $\kappa \in (0,1]$. The open set Ω is a $C^{k,\kappa}$-*domain *if the boundary $\Gamma := \partial\Omega$ is compact and there exist finite families $\{W_j\}$ and $\{\Omega_j\}$ with the following properties:*

- *The family $\{W_j\}$ is a finite cover of Γ. This means, that W_j are open subsets of $\mathbb{R}^d$ and $\Gamma \subset \bigcup_j W_j$,*
- *each Ω_j can be transformed to a $C^{k,\kappa}$-hypograph by a rotation and a translation,*
- *for Ω it holds $W_j \cap \Omega = W_j \cap \Omega_j$ for every j.*

Notice that a Lipschitz domain is thus a $C^{0,1}$-domain. If Ω is a Lipschitz hypograph as in (II.1.5), we have that

$$\Gamma = \big\{\mathbf{x} \in \mathbb{R}^d \colon x_d = \xi(x_1, \ldots, x_{d-1})\big\}.$$

Every Lipschitz domain Ω has a surface measure σ and an outward pointing unit normal $\mathbf{n}$ almost everywhere.

Under a sufficiently smooth mapping, the Lipschitz property of the domain is conserved. More precisely, let $\boldsymbol{\kappa} \colon \mathbb{R}^d \to \mathbb{R}^d$ be a C^1-diffeomorphism. Then, if Ω is a Lipschitz domain, also the set $\boldsymbol{\kappa}(\Omega)$ is a Lipschitz domain, see [McL00, p. 90]. [McL00, Theorem 3.33] and [McL00, Theorem 3.30] provide the following statement.

Lemma II.1.23. *Let $s \in \mathbb{R}_{\geq 0}$ and Ω be a Lipschitz domain. We then have*

$$\widetilde{H}^s(\Omega) \subset H^s_0(\Omega)$$

and

$$\widetilde{H}^s(\Omega) = H^s_0(\Omega) \text{ for all } s \neq \left\{\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\right\}.$$

Moreover,

$$H^s(\Omega)' = \widetilde{H}^{-s}(\Omega), \quad \widetilde{H}^s(\Omega)' = H^{-s}(\Omega) \quad \text{for all } s \in \mathbb{R}.$$

Additionally, we can state the equivalence of the Sobolev spaces, see [McL00, Theorem 3.30], [McL00, Theorem 3.16], [Wlo87, Lemma 5.1] and [McL00, Theorem 3.19].

Lemma II.1.24. *Let Ω be a Lipschitz domain or $\Omega = \mathbb{R}^d$. Then, it holds*

$$W^{s,2}(\Omega) = H^s(\Omega) \text{ and } W^{s,2}_0(\Omega) = H^s_0(\Omega) \text{ for all } s \in \mathbb{R}_{\geq 0}.$$

Moreover, for any non-empty set $\Omega \subset \mathbb{R}^d$ and any $k \in \mathbb{N}_0$, it holds

$$H^{-k}(\Omega) = W^{-k,2}(\Omega)$$

with equivalent norms.

II.1.5 Sobolev spaces on manifolds

To construct Sobolev spaces on manifolds, for example on the boundary Γ of a domain Ω, we use the Sobolev spaces on $\mathbb{R}^{d-1}$, as shown in [McL00, Chapter 3, p. 98ff.]. The well-definedness of the Sobolev spaces depends on the regularity of the boundary and a reasonable notion of integration on submanifolds which relies in particular on the surface measure σ. Due to the required differential geometric technicalities we postpone a detailed discussion thereof to Section II.2.2. We first need to introduce the notion of a partition of unity along the lines of [McL00, Chapter 3, p. 83].

Definition II.1.25. *Let $\Omega \subset \mathbb{R}^d$ be an open set. A* partition of unity *is a finite or infinite sequence of functions $\varphi_1, \varphi_2, \ldots \in C^\infty(\mathbb{R}^d)$ such that*

1. *$\varphi_i \geq 0$ on $\mathbb{R}^d$ for all i,*
2. *each point of Ω has a neighbourhood that intersects $\operatorname{supp} \varphi_i$ for only finitely many i,*
3. *$\sum_i \varphi_i(\mathbf{x}) = 1$ for all $\mathbf{x} \in \Omega$.*

From the second property, it follows that the sum in the third property is a finite sum for every $\mathbf{x} \in \Omega$. Moreover, if Ω is not open, we speak of a partition of unity of Ω if the φ_i form a partition of unity for an open neighbourhood of Ω.

Let $\mathcal{W}$ be an open cover of Ω. Following [McL00, p. 84], we say that a partition of unity $\{\varphi_i\}_{i\geq 1}$ is *subordinate* to $\mathcal{W}$ if for each i there exists a $W \in \mathcal{W}$ such that $\operatorname{supp} \varphi_i \subset W$. We can now state the following lemma for the existence of a partition of unity along the lines of [McL00, Theorem 3.21, p. 84].

Lemma II.1.26. *Given any open cover $\mathcal{W}$ of a set $\Omega \subset \mathbb{R}^d$, there exists a partition of unity $\{\varphi_i\}_{i\geq 1}$ for Ω subordinate to $\mathcal{W}$. Moreover, the φ_i can be chosen in such a way that $\operatorname{supp} \varphi_i$ is compact for each i.*

Definition II.1.27. *Let $k \in \mathbb{N}$ and Ω be a $C^{k-1,1}$-domain. Let $\{\varphi_j\}_{j\geq 1}$ be a partition of unity subordinate to the open cover $\{W_j\}_{j\geq 1}$ of $\Gamma := \partial\Omega$, where the W_j are introduced in Definition II.1.22. Thus, there exist $C^{k-1,k}$-mappings $\boldsymbol{\psi}_j \colon \mathbb{R}^{d-1} \to \mathbb{R}^d$, for example given by $\mathbf{x} \mapsto \big(x_1, \ldots, x_{d-1}, \xi_j(x_1, \ldots, x_{d-1})\big)$. With the aid of the partition of unity, we can write every function u defined on Γ as*

$$u = \sum_j \varphi_j u.$$

We then set, using $L^2(\Gamma) = L^2_\sigma(\Gamma)$,

$$H^s(\Gamma) := \big\{u \in L^2(\Gamma) \colon (\varphi_j u) \circ \boldsymbol{\psi}_j \in H^s(\mathbb{R}^{d-1}) \text{ for all } j\big\} \text{ for all } 0 \leq s \leq k$$

and endow it with the scalar product

$$(u, v)_{H^s(\Gamma)} = \sum_j \big((\varphi_j u) \circ \boldsymbol{\psi}_j, (\varphi_j v) \circ \boldsymbol{\psi}_j\big)_{H^s(\mathbb{R}^{d-1})}.$$

For $-k \leq s < 0$, we define the Sobolev spaces by duality, thus

$$H^s(\Gamma) = \big(H^{-s}(\Gamma)\big)',$$

equipped with the dual norm

$$\|u\|_{H^s(\Gamma)} = \sup_{0\neq v\in H^{-s}(\Gamma)} \frac{(u,v)_{L^2(\Gamma)}}{\|v\|_{H^{-s}(\Gamma)}}.$$

The use of the L^2 inner product instead of the duality pairing is justified by Remark II.1.18.

Notice that, according to [McL00, Chapter 3], the definition is independent of the choice of $\{W_j\}_{j\geq 1}$, $\{\Omega_j\}_{j\geq 1}$ and $\{\varphi_j\}_{j\geq 1}$.

With an analogous procedure as above, we can define the spaces $C^k(\Gamma)$ for $k \in \mathbb{N}_0$.

To introduce Sobolev spaces which are only defined on a part of the boundary, we follow [McL00, p. 99]. Let Ω be a Lipschitz hypograph. Let $\Gamma = \Gamma_1 \cup \Pi \cup \Gamma_2$, where Γ_1 and Γ_2 are disjoint, non-empty, relatively open subsets of Γ and have Π as their common boundary in Γ. We call this a *Lipschitz dissection* of Γ if there exists a Lipschitz function $\rho\colon \mathbb{R}^{d-2} \to \mathbb{R}$ such that

$$\begin{aligned}
\Gamma_1 &= \big\{\mathbf{x} \in \Gamma\colon x_{d-1} < \rho(x_1,\dots,x_{d-2})\big\},\\
\Pi &= \big\{\mathbf{x} \in \Gamma\colon x_{d-1} = \rho(x_1,\dots,x_{d-2})\big\},\\
\Gamma_2 &= \big\{\mathbf{x} \in \Gamma\colon x_{d-1} > \rho(x_1,\dots,x_{d-2})\big\}.
\end{aligned}$$

This can be naturally extended to Ω being a Lipschitz domain. We define

$$H^s(\Gamma_1) := \big\{U|_{\Gamma_1}\colon U \in H^s(\Gamma)\big\}.$$

Let $\mathcal{D}(\Gamma_1) = \{\phi \in \mathcal{D}(\Gamma)\colon \operatorname{supp}\phi \subset \Gamma_1\}$. Then, we set

$$\widetilde{H}^s(\Gamma_1) = \overline{\mathcal{D}(\Gamma_1)}^{H^s(\Gamma)}$$

in analogy to (II.1.4).

II.1.6 Gâteaux and Fréchet derivative

In the following, we introduce the notions of the first variation, the Gâteaux derivative and the Fréchet derivative along the lines of [Trö05, Section 2.6, p. 44–46], see also [Alt12, p. 149]. We let X and Y be real Banach spaces, $\Omega \subset X$ an open set and $f\colon \Omega \to Y$ a mapping.

Definition II.1.28. *If the limes*

$$\nabla f(\mathbf{x})[\mathbf{h}] := \lim_{t\searrow 0} \frac{f(\mathbf{x}+t\mathbf{h}) - f(\mathbf{x})}{t} = \frac{\mathrm{d}}{\mathrm{d}t} f(\mathbf{x}+t\mathbf{h})|_{t=0}$$

exists in Y for given $\mathbf{x} \in \Omega$ and $\mathbf{h} \in X$, then we call it the directional derivative *of f at $\mathbf{x}$ in the direction $\mathbf{h}$. If the limes exists for all $\mathbf{h} \in X$, then we call the map $\mathbf{h} \mapsto \nabla f(\mathbf{x},\mathbf{h})$ the* first variation *of f at $\mathbf{x}$.*

This map does not have to be linear, see [Trö05, p. 44] for an example.

Definition II.1.29. *If the first variation $\nabla f(\mathbf{x})[\mathbf{h}]$ at $\mathbf{x}$ and a linear continuous operator $A\colon X \to Y$ with*

$$\nabla f(\mathbf{x})[\mathbf{h}] = A\mathbf{h} \quad \textit{for all } \mathbf{h} \in X$$

exist, then we call f Gâteaux differentiable *at $\mathbf{x}$ and A is the* Gâteaux derivative *of f at $\mathbf{x}$. We write $A = f'_G(\mathbf{x})$.*

Thus, if $f\colon \Omega \to \mathbb{R}$ is Gâteaux differentiable at $\mathbf{x}$, then $f'_G(\mathbf{x})$ is an element of the dual space X'.

Definition II.1.30. *A map $f\colon \Omega \to Y$ is called* Fréchet differentiable *at $\mathbf{x} \in \Omega$, if there exists an operator $A \in \mathcal{L}(X;Y)$ and a map $r(\mathbf{x},\cdot)\colon X \to Y$ with the following property: For all $\mathbf{h} \in X$ with $\mathbf{x}+\mathbf{h} \in \Omega$ it holds*

$$f(\mathbf{x}+\mathbf{h}) = f(\mathbf{x}) + A\mathbf{h} + r(\mathbf{x},\mathbf{h}),$$

where r satisfies

$$\frac{\|r(\mathbf{x},\mathbf{h})\|_Y}{\|\mathbf{x}\|_X} \to 0 \quad \textit{for } \|\mathbf{h}\|_X \to 0.$$

A is called the Fréchet derivative *of f at $\mathbf{x}$ and we write $A = f'_F(\mathbf{x})$.*

Notice that, in general, not every Gâteaux differentiable function is also Fréchet differentiable, see [AH10, p. 242] for an example. The inverse is true, thus if f is Fréchet differentiable at $\mathbf{x}$, then f is continuous at $\mathbf{x}$ and Gâteaux differentiable with $f'_G(\mathbf{x}) = f'_F(\mathbf{x})$, see [IT79, Hilfssatz 1, p. 37].

The following theorem can be found in [IT79, Folgerung, p. 41] or [AH10, Proposition A.3, p. 242] and gives a criterion when a Gâteaux derivative is also a Fréchet derivative.

Theorem II.1.31. *Let X be a Banach space and f a continuous map from the open neighbourhood U of $\mathbf{x}$ into the Banach space Y. If f is Gâteaux differentiable on U, i.e. for all $\mathbf{y} \in U$, and the map $U \to \mathcal{L}(X;Y)$ given by $\mathbf{y} \mapsto f'_G(\mathbf{y})$ is continuous, then f is Fréchet differentiable at $\mathbf{x}$.*

II.2 Differential geometry

In the following section, we will recall how to transform domain and boundary integrals when having a diffeomorphism at hand, and introduce some general terms and facts of differential geometry.

II.2.1 Fundamental terms

We first introduce the notion of a parametrization along the lines of [FK14, Paragraph 11, p. 257ff.].

Lemma II.2.1. *Let $1 \le m < d$ and $1 \le k \le \infty$. For every point $\mathbf{a}$ of an m-dimensional C^k-submanifold $S \subset \mathbb{R}^d$ there exists a neighbourhood $V \subset \mathbb{R}^d$, a domain $U \subset \mathbb{R}^m$ and a C^k-map $\boldsymbol{\gamma}\colon U \to S$ with*

- $\boldsymbol{\gamma}(U) = V \cap S$,
- $\mathrm{D}\boldsymbol{\gamma}(\mathbf{u})$ *has the maximal rank m for every $\mathbf{u} \in U$,*
- *the inverse map $\boldsymbol{\gamma}^{-1}\colon V \cap S \to U$ exists and is continuous.*

We call such maps $\boldsymbol{\gamma}$ a parametrization *of S and the image $V \cap S$ a* parameter neighbourhood *of $\mathbf{a}$.*

Following [FK14, p. 264], we can define the tangent space of a submanifold and characterize it as the span of the derivatives of the parametrization.

Definition II.2.2. *Let S be an m-dimensional submanifold of $\mathbb{R}^d$. A vector $\mathbf{v} \in \mathbb{R}^d$ is called a* tangent vector *of S at the point $\mathbf{a} \in S$ if there exists a C^1-curve $\boldsymbol{\alpha}\colon (-\epsilon, \epsilon) \to S$ with*

$$\boldsymbol{\alpha}(0) = \mathbf{a}, \quad \boldsymbol{\alpha}'(0) = \mathbf{v}.$$

Lemma II.2.3. *The set of all tangent vectors of S at a point $\mathbf{a} \in S$ builds an m-dimensional vector space, called the* tangent space *$T_{\mathbf{a}}S$. It is characterized by*

$$T_{\mathbf{a}}S = \operatorname{span}\left\{\partial_1\boldsymbol{\gamma}(\mathbf{u}), \dots, \partial_m\boldsymbol{\gamma}(\mathbf{u})\right\}$$

and is the image of $\mathrm{D}\boldsymbol{\gamma}(\mathbf{u})$ for every parametrization $\boldsymbol{\gamma}$ with $\boldsymbol{\gamma}(\mathbf{u}) = \mathbf{a}$.

Definition II.2.4. *Let $S \subset \mathbb{R}^d$ be a C^r-submanifold. A function $f\colon S \to \mathbb{R}$ is called* C^k-differentiable *($f \in C^k(S), 0 \leq k \leq r$), if $f \circ \boldsymbol{\gamma}$ is C^k-differentiable for every C^r-parametrization $\boldsymbol{\gamma}$ of S. It suffices that for every point $\mathbf{a} \in S$ there exists at least one C^k-parametrization of a neighbourhood $V \cap S$ of $\mathbf{a}$, such that $f \circ \boldsymbol{\gamma}$ is C^k-differentiable. A vector field $\mathbf{V}\colon S \to \mathbb{R}^d$ is called C^k-differentiable, if every component is C^k-differentiable.*

In the following, we introduce the Gram matrix along the lines of [FK14, p. 265]. Let $\boldsymbol{\gamma}$ be a parametrization of an m-dimensional submanifold $S \subset \mathbb{R}^d$. Then, the *Gram matrix*

$$G(\mathbf{u}) = \mathrm{D}\boldsymbol{\gamma}(\mathbf{u})^\mathsf{T}\, \mathrm{D}\boldsymbol{\gamma}(\mathbf{u})$$

has the coefficients

$$g_{i,k} = \partial_i\boldsymbol{\gamma}(\mathbf{u})^\mathsf{T}\partial_k\boldsymbol{\gamma}(\mathbf{u}), \quad 1 \leq i, k \leq m.$$

The *Gram determinant* is defined as

$$g(\mathbf{u}) := \det\big(G(\mathbf{u})\big).$$

II.2.2 Integration on submanifolds

We can now define the integration on submanifolds according to [FK14, p. 266]. Let $f\colon S \to \mathbb{R}$ be a continuous function on an m-dimensional submanifold $S \subset \mathbb{R}^d$. Let K be a compact subset of S. Then, we can define the integral $\int_K f\,\mathrm{d}\sigma$ in two steps.

Step 1 If K lies within a parameter neighbourhood (see Lemma II.2.1), thus in the image of a parametrization $\boldsymbol{\gamma}\colon \mathbb{R}^m \supset U \to S \cap V$, we set

$$\int_K f\,\mathrm{d}\sigma := \int_{\boldsymbol{\gamma}^{-1}(K)} f\big(\boldsymbol{\gamma}(\mathbf{u})\big)\sqrt{g(\mathbf{u})}\,\mathrm{d}\mathbf{u}. \tag{II.2.1}$$

Notice that the right-hand side is independent of the choice of the parametrization.

Step 2 Let K be an arbitrary compact subset of S. There exist finitely many parameter neighbourhoods $V_k \cap S$ and corresponding parametrizations $\boldsymbol{\gamma}_k\colon \mathbb{R}^m \supset U_k \to V_k \cap S$ such that $K \subset \bigcup_k V_k$. Moreover, there exists a partition of unity $\{\varphi_k\}$

with $\operatorname{supp}\varphi_k \subset V_k$ (see Definition II.1.25). We set $A_k := K \cap \operatorname{supp}\varphi_k$ and define the integral as

$$\int_K f \,\mathrm{d}\sigma := \sum_k \int_{A_k} f\varphi_k \,\mathrm{d}\sigma. \tag{II.2.2}$$

This definition is independent of the choice of cover and partition of unity.

Notice that the integral transformation formula for domain integrals, see e.g. [For17, Satz 1, p. 104], is a special case of (II.2.1) and reads:

Lemma II.2.5. *Let U and V be open sets of $\mathbb{R}^d$ and $\boldsymbol{\kappa}\colon U \to V$ a C^1-diffeomorphism. Then, for every continuous function $f\colon V \to \mathbb{R}$ with compact support, it holds*

$$\int_V f(\mathbf{y}) \,\mathrm{d}\mathbf{y} = \int_U f\big(\boldsymbol{\kappa}(\mathbf{x})\big) \Big| \det\big(\mathrm{D}\boldsymbol{\kappa}(\mathbf{x})\big)\Big| \,\mathrm{d}\mathbf{x}.$$

For the computation of the integral $\int_S f \,\mathrm{d}\sigma$, one can apply the definition above if S is compact or allows to be covered with finitely many parameter neighbourhoods. Otherwise, we can find countable many compact sets $K_i \subset S$ as described in (II.1.1). A continuous function $f\colon S \to \mathbb{R}$ is *integrable over* S, if the sequence of integrals $\int_{K_i} |f| \,\mathrm{d}\sigma$ is bounded. In this case, we define

$$\int_S f \,\mathrm{d}\sigma := \lim_{i\to\infty} \int_{K_i} f \,\mathrm{d}\sigma.$$

This definition is again independent of the choice of K_i, see [FK14, p. 266].

II.2.3 Boundary integral transformation

We introduce the change of variables for boundary integrals, whose proof is in complete analogy to [SZ92, Proposition 2.47] or [SS10b, Remark 3].

Lemma II.2.6. *Let $\Gamma \subset \mathbb{R}^d$ be a C^k-manifold, $1 \leq k \leq \infty$. We denote the mapped boundary by $\Gamma_{\boldsymbol{\kappa}} = \boldsymbol{\kappa}(\Gamma)$, where $\boldsymbol{\kappa}\colon \mathbb{R}^d \to \mathbb{R}^d$ is a C^k-diffeomorphism. Let $g \in L^1(\Gamma_{\boldsymbol{\kappa}})$. We have the integral transformation*

$$\int_{\Gamma_{\boldsymbol{\kappa}}} g \,\mathrm{d}\sigma_{\boldsymbol{\kappa}} = \int_\Gamma g \circ \boldsymbol{\kappa}\omega_{\boldsymbol{\kappa}} \,\mathrm{d}\sigma$$

with the density term

$$\omega_{\boldsymbol{\kappa}} = \big|\det(\mathrm{D}\boldsymbol{\kappa})\big| \big\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}\big\| \tag{II.2.3}$$

and $\mathbf{n}$ being the unit normal of Γ.

Notice that the density term can be computed by a general procedure, see [DZ11, Chapter 2, Section 3.2.2].

The following is along the lines of [SS10b, Lemma 9].

Lemma II.2.7. *The unit normal field $\mathbf{n}_{\boldsymbol{\kappa}}$ on the mapped boundary $\Gamma_{\boldsymbol{\kappa}}$ reads*

$$\mathbf{n}_{\boldsymbol{\kappa}}\big(\boldsymbol{\kappa}(\mathbf{x})\big) = \frac{\big(\mathrm{D}\boldsymbol{\kappa}(\mathbf{x})\big)^{-\intercal}\mathbf{n}(\mathbf{x})}{\Big\|\big(\mathrm{D}\boldsymbol{\kappa}(\mathbf{x})\big)^{-\intercal}\mathbf{n}(\mathbf{x})\Big\|},$$

where $\mathbf{n}$ is the unit normal on Γ.

II.2.4 Curvature

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain with boundary Γ and $\mathbf{n}$ be the outward pointing normal. Let us introduce how to describe a surface implicitly. According to [OF03, Formula (2.1)] or [Néd01, Formula (2.5.138)], we have the following definition.

Definition II.2.8. *A* distance function a *is defined as*

$$a(\mathbf{x}) = \inf_{\mathbf{y}\in\Gamma} |\mathbf{x}-\mathbf{y}| \qquad \textit{for } \mathbf{x} \in \mathbb{R}^d.$$

It holds $a(\mathbf{x}) = 0$ *for* $\mathbf{x} \in \Gamma$*.*

Notice that distance functions have a kink at Γ. We can therefore introduce *signed (oriented) distance functions* (see [DZ11, Chapter 7, Section 2] or [Néd01, Section 2.5.6]).

Definition II.2.9. *A* signed distance function *is a function* $b(\mathbf{x})$ *with* $\big|b(\mathbf{x})\big| = a(\mathbf{x})$ *for all* $\mathbf{x}$*. Having a domain* Ω*, we can divide the space into the interior and the exterior. If* $b(\mathbf{x}) = a(\mathbf{x}) = 0$*, the point* $\mathbf{x}$ *lies on the boundary* Γ*. If* $b(\mathbf{x}) = -a(\mathbf{x})$*, then the point* $\mathbf{x}$ *lies in the interior and for* $b(\mathbf{x}) = a(\mathbf{x})$ *the point* $\mathbf{x}$ *lies in the exterior or vice versa.*

With this definition, we also removed the kink of the distance function (see [OF03, Chapter 2]). Notice that the more general case of signed distance functions are implicit functions ϕ. They have the same sign convention as a signed distance function, but not the distance property. Taking the level set of ϕ, thus the set where ϕ assumes a constant value, also allows to describe a boundary Γ. Using the sign convention then divides the space into the interior and exterior of a domain in an analogous fashion as the signed distance function. We call ϕ a *level set function*.

Along the lines of [DZ11, p. 485], we have the following definition.

Definition II.2.10. *For a* $\epsilon > 0$*, we can define the* tubular neighbourhood *of* $\Gamma \subset \mathbb{R}^d$ *as*

$$S_\epsilon(\Gamma) := \Big\{\mathbf{x} \in \mathbb{R}^d \colon \big|b(\mathbf{x})\big| < \epsilon\Big\}$$

for the oriented distance function b *associated to* Ω*. If* Γ *is compact and* C^2*, then there exists an* $\epsilon > 0$ *such that* $b \in C^2\big(S_{2\epsilon}(\Gamma)\big)$*.*

For smooth surfaces, it holds that the normal $\mathbf{n}$ to the surface corresponds to the gradient of b. Thus, we have a canonical extension $\boldsymbol{\mathcal{N}}$ of the normal from the surface into a tubular neighbourhood of the surface by setting $\boldsymbol{\mathcal{N}} = \nabla b$. We denote the *curvature operator* by

$$\boldsymbol{\mathcal{R}} := \mathrm{D}\boldsymbol{\mathcal{N}} = \mathrm{D}^2 b. \tag{II.2.4}$$

In here, $\mathrm{D}^2 b$ is the second fundamental form, see [DZ11, Chapter 9, Section 5]. According to [Néd01, Theorem 2.5.18] and [Gra91, Chapter 13.1], the curvature operator is a symmetric linear operator acting in the tangent plane (see also Lemma II.2.3). Thus, it holds

$$\boldsymbol{\mathcal{R}}\mathbf{n} = 0, \tag{II.2.5}$$

see also [Néd01, Formula (2.5.162)].

We can define the curvature along the lines of [MZ06, Definition 5.4] or [DZ11, Chapter 9, Section 4.2]:

Definition II.2.11. *For a smooth surface $\Gamma \subset \mathbb{R}^d$, $d \in \mathbb{N}$, the* additive curvature $\mathcal{H}$ *of Γ is defined as*

$$\mathcal{H} = \Delta b = \operatorname{tr}(\boldsymbol{\mathcal{R}}) = (d-1)\overline{H}.$$

Here, $\overline{H}$ is referred to as the mean curvature.

II.2.5 Tangential differential operators

Let us consider again a Lipschitz domain Ω with boundary Γ and let $\mathbf{n}$ be the outward pointing normal. Along the lines of [DZ11, Chapter 9, Sections 5.1 and 5.2], we introduce the following definitions of the tangential differential operators.

Definition II.2.12. *Let Γ be compact and let us associate to $f \in C^1(\Gamma)$ an extension $F \in C^1\big(S_{2\epsilon}(\Gamma)\big)$. Then the* tangential gradient *of f is defined as*

$$\nabla_\Gamma f := \nabla F|_\Gamma - \frac{\partial F}{\partial \mathbf{n}}\mathbf{n}.$$

Moreover, if we have an extension $\mathbf{V} \in C^1\big(S_{2\epsilon}(\Gamma); \mathbb{R}^d\big)$ of a vector field $\mathbf{v} \in C^1(\Gamma; \mathbb{R}^d)$, $d \geq 1$, we can define the tangential Jacobian matrix *as*

$$\mathrm{D}_\Gamma \mathbf{v} := \mathrm{D}\mathbf{V}|_\Gamma - \mathrm{D}\mathbf{V}\mathbf{n}\mathbf{n}^\intercal. \tag{II.2.6}$$

The tangential divergence *is defined as*

$$\operatorname{div}_\Gamma \mathbf{v} := \operatorname{tr}\big(\mathrm{D}\mathbf{V}|_\Gamma - \mathrm{D}\mathbf{V}\mathbf{n}\mathbf{n}^\intercal\big) = \operatorname{div}\mathbf{V}|_\Gamma - \langle \mathrm{D}\mathbf{V}\mathbf{n}, \mathbf{n}\rangle.$$

Notice that we can also introduce these tangential differential operators by using projection operators instead of extensions, compare [DZ11, Chapter 9, Section 5].

With Definition II.2.12 at hand, we can write the additive curvature also as

$$\mathcal{H} = \operatorname{div}_\Gamma \mathbf{n}$$

since

$$\operatorname{div}_\Gamma \mathbf{n} = \operatorname{div}\boldsymbol{\mathcal{N}}|_\Gamma - \mathrm{D}\boldsymbol{\mathcal{N}}\mathbf{n}\mathbf{n}^\intercal = \Delta b|_\Gamma,$$

where we used (II.2.5) and Definition II.2.11.

According to [DZ11, Chapter 9, Theorem 5.2], it holds

$$\langle \mathbf{n}, \nabla_\Gamma f\rangle = \langle \nabla b, \nabla_\Gamma f\rangle = 0 \tag{II.2.7}$$

on Γ under the assumptions that Γ is compact and C^2.

The following lemma gives a formula of tangential calculus, which can be found in [DZ11, Chapter 9, Section 5.4, p. 497].

Lemma II.2.13. *Let $\mathbf{W} \in C^1\big(S_{2h}(\Gamma); \mathbb{R}^d\big)$. We set*

$$\mathbf{w} := \mathbf{W}|_\Gamma, \quad w_\mathbf{n} := \langle \mathbf{W}, \mathbf{n}\rangle, \quad \mathbf{w}_\Gamma := \mathbf{W} - w_\mathbf{n}\mathbf{n}.$$

Then, there holds

$$\nabla_\Gamma w_\mathbf{n} = (\mathrm{D}_\Gamma \mathbf{w})^\intercal \mathbf{n} + \boldsymbol{\mathcal{R}}\mathbf{w}_\Gamma. \tag{II.2.8}$$

II.2.6 Divergence theorems

We recall the well-known divergence theorem on domains, also known as Gauß' theorem (see [For17, Satz 3, p. 182]).

Lemma II.2.14. *Let $\Omega \subset \mathbb{R}^d$ be a compact subset with smooth boundary, $\mathbf{n}$ the outward pointing normal vector field and $U \supset \Omega$ an open subset of $\mathbb{R}^d$. Then, for every continuously differentiable vector field $\mathbf{F}\colon U \to \mathbb{R}^d$, it holds*

$$\int_\Omega \operatorname{div}\big(\mathbf{F}(\mathbf{x})\big)\,\mathrm{d}\mathbf{x} = \int_{\partial\Omega} \big\langle \mathbf{F}(\mathbf{x}), \mathbf{n}(\mathbf{x}) \big\rangle \,\mathrm{d}\sigma.$$

Notice that we can also relax the assumptions of the above lemma. According to [McL00, Theorem 3.34] it suffices, that the domain is a Lipschitz domain. By a density argument, we can also make use of this relation for $\mathbf{F}$ being weakly differentiable.

When considering a surface having a boundary itself, we can find an analogous formula for boundary integrals in [DZ97, Corollary 3.1] and [SZ92, Proposition 2.58]. The formula is called the *tangential Stokes formula.*

Lemma II.2.15. *Let $S \subset \Gamma$ be a C^2-manifold and ∂S be the boundary of S. For $\mathbf{v} \in H^1(\Gamma;\mathbb{R}^d)$, it holds*

$$\int_S \operatorname{div}_S \mathbf{v}\,\mathrm{d}S = \int_S \mathcal{H}\langle \mathbf{v}, \mathbf{n}\rangle \,\mathrm{d}S - \int_{\partial S} \langle \mathbf{v}, \boldsymbol{\tau}\rangle \,\mathrm{d}\partial S,$$

where $\mathcal{H}$ denotes the additive curvature (see Definition II.2.11) and $\boldsymbol{\tau}$ is the unique unit tangent vector to S, which is outward pointing from S and normal to the boundary ∂S.

The classical tangential Stokes formula for a closed surface is for example stated in [DZ11, Chapter 9, Section 5.5, p. 498]. Notice that with the relation $\operatorname{div}_S(f\mathbf{v}) = f \operatorname{div}_S \mathbf{v} + \langle \nabla_S f, \mathbf{v}\rangle$ for $f \in H^1(\Gamma)$ and $\mathbf{v}$ as above (compare [DZ11, Chapter 9, Section 5.5]), also a tangential Green's formula can be straightforwardly derived from Lemma II.2.15.

Chapter III

Parabolic equations on tubes

This chapter treats the necessary background for handling parabolic equations on cylindrical domains and non-cylindrical domains, reflecting moving domains. While the former is standard, the latter is not well-established. We can prove an existence and uniqueness result for the heat equation on moving domains with Dirichlet boundary condition by using a variational formulation in anisotropic Sobolev spaces. Introducing boundary integral operators and proving their mapping properties allows to state also an existence and uniqueness result of a Neumann problem, where the Neumann trace contains an additional term accounting for the moving boundary.

Although we follow the argumentation line of Costabel [Cos90], we repeat the proofs here in the non-cylindrical setting for the reader's convenience, since we have to use the appropriate function spaces and the correct Neumann traces. We indicate the needed adaptations.

To avoid cluttering of the notation, we use $\langle\cdot,\cdot\rangle$ to denote the standard inner product on $\mathbb{R}^d$ as well as to denote the duality product in this chapter, since the meaning is clear from the context.

III.1 Anisotropic Sobolev spaces

In order to study the heat equation, we shall introduce appropriate anisotropic Sobolev spaces on cylindrical domains. From these spaces, we will then derive Sobolev spaces on time-dependent domains.

III.1.1 Anisotropic Sobolev spaces on cylindrical domains

Let $\Omega_0 \subset \mathbb{R}^d$, $d \geq 2$, be a Lipschitz domain in the spatial variable with boundary $\Gamma_0 := \partial\Omega_0$ and let $0 < T < \infty$. Then, the product set $Q_0 := (0,T) \times \Omega_0 \subset \mathbb{R}^{1+d}$ forms a time-space cylinder with the lateral boundary $\Sigma_0 := (0,T) \times \Gamma_0$. The appropriate function spaces for parabolic problems in time invariant domains, i.e. in cylindrical domains, are the anisotropic Sobolev spaces defined by

$$H^{r,s}(Q_0) := L^2\big((0,T); H^r(\Omega_0)\big) \cap H^s\big((0,T); L^2(\Omega_0)\big)$$

for $r, s \in \mathbb{R}_{\geq 0}$, see, e.g., [CKY98, Cos90, LM72b]. The corresponding boundary spaces are

$$H^{r,s}(\Sigma_0) := L^2\big((0,T); H^r(\Gamma_0)\big) \cap H^s\big((0,T); L^2(\Gamma_0)\big)$$

Note that these spaces are well-defined for $r \leq 1$ (while $s \geq 0$ is arbitrary) if Γ_0 is Lipschitz.

Remark III.1.1. *The space $H^{r,s}(Q_0)$ consists of all functions $u \in L^2(Q_0)$, where the $L^2(Q_0)$-norm of the partial derivatives $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^{\beta} u(t,\mathbf{x})$ is finite for all $|\boldsymbol{\alpha}| \leq \lambda r$, $\beta \leq (1-\lambda)s$, and $\lambda \in [0,1]$.*

With these definitions at hand, we can define spaces for functions with zero initial condition by setting

$$H^{r,s}_{;0,}(Q_0) := L^2\big((0,T); H^r(\Omega_0)\big) \cap H^s_{0,}\big((0,T); L^2(\Omega_0)\big),$$

where

$$H^s_{0,}\big((0,T); L^2(\Omega_0)\big) := \Big\{ u = U|_{(0,T)} \colon U \in H^s\big((-\infty,T); L^2(\Omega_0)\big) \colon U(t) = 0 \text{ for } t < 0 \Big\}.$$

Note that we adopted the notation from [DNS19, Doh19]. In addition, we can define functions which vanish at $t = T$ by setting

$$H^{r,s}_{;,0}(Q_0) := L^2\big((0,T); H^r(\Omega_0)\big) \cap H^s_{,0}\big((0,T); L^2(\Omega_0)\big),$$

where in complete analogy

$$H^s_{,0}\big((0,T); L^2(\Omega_0)\big) := \Big\{ u = U|_{(0,T)} \colon U \in H^s\big((0,\infty); L^2(\Omega_0)\big) \colon U(t) = 0 \text{ for } t > T \Big\}.$$

As in the elliptic case, we can also include (spatial) zero boundary conditions into the function spaces by setting

$$\begin{aligned} H^{r,s}_{0;0,}(Q_0) &:= L^2\big((0,T); H^r_0(\Omega_0)\big) \cap H^s_{0,}\big((0,T); L^2(\Omega_0)\big), \\ H^{r,s}_{0;,0}(Q_0) &:= L^2\big((0,T); H^r_0(\Omega_0)\big) \cap H^s_{,0}\big((0,T); L^2(\Omega_0)\big), \end{aligned}$$

where the spaces include zero initial and end conditions, respectively. On the boundary, we introduce

$$\begin{aligned} H^{r,s}_{;0,}(\Sigma_0) &:= L^2\big((0,T); H^r(\Gamma_0)\big) \cap H^s_{0,}\big((0,T); L^2(\Gamma_0)\big), \\ H^{r,s}_{;,0}(\Sigma_0) &:= L^2\big((0,T); H^r(\Gamma_0)\big) \cap H^s_{,0}\big((0,T); L^2(\Gamma_0)\big). \end{aligned}$$

These spaces are the closures of $H^{r,s}(\Sigma_0)$ for zero initial and end condition, respectively, compare [Doh19, Section 2.3].

By duality we have

$$H^{-r,-s}_{;0,}(Q_0) = \big[H^{r,s}_{0;,0}(Q_0)\big]' \quad \text{for } r - \frac{1}{2} \notin \mathbb{Z}$$

according to [Cos90]. The anisotropic Sobolev spaces on the boundary with negative smoothness index are defined by

$$\begin{aligned} H^{-r,-s}_{;,0}(\Sigma_0) &:= \big[H^{r,s}_{;0,}(\Sigma_0)\big]', \\ H^{-r,-s}_{;0,}(\Sigma_0) &:= \big[H^{r,s}_{;,0}(\Sigma_0)\big]', \\ \widetilde{H}^{-r,-s}(\Sigma_0) &:= \big[H^{r,s}(\Sigma_0)\big]', \end{aligned}$$

see [Doh19, Section 2.3]. Moreover, according to [Doh19, Remark 2.1], for $r \geq 0$ and $0 \leq s < \frac{1}{2}$ it holds $H^{r,s}(\Sigma_0) = H^{r,s}_{;0,}(\Sigma_0) = H^{r,s}_{;,0}(\Sigma_0)$ and, therefore, the above introduced dual spaces are equal and we simply write $H^{-r,-s}(\Sigma_0)$.

Remark III.1.2. *We would like to clarify the intuition behind the slightly cumbersome notation. In $H^{r,s}_{0;,}(Q_0)$, a zero before the semicolon indicates a zero boundary condition in space. After the semicolon, a zero initial condition can be indicated by writing a zero between the semicolon and the comma. Whereas, a zero after the comma stands for a zero end condition. Thus, the notation allows to see the spatial and temporal boundary condition at a glance.*

III.1.2 Anisotropic Sobolev spaces on non-cylindrical domains

Having at hand the Sobolev spaces defined on cylindrical domains, we can also introduce Sobolev spaces on non-cylindrical domains. They include a spatial domain, which we denote by Ω_t. The subscript t indicates that the spatial domain might differ for every point of time. To obtain a non-cylindrical domain, also called *tube*, Q_T we set

$$Q_T := \bigcup_{0<t<T} \big(\{t\} \times \Omega_t\big). \tag{III.1.1}$$

This domain has a lateral boundary Σ_T defined by

$$\Sigma_T := \bigcup_{0<t<T} \big(\{t\} \times \Gamma_t\big), \tag{III.1.2}$$

where $\Gamma_t := \partial\Omega_t$. The domains Ω_t each have a spatial normal $\mathbf{n}_t$, which we will also denote by $\mathbf{n}$ if it is clear from the context.

For every point of time t, we assume to have a smooth diffeomorphism $\boldsymbol{\kappa}$, which maps the initial domain Ω_0 onto the time-dependent domain Ω_t. In accordance with [MZ06], we write

$$\boldsymbol{\kappa}\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d, \quad (t,\mathbf{x}) \mapsto \boldsymbol{\kappa}(t,\mathbf{x}) \tag{III.1.3}$$

to emphasize the dependence of the mapping $\boldsymbol{\kappa}$ on the time, where we have $\boldsymbol{\kappa}(t,\Omega_0) = \Omega_t$. Especially, Ω_t is also a Lipschitz domain for all $t \in [0,T]$.

We introduce the non-cylindrical analogues of the Sobolev spaces by setting

$$H^{r,s}(Q_T) := \big\{ v \in L^2(Q_T) \colon v \circ \boldsymbol{\kappa} \in H^{r,s}(Q_0) \big\}$$

where the composition with $\boldsymbol{\kappa}$ only acts on the spatial component. Due to the chain rule, $v \circ \boldsymbol{\kappa}$ and v have the same Sobolev regularity, provided that the mapping $\boldsymbol{\kappa}$ is smooth enough, see for example [McL00, Theorem 3.23] for the elliptic case. For what follows, we assume that $\boldsymbol{\kappa} \in C^2\big([0,T] \times \mathbb{R}^d\big)$ satisfies

$$\|\boldsymbol{\kappa}(t,\mathbf{x})\|_{C^2([0,T]\times\mathbb{R}^d;\mathbb{R}^d)}, \|\boldsymbol{\kappa}(t,\mathbf{x})^{-1}\|_{C^2([0,T]\times\mathbb{R}^d;\mathbb{R}^d)} \leq C_{\boldsymbol{\kappa}} \tag{III.1.4}$$

for some constant $C_{\boldsymbol{\kappa}} \in (0,\infty)$ as in [HPS16, p. 826]. We define the norm of $H^{r,s}(Q_T)$ as

$$\|u\|_{H^{r,s}(Q_T)} = \|u \circ \boldsymbol{\kappa}\|_{H^{r,s}(Q_0)}$$

for $r, s \geq 0$. Notice that the Sobolev spaces on the boundary are defined in a similar manner.

Remark III.1.3. *(i) The space $H^{r,s}(Q_T)$ contains all functions such that $u \circ \boldsymbol{\kappa} \in H^{r,s}(Q_0)$. This means that $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^{\beta}(u \circ \boldsymbol{\kappa}) \in L^2(Q_0)$ for all $|\boldsymbol{\alpha}| \leq \lambda r$, $\beta \leq (1-\lambda)s$, and $\lambda \in [0,1]$. According to (III.1.4), the partial derivatives $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^{\beta} \boldsymbol{\kappa}$ exist and are uniformly bounded for all $|\boldsymbol{\alpha}| + \beta \leq 2$.*

(ii) Consider a function $u \in L^2(Q_T)$ *with partial derivatives* $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^{\beta} u \in L^2(Q_T)$ *for all* $|\boldsymbol{\alpha}| \leq \lambda r$, $\beta \leq (1-\lambda)s$, *and* $\lambda \in [0,1]$. *When computing the time-derivative of* $u \circ \boldsymbol{\kappa}$, *we obtain also a spatial derivative as the following shows*

$$(\partial_t u) \circ \boldsymbol{\kappa} = \partial_t (u \circ \boldsymbol{\kappa}) - \big\langle (\mathrm{D}\,\boldsymbol{\kappa})^{-\intercal} \nabla (u \circ \boldsymbol{\kappa}), \partial_t \boldsymbol{\kappa} \big\rangle. \tag{III.1.5}$$

This expression, which is also stated in [MZ06, pg. 43], can be proven by applying the multivariate chain rule since only the spatial component is affected by the composition with $\boldsymbol{\kappa}$. *Hence, it holds* $u \in H^{r,s}(Q_T)$ *only if* $r \geq s$ *since the temporal derivative* $\partial_t^{\beta}(u \circ \boldsymbol{\kappa})$ *involves also spatial partial derivatives* $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} u$ *up to the order* $|\boldsymbol{\alpha}| = \beta$ *besides the temporal derivative* $\partial_t^{\beta} u$.

(iii) Due to the uniformity condition (III.1.4), *we have as in [HPS16]*

$$0 < \underline{\sigma} \leq \min\{\sigma(\mathrm{D}\boldsymbol{\kappa})\} \leq \max\{\sigma(\mathrm{D}\boldsymbol{\kappa})\} \leq \overline{\sigma} < \infty,$$

where $\mathrm{D}\boldsymbol{\kappa}$ *denotes the Jacobian of* $\boldsymbol{\kappa}$ *and* $\sigma(\mathrm{D}\boldsymbol{\kappa})$ *denotes its singular values. Especially, as in [HPS16, Remark 1, p. 827], we may assume* $\det(\mathrm{D}\boldsymbol{\kappa})$ *to be positive.*

(iv) We can define the dual space of $H^{r,s}_{0;,0}(Q_T)$ *in two different ways, namely*

$$\|u\|_{H^{-r,-s}_{;0,}(Q_T)} = \sup_{\widetilde{v} \in H^{r,s}_{0;,0}(Q_0)} \frac{\int_{Q_0} (u \circ \boldsymbol{\kappa}) \widetilde{v} \, \mathrm{d}(\mathbf{x},t)}{\|\widetilde{v}\|_{H^{r,s}_{0;,0}(Q_0)}}$$

and

$$|||u|||_{H^{-r,-s}_{;0,}(Q_T)} = \sup_{v \in H^{r,s}_{0;,0}(Q_T)} \frac{\int_{Q_T} uv \, \mathrm{d}(\mathbf{x},t)}{\|v\|_{H^{r,s}_{0;,0}(Q_T)}}.$$

We show that these norms are equivalent. On the one hand, there holds

$$\begin{aligned}
|||u|||_{H^{-r,-s}_{;0,}(Q_T)} &= \sup_{v \in H^{r,s}_{0;,0}(Q_T)} \frac{\int_{Q_0} (u \circ \boldsymbol{\kappa})(v \circ \boldsymbol{\kappa}) \det(\mathrm{D}\boldsymbol{\kappa}) \, \mathrm{d}(\mathbf{x},t)}{\|v\|_{H^{r,s}_{0;,0}(Q_T)}} \\
&\leq \|u\|_{H^{-r,-s}_{;0,}(Q_T)} \sup_{v \in H^{r,s}_{0;,0}(Q_T)} \frac{\big\|(v \circ \boldsymbol{\kappa}) \det(\mathrm{D}\boldsymbol{\kappa})\big\|_{H^{r,s}_{0;,0}(Q_0)}}{\|v \circ \boldsymbol{\kappa}\|_{H^{r,s}_{0;,0}(Q_0)}} \\
&\lesssim \|u\|_{H^{-r,-s}_{;0,}(Q_T)},
\end{aligned}$$

where we used the definition of the norm on $H^{r,s}_{0;,0}(Q_T)$ *for* $s, r \geq 0$ *and that the pointwise multiplication with a smooth function is a continuous operation. On the other hand, we likewise find*

$$\begin{aligned}
\|u\|_{H^{-r,-s}_{;0,}(Q_T)} &= \sup_{\widetilde{v} \in H^{r,s}_{0;,0}(Q_0)} \frac{\int_{Q_T} u(\widetilde{v} \circ \boldsymbol{\kappa}^{-1}) \det(\mathrm{D}\boldsymbol{\kappa}^{-1}) \, \mathrm{d}(\mathbf{x},t)}{\|\widetilde{v}\|_{H^{r,s}_{0;,0}(Q_0)}} \\
&\leq |||u|||_{H^{-r,-s}_{;0,}(Q_T)} \sup_{\widetilde{v} \in H^{r,s}_{0;,0}(Q_0)} \frac{\big\|(\widetilde{v} \circ \boldsymbol{\kappa}^{-1}) \det(\mathrm{D}\boldsymbol{\kappa}^{-1})\big\|_{H^{r,s}_{0;,0}(Q_T)}}{\|\widetilde{v}\|_{H^{r,s}_{0;,0}(Q_0)}} \\
&\lesssim |||u|||_{H^{-r,-s}_{;0,}(Q_T)},
\end{aligned}$$

Hence, both duality pairings result in the same dual spaces and we can say that $H^{r,s}_{0;,0}(Q_T)$ *and* $H^{-r,-s}_{;0,}(Q_T)$ *are indeed dual, in the same way as for the other pairings. For similar considerations see also [DS99, Section 4.5].*

Finally, let the space $\mathcal{V}(Q_T)$ consist of all functions v with $v \circ \boldsymbol{\kappa} \in \mathcal{V}(Q_0)$ and

$$\mathcal{V}(Q_0) := \Big\{ u \in L^2\big((0,T); H^1(\Omega_0)\big) \colon \partial_t u \in L^2\big((0,T); H^{-1}(\Omega_0)\big) \Big\}. \tag{III.1.6}$$

The norm on this space is given by

$$\|u\|^2_{\mathcal{V}(Q_0)} := \|u\|^2_{H^{1,0}(Q_0)} + \|\partial_t u\|^2_{L^2((0,T);H^{-1}(\Omega_0))}.$$

Note that the space $\mathcal{V}(Q_0)$ is a dense subspace of $H^{1,\frac{1}{2}}_{;,}(Q_0)$, which follows according to [Cos90, Formula (2.2)] from the interpolation result

$$L^2(I;X) \cap H^1(I;Y) \subset H^{\frac{1}{2}}\big(I;[X,Y]_{\frac{1}{2}}\big) \cap C\big(\overline{I};[X,Y]_{\frac{1}{2}}\big) \tag{III.1.7}$$

for $X \subset Y$ being Hilbert spaces. We will not go into the depths of interpolation theory and refer the reader to [BL12, Lun18, LM72a] for further information. Analogously to the space $\mathcal{V}(Q_T)$, we can define the space $\mathcal{V}_0(Q_T)$, which includes zero boundary conditions, as the space consisting of all the functions v with $v \circ \boldsymbol{\kappa} \in \mathcal{V}_0(Q_0)$ and

$$\mathcal{V}_0(Q_0) := \Big\{ u \in L^2\big((0,T); H^1_0(\Omega_0)\big) : \partial_t u \in L^2\big((0,T); H^{-1}(\Omega_0)\big) \Big\}. \tag{III.1.8}$$

III.2 Dirichlet trace operator

III.2.1 Dirichlet trace operator on cylindrical domains

We first introduce the notion of traces with respect to cylindrical domains. According to [Doh19, Section 2.3], we can define the (interior) Dirichlet trace for a function $u \in C^1(\overline{Q}_0)$ as

$$\gamma_0 u(t,\mathbf{x}) := \lim_{\Omega_0 \ni \mathbf{y} \to \mathbf{x} \in \Gamma_0} u(t,\mathbf{y}) \quad \text{for } (t,\mathbf{x}) \in \Sigma_0.$$

We thus have $\gamma_0 u = u|_{\Sigma_0}$. We can introduce a similar operator on anisotropic Sobolev spaces, see the following lemma, being along the lines of [LM68, Theorem 2.1]. It has been proven for $\Gamma_0 \in C^\infty$, but it is also true for a Lipschitz boundary in accordance with [Cos90, p. 504ff.].

Lemma III.2.1. *The map*

$$\gamma_0 \colon H^{1,\frac{1}{2}}(Q_0) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)$$

is linear and continuous.

We find the following statement in [Cos90, Lemma 2.4], which holds in the case of a Lipschitz domain Ω_0.

Lemma III.2.2. *The Dirichlet trace operator γ_0 is continuous and surjective as an operator from $H^{1,\frac{1}{2}}_{;0,}(Q_0)$ to $H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)$.*

According to [Doh19, Theorem 2.4], there exists also an extension operator. The extension operator is a right inverse to the surjective Dirichlet trace operator γ_0 and, thus, extends a function defined only on the boundary to the space (see also [DNS19, p. 12] and [Cos90, Definition 2.17]).

Lemma III.2.3. *The Dirichlet trace operator*

$$\gamma_0 \colon H^{1,\frac{1}{2}}_{;0,}(Q_0) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)$$

has a continuous right inverse operator

$$\mathcal{E}_0 \colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0) \to H^{1,\frac{1}{2}}_{;0,}(Q_0),$$

satisfying $\gamma_0\mathcal{E}_0 v = v$ *for all* $v \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)$.

III.2.2 Dirichlet trace operator on non-cylindrical domains

In this section, we denote the (interior) Dirichlet trace operator with respect to a non-cylindrical domain by $\gamma_{0,t}$ in order to distinguish it from the Dirichlet trace operator with respect to a cylindrical domain introduced above. When no confusion can happen, we will drop the subscript t in the trace operator for a non-cylindrical domain.

For a smooth function $u \in C^1(\overline{Q}_T)$, defined on a non-cylindrical domain, we set

$$\gamma_{0,t}u(t, \mathbf{x}_t) := \lim_{\Omega_t \ni \mathbf{y}_t \to \mathbf{x}_t \in \Gamma_t} u(t, \mathbf{y}_t).$$

It obviously holds

$$\gamma_{0,t}u(t, \mathbf{x}_t) = \lim_{\substack{\Omega_0 \ni \mathbf{y} \to \mathbf{x} \in \Gamma_0,\\ \boldsymbol{\kappa}(t,\mathbf{x}) = \mathbf{x}_t}} u\big(t, \boldsymbol{\kappa}(t, \mathbf{y})\big) = \gamma_0(u \circ \boldsymbol{\kappa})(t, \mathbf{x}) = \gamma_0(u \circ \boldsymbol{\kappa})\big(t, \boldsymbol{\kappa}^{-1}(t, \mathbf{x}_t)\big)$$

for the diffeomorphism $\boldsymbol{\kappa}$ from (III.1.3). By density of the smooth functions in the Sobolev spaces, we can also extend this notion to Sobolev spaces. Moreover, we have the same mapping properties for $\gamma_{0,t}$ as for γ_0, since

$$\begin{aligned}
\|\gamma_{0,t}u\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)} &= \|\gamma_{0,t}u \circ \boldsymbol{\kappa}\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)} \\
&= \left\|\big(\gamma_0(u \circ \boldsymbol{\kappa}) \circ \boldsymbol{\kappa}^{-1}\big) \circ \boldsymbol{\kappa}\right\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)} \\
&\lesssim \|u \circ \boldsymbol{\kappa}\|_{H^{1,\frac{1}{2}}(Q_0)} \\
&= \|u\|_{H^{1,\frac{1}{2}}(Q_T)}.
\end{aligned}$$

Due to this consideration, all the properties of Section III.2.1 remain valid for the Dirichlet trace operator on non-cylindrical domains. The surjectivity follows for example from the following consideration: Let $v \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$. By the definition of the norm, we thus have $v \circ \boldsymbol{\kappa} \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_0)$. By the surjectivity of the Dirichlet trace operator with respect to Q_0, there exists a $w \in H^{1,\frac{1}{2}}_{;0,}(Q_0)$ with $\gamma_0 w = v \circ \boldsymbol{\kappa}$. Due to the bijectivity of $\boldsymbol{\kappa}$, we may define

$$\hat{w} := w \circ \boldsymbol{\kappa}^{-1} \in H^{1,\frac{1}{2}}_{;0,}(Q_T).$$

We hence have

$$\gamma_{0,t}\hat{w}(t, \mathbf{x}_t) = \gamma_0 w\big(t, \boldsymbol{\kappa}^{-1}(t, \mathbf{x}_t)\big) = v(t, \mathbf{x}_t),$$

from where the surjectivity follows and we can also infer the existence of the right inverse operator $\mathcal{E}_0$.

III.3 Existence and uniqueness of solutions to Dirichlet problems

In the sequel, we are going to consider the Dirichlet problem and introduce a variational formulation for it. We then show that under certain conditions, the Dirichlet problem is uniquely solvable.

For the cylindrical case it is well known that the solution operator $g \mapsto \mathcal{T}_0 g := u$ of the heat equation

$$\begin{aligned} (\partial_t - \Delta)u &= 0 \quad \text{in } Q_0, \\ u &= g \quad \text{on } \Sigma_0, \end{aligned}$$

with homogeneous initial conditions is an isomorphism between the spaces

$$\mathcal{T}_0\colon H_{;0,}^{\frac{1}{2}+s,(\frac{1}{2}+s)/2}(\Sigma_0) \to H_{;0,}^{1+s,(1+s)/2}(Q_0)$$

for $s > -\frac{1}{2}$ when Ω_0 is smooth and for $|s| < \frac{1}{2}$ when Ω_0 is Lipschitz, see [LM72b, Theorem 5.3] and [Cos90, Proposition 4.13].

For the existence, uniqueness and regularity of solutions of the Dirichlet problem on non-cylindrical domains, we have to make sure that the analogous result also holds. The main technique of the argument is to transport the heat equation to a parabolic problem with variable coefficients in the space-time cylinder Q_0 and apply the functional analytic tools of the above references there. To that end, we first state the transportation of domain integrals.

III.3.1 Transportation of domain integrals

We consider a mapping $\boldsymbol{\xi}$, which maps a domain Ω_τ to a domain Ω_ς and satisfies a uniformity condition as in (III.1.4). Let us denote $Q_\tau = \bigcup_\tau \big(\{\tau\}\times\Omega_\tau\big)$ and analogously for Q_ς and the lateral area by Σ_τ or Σ_ς, respectively.

First notice that for v smooth enough it holds

$$(\nabla v)\circ\boldsymbol{\xi} = (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi}), \tag{III.3.1}$$

which can be proven by using the chain rule. We mention that this identity is also stated in [MZ06, p. 43].

Lemma III.3.1. *Let $v \in H_{;0,}^{1,\frac{1}{2}}(Q_\varsigma)$ and $\varphi \in H_{0;,0}^{1,\frac{1}{2}}(Q_\varsigma)$. Then, the transport of*

$$S(v,\varphi) := \int_0^T \int_{\Omega_\varsigma} \big\{\langle\nabla v, \nabla\varphi\rangle + \partial_t v\varphi\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t = \int_0^T \int_{\Omega_\varsigma} f\varphi\,\mathrm{d}\mathbf{x}\mathrm{d}t \tag{III.3.2}$$

from Q_ς to Q_τ gives the parabolic problem

$$\int_0^T \int_{\Omega_\tau} \partial_t v^{\tau,\varsigma}\varphi^{\tau,\varsigma}\,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T a(t; v^{\tau,\varsigma}, \varphi^{\tau,\varsigma})\,\mathrm{d}t = \int_0^T \int_{\Omega_\tau} f^{\tau,\varsigma}\varphi^{\tau,\varsigma}\,\mathrm{d}\mathbf{x}\mathrm{d}t \tag{III.3.3}$$

with

$$\begin{aligned}
a(t; v^{\tau,\varsigma}, \varphi^{\tau,\varsigma}) := &\int_{\Omega_\tau} \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla \varphi^{\tau,\varsigma}\big\rangle \,\mathrm{d}\mathbf{x} \\
&- \int_{\Omega_\tau} \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, \partial_t\boldsymbol{\xi}\varphi^{\tau,\varsigma}\big\rangle \,\mathrm{d}\mathbf{x} \\
&- \int_{\Omega_\tau} \Big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\frac{1}{\det(\mathrm{D}\boldsymbol{\xi})}\nabla\big(\det(\mathrm{D}\boldsymbol{\xi})\big)\varphi^{\tau,\varsigma}, (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\Big\rangle \,\mathrm{d}\mathbf{x},
\end{aligned}$$

where $v^{\tau,\varsigma} = v\circ\boldsymbol{\xi}$ *and similarly for* $\varphi^{\tau,\varsigma}$ *and* $f^{\tau,\varsigma}$.

Proof. With the aid of (III.3.1) and (III.1.5), the transport of (III.3.2) from Q_ς onto Q_τ gives

$$\begin{aligned}
&\int_0^T \int_{\Omega_\tau} \det(\mathrm{D}\boldsymbol{\xi})\big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi}), (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(\varphi\circ\boldsymbol{\xi})\big\rangle \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad+ \int_0^T \int_{\Omega_\tau} \det(\mathrm{D}\boldsymbol{\xi})\Big[\partial_t(\varphi\circ\boldsymbol{\xi})(v\circ\boldsymbol{\xi}) - \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi}), \partial_t\boldsymbol{\xi}(\varphi\circ\boldsymbol{\xi})\big\rangle\Big] \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad\quad= \int_0^T \int_{\Omega_\tau} \det(\mathrm{D}\boldsymbol{\xi})(f\circ\boldsymbol{\xi})(\varphi\circ\boldsymbol{\xi}) \,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}$$

Using Green's first identity and the zero boundary condition yields

$$\begin{aligned}
&\int_0^T \int_{\Omega_\tau} -\operatorname{div}\big(\det(\mathrm{D}\boldsymbol{\xi})(\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi})\big)(\varphi\circ\boldsymbol{\xi}) \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad+ \int_0^T \int_{\Omega_\tau} \det(\mathrm{D}\boldsymbol{\xi})\Big[\partial_t(v\circ\boldsymbol{\xi}) - \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi}), \partial_t\boldsymbol{\xi}\big\rangle\Big](\varphi\circ\boldsymbol{\xi}) \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad\quad= \int_0^T \int_{\Omega_\tau} \det(\mathrm{D}\boldsymbol{\xi})(f\circ\boldsymbol{\xi})(\varphi\circ\boldsymbol{\xi}) \,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}$$

Thus, in the strong formulation, we have when dividing by $\det(\mathrm{D}\boldsymbol{\xi})$ that

$$\begin{aligned}
&-\frac{1}{\det(\mathrm{D}\boldsymbol{\xi})}\operatorname{div}\Big(\det(\mathrm{D}\boldsymbol{\xi})(\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi})\Big) \\
&\qquad\qquad + \partial_t(v\circ\boldsymbol{\xi}) - \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla(v\circ\boldsymbol{\xi}), \partial_t\boldsymbol{\xi}\big\rangle = f\circ\boldsymbol{\xi} \quad \text{in } Q_\tau.
\end{aligned}$$

Rewriting gives

$$\begin{aligned}
&-\operatorname{div}\Big((\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\Big) + \partial_t v^{\tau,\varsigma} - \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, \partial_t\boldsymbol{\xi}\big\rangle \\
&\qquad - \frac{1}{\det(\mathrm{D}\boldsymbol{\xi})}\Big\langle \nabla\big(\det(\mathrm{D}\boldsymbol{\xi})\big), (\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\Big\rangle = f^{\tau,\varsigma} \quad \text{in } Q_\tau.
\end{aligned} \tag{III.3.4}$$

Testing again with a function $\varphi^{\tau,\varsigma}$ gives the weak formulation

$$\begin{aligned}
&\int_0^T \int_{\Omega_\tau} -\operatorname{div}\Big((\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\Big)\varphi^{\tau,\varsigma} \,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T \int_{\Omega_\tau} \partial_t v^{\tau,\varsigma}\varphi^{\tau,\varsigma} \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad - \int_0^T \int_{\Omega_\tau} \big\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, \partial_t\boldsymbol{\xi}\big\rangle\varphi^{\tau,\varsigma} \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad - \int_0^T \int_{\Omega_\tau} \frac{1}{\det(\mathrm{D}\boldsymbol{\xi})}\Big\langle \nabla\big(\det(\mathrm{D}\boldsymbol{\xi})\big), (\mathrm{D}\boldsymbol{\xi})^{-1}(\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\Big\rangle\varphi^{\tau,\varsigma} \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad\quad = \int_0^T \int_{\Omega_\tau} f^{\tau,\varsigma}\varphi^{\tau,\varsigma} \,\mathrm{d}\mathbf{x}\mathrm{d}t,
\end{aligned}$$

which can be reformulated by using the divergence theorem with vanishing boundary terms to

$$\begin{aligned}
&\int_0^T \int_{\Omega_\tau} \left\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla \varphi^{\tau,\varsigma}\right\rangle \mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T \int_{\Omega_\tau} \partial_t v^{\tau,\varsigma}\varphi^{\tau,\varsigma}\,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad - \int_0^T \int_{\Omega_\tau} \langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}, \partial_t\boldsymbol{\xi}\varphi^{\tau,\varsigma}\rangle\,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad - \int_0^T \int_{\Omega_\tau} \left\langle (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\frac{1}{\det(\mathrm{D}\boldsymbol{\xi})}\nabla\big(\det(\mathrm{D}\boldsymbol{\xi})\big)\varphi^{\tau,\varsigma}, (\mathrm{D}\boldsymbol{\xi})^{-\intercal}\nabla v^{\tau,\varsigma}\right\rangle \mathrm{d}\mathbf{x}\mathrm{d}t \\
&\quad = \int_0^T \int_{\Omega_\tau} f^{\tau,\varsigma}\varphi^{\tau,\varsigma}\,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned} \tag{III.3.5}$$

From here, the claim follows immediately. □

III.3.2 General theory on existence and uniqueness

In the following, we will state a general result for parabolic equations, which can be used to show existence and uniqueness of solutions on non-cylindrical domains.

Let us first give the following definition along the lines of [Wlo87, Definition 25.3].

Definition III.3.2. *Let V be a Hilbert space. We define*

$$W(0,T) := \Big\{ f \in L^2\big((0,T);V\big) :\ \partial_t f \in L^2\big((0,T);V'\big)\Big\}$$

with the scalar product

$$(f,g)_W := \int_0^T \big(f(t),g(t)\big)_V\,\mathrm{d}t + \int_0^T (\partial_t f(t), \partial_t g(t))_{V'}\,\mathrm{d}t.$$

Notice that the space $\mathcal{V}_0(Q_0)$ introduced in (III.1.8) is a specific case of the spaces $W(0,T)$.

Let us now cite the mentioned abstract existence and uniqueness result for the solution of a parabolic differential equation according to [Wlo87, Paragraph 26]. We consider two given separable Hilbert spaces V and H, with $V \hookrightarrow H$ injective, continuous and dense. Thus, we can extend these Hilbert spaces to a Gelfand triple $V \hookrightarrow H \hookrightarrow V'$ (see Remark II.1.18). Let $0 < T < \infty$. For $t \in [0,T]$, consider the form $a(t;\varphi,\psi)$, which is sesquilinear in $\varphi,\psi \in V$. The form should satisfy the following three requirements:

- $a(t;\varphi,\psi)$ is measurable on $[0,T]$ for fixed $\varphi,\psi \in V$.
- There exits some $c > 0$, independent of t, with

$$\big|a(t;\varphi,\psi)\big| \le c\|\varphi\|_V\|\psi\|_V \quad \forall t \in [0,T], \varphi,\psi \in V.$$

- There exist real $\lambda \ge 0$, $\alpha > 0$ independent of t and φ, with

$$\operatorname{Re} a(t;\varphi,\varphi) + \lambda\|\varphi\|_H^2 \ge \alpha\|\varphi\|_V^2 \quad \forall t \in [0,T], \varphi \in V.$$

According to [Wlo87, Theorem 17.9], the second requirement ensures the existence of a representation operator $\mathcal{L}(t)\colon a(t,\varphi,\psi) = \big(\mathcal{L}(t)\varphi,\psi\big)_H$, where $\mathcal{L}(t)\colon V \to V'$ is linear and continuous for fixed t.

For given $f \in L^2\big((0,T);V'\big)$ and $u_0 \in H$, we consider the problem

$$\begin{aligned} \mathcal{L}(t)u + \partial_t u &= f \text{ in } V' \\ u(0) &= u_0. \end{aligned} \tag{III.3.6}$$

We can now state the existence and uniqueness result found in [LM72b, Chapter 3, Theorem 4.1] or [Wlo87, Theorem 26.1].

Theorem III.3.3. *Suppose the three requirements on $a(t;\varphi,\psi)$ introduced above hold. For $T < \infty$, the problem (III.3.6) has a unique solution u, depending continuously on f and u_0. This means that the map*

$$(f,u_0) \mapsto u,$$

is continuous from $L^2\big((0,T);V'\big) \times H$ into $W(0,T)$.

Remark III.3.4. *Note that we only prescribe boundedness and coercivity of $a(t;\varphi,\psi)$. Usually one would also need injectivity to have an existence and uniqueness result, see [SS10a] for example. But the proof of [Wlo87, Theorem 26.1] states that λ can be chosen as 0 and, therefore, we do not need to prove the injectivity here.*

III.3.3 Existence and uniqueness of Dirichlet problems on tubes

We consider the following non-cylindrical Dirichlet problem with homogeneous initial datum

$$\begin{aligned} (\partial_t - \Delta)u &= f && \text{in } Q_T, \\ \gamma_0 u &= g && \text{on } \Sigma_T, \\ u(0,\cdot) &= 0 && \text{in } \Omega_0. \end{aligned} \tag{III.3.7}$$

We have the following existence and uniqueness theorem for its solution.

Theorem III.3.5. *Let $f \in H^{-1,-\frac{1}{2}}_{;0,}(Q_T)$ and $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$. Then, there exists a unique solution $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$, satisfying the boundary condition in (III.3.7) and*

$$\begin{aligned} S(u,\varphi) &:= \int_0^T \int_{\Omega_t} \big\{\langle \nabla u, \nabla\varphi\rangle + \partial_t u\varphi\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t \\ &= \int_0^T \int_{\Omega_t} fu\,\mathrm{d}\mathbf{x}\mathrm{d}t \text{ for all } \varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q_T). \end{aligned} \tag{III.3.8}$$

Proof. We set $u^t = u \circ \boldsymbol{\kappa}$ and similarly for φ^t and f^t. We first show the analogue of [Cos90, Lemma 2.3]: Let $g = 0$. For every $f \in L^2\big((0,T);H^{-1}(\Omega_t)\big)$, there exists a unique solution $u \in \mathcal{V}_0(Q_T)$ of (III.3.7), where the space $\mathcal{V}_0(Q_T)$ is defined in (III.1.6).

Transforming (III.3.8) back to Q_0 by using Lemma III.3.1 with $\boldsymbol{\xi} = \boldsymbol{\kappa}$, $Q_\varsigma = Q_T$ and $Q_\tau = Q_0$ gives

$$\begin{aligned} &\int_0^T \Big\{ \big(\partial_t u^t(t), \varphi^t(t)\big)_{L^2(\Omega_0)} + a\big(t; u^t(t), \varphi^t(t)\big)\Big\}\,\mathrm{d}t \\ &= \int_0^T \big(f^t(t), u^t(t)\big)_{L^2(\Omega_0)}\,\mathrm{d}t, \end{aligned} \tag{III.3.9}$$

where a is defined in Lemma III.3.1.

To show solvability of (III.3.8), we apply Theorem III.3.3 to its equivalent formulation (III.3.9). Theorem III.3.3 requires boundedness and coercivity of a. The boundedness follows easily from Remark III.1.3. It remains to show coercivity, that is, there exist some constants $\alpha > 0$ and $\lambda \geq 0$, such that for almost all $t \in (0, T)$

$$a(t; u^t, u^t) \geq \alpha \|u^t\|^2_{H^1(\Omega_0)} - \lambda \|u^t\|^2_{L^2(\Omega_0)} \tag{III.3.10}$$

holds for all $u^t \in H^1_0(\Omega_0)$. With the help of the Cauchy-Schwarz inequality, we have

$$\begin{aligned} a(t; u^t, u^t) \geq &\int_{\Omega_0} \left\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla u^t\right\|^2 \mathrm{d}\mathbf{x} \\ &- \int_{\Omega_0} \left\| \Big(\underbrace{(\mathrm{D}\boldsymbol{\kappa})^{-\intercal} \frac{1}{\det(\mathrm{D}\boldsymbol{\kappa})} \nabla\big(\det(\mathrm{D}\boldsymbol{\kappa})\big)}_{=:a_1} + \underbrace{\partial_t \boldsymbol{\kappa}}_{=:a_2} \Big) u^t \right\| \left\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla u^t\right\| \mathrm{d}\mathbf{x}. \end{aligned}$$

Completing the square gives

$$\begin{aligned} a(t; u^t, u^t) \geq &\underbrace{\int_{\Omega_0} \frac{1}{2}\Big(\left\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla u^t\right\| - \left\|(a_1 + a_2) u^t\right\|\Big)^2 \mathrm{d}\mathbf{x}}_{\geq 0} \\ &+ \int_{\Omega_0} \frac{1}{2}\left\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla u^t\right\|^2 \mathrm{d}\mathbf{x} - \int_{\Omega_0} \frac{1}{2}\left\|(a_1 + a_2) u^t\right\|^2 \mathrm{d}\mathbf{x}. \end{aligned}$$

Discarding the positive term and due to Remark III.1.3, we have

$$a(t; u^t, u^t) \geq C|u^t|^2_{H^1(\Omega_0)} - \frac{1}{2}\int_{\Omega_0} |u^t|^2 \|a_1 + a_2\|^2 \,\mathrm{d}\mathbf{x}$$

and, therefore, by using the parallelogram law

$$a(t; u^t, u^t) \geq C|u^t|^2_{H^1(\Omega_0)} - \int_{\Omega_0} |u^t|^2 \big(\|a_1\|^2 + \|a_2\|^2\big) \,\mathrm{d}\mathbf{x}.$$

Now we can apply again Remark III.1.3 to a_1 and a_2 and the Poincaré-Friedrichs inequality to the first term to arrive at the desired estimate (III.3.10).

Secondly, following the lines of [Cos90], the analogue of [Cos90, Lemma 2.8] reads: For every $f \in H^{-1,-\frac{1}{2}}_{;0,}(Q_T)$, there exists a unique $u \in H^{1,\frac{1}{2}}_{0;0,}(Q_T)$ satisfying $(\partial_t - \Delta)u = f$ in Q_T. For the proof, we can straightforwardly modify the proof [Cos90, Lemma 2.8], which is based on adjoint operators and interpolation results. The interpolation results also hold on the spaces with respect to the tube Q_T and the adjoint operators with respect to Q_T have the same structure as the adjoint operators in [Cos90] with respect to Q_0.

Thirdly, due to the surjectivity (see Lemma III.2.2 and Section III.2.2) of the trace operator, we can then follow the proof of [Cos90, Theorem 2.9] to finally obtain the statement of the theorem. □

For a non-homogeneous initial datum, we consider the Dirichlet problem

$$\begin{aligned} (\partial_t - \Delta)u &= f && \text{in } Q_T, \\ \gamma_0 u &= g && \text{on } \Sigma_T, \\ u(0, \cdot) &= u_0 && \text{in } \Omega_0. \end{aligned} \tag{III.3.11}$$

Theorem III.3.6. *Let $f \in H^{-1,-\frac{1}{2}}_{;0,}(Q_T)$, $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$. There exists a unique solution $u \in H^{1,\frac{1}{2}}(Q_T)$ satisfying (III.3.11) for $u_0 \in L^2(\Omega_0)$.*

Proof. For the proof, we follow the strategy taken in [DNS19]. We first consider the problem with homogeneous initial condition. In Theorem III.3.5, it is shown that this differential equation has a unique solution in $H^{1,\frac{1}{2}}_{;0,}(Q_T)$, which we denote by u_{hom}. Considering the problem with inhomogeneous initial condition $u_0 \in L^2(\Omega_0)$, but homogeneous boundary condition and source term, there exists a unique solution $u_{\mathrm{inhom}} \in \mathcal{V}_0(Q_T)$ according to Theorem III.3.3, since all the requested assumptions of this theorem have already been shown in the proof of Theorem III.3.5. Now as in [DNS19], the unique solution $u \in H^{1,\frac{1}{2}}(Q_T)$ is given by $u = u_{\mathrm{hom}} + u_{\mathrm{inhom}}$. □

Remark III.3.7. *In [LMZ02, Theorem 2.2], it is proven that for given $u_0 \in L^2(\Omega_0)$, $f \in L^2\big((0,T); H^{-1}(\Omega_t)\big)$ and $g = 0$, the Dirichlet problem (III.3.11) has a unique solution $u \in C^0\big([0,T]; L^2(\Omega_t)\big) \cap L^2\big([0,T]; H^1_0(\Omega_t)\big)$. Therefore, also in the setting of Theorem III.3.6 for $g = 0$, the solution u lies in $C^0\big([0,T]; L^2(\Omega_t)\big)$ and thus the initial trace $\tau_0 u := u|_{t=0} \in L^2(\Omega_0)$ is well defined. For the cylindrical case, compare [DNS19, p. 14].*

Remark III.3.8. *If the Dirichlet data in (III.3.7) satisfy $g \in H^{\frac{3}{2},\frac{3}{4}}(\Sigma_T)$, the right-hand side $f \in L^2(Q_T)$, and the initial datum $u_0 \in H^1(\Omega_0)$, then the solution u of (III.3.8) lies in $H^{2,1}(Q_T)$. This is a consequence of [LSU68, Chapter IV, Theorem 9.1].*

III.4 Neumann trace operator

Similarly as we defined the Dirichlet trace operator, we can also introduce an (interior) Neumann trace operator. In the following, we will first introduce this concept on cylindrical domains. Then, we will introduce the notion of a Neumann trace on a non-cylindrical domain formally and rigorously.

III.4.1 Neumann trace operator on cylindrical domains

Let us introduce the Neumann trace operator, also called the conormal derivative, on a cylindrical domain along the lines of [Cos90]. We define the space

$$H^{1,\frac{1}{2}}(Q_0;\mathcal{L}) := \big\{u \in H^{1,\frac{1}{2}}(Q_0) \colon \mathcal{L}u \in L^2(Q_0)\big\},$$

where $\mathcal{L} := \partial_t - \Delta$ is the partial differential operator under consideration. The norm on this space is given by

$$\|u\|^2_{H^{1,\frac{1}{2}}(Q_0;\mathcal{L})} := \|u\|^2_{H^{1,\frac{1}{2}}(Q_0)} + \big\|(\partial_t - \Delta)u\big\|^2_{L^2(Q_0)}.$$

According to [Cos90, Lemma 2.16], the bilinear form

$$b(u,v) := \int_{Q_0} \big\{\langle \nabla u, \nabla v\rangle - (\partial_t - \Delta)uv\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t + d(u,v)$$

is continuous on $H^{1,\frac{1}{2}}(\mathbb{R}\times\Omega_0;\mathcal{L})\times H^{1,\frac{1}{2}}(\mathbb{R}\times\Omega_0)$, where

$$d(u,v) := \int_{\mathbb{R}\times\Omega_0} \partial_t u v \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

The bilinear form $d(u,v)$ has a continuous extension from $C_0^\infty(\mathbb{R}^{d+1})\times C_0^\infty(\mathbb{R}^{d+1})$ to $H^{\frac{1}{2}}(\mathbb{R};L^2(\Omega_0))\times H^{\frac{1}{2}}(\mathbb{R};L^2(\Omega_0))$ and it holds $d(u,v) = -d(v,u)$ for all $u,v\in H^{\frac{1}{2}}(\mathbb{R};L^2(\Omega_0))$, compare [Cos90, Lemma 2.6].

The (interior) Neumann trace is defined for $u\in C^1(\overline{Q}_0)$ by

$$\gamma_1^{\mathrm{int}}u(t,\mathbf{x}) := \lim_{\Omega_0\ni\mathbf{y}\to\mathbf{x}\in\Gamma_0} \langle \nabla_{\mathbf{y}}u(t,\mathbf{y}),\mathbf{n}_{\mathbf{x}}\rangle \quad \text{for } (t,\mathbf{x})\in\Sigma_0$$

and coincides with the normal derivative on Σ_0, thus $\gamma_1^{\mathrm{int}}u = \partial u/\partial\mathbf{n}$ on Σ_0, see [Doh19, Section 3.3] and also [Wlo87, Satz 8.7] for the elliptic case. Since it holds

$$b(u,v) = \int_{\Sigma_0} \frac{\partial u}{\partial \mathbf{n}} v \,\mathrm{d}\sigma\mathrm{d}t$$

for $u,v\in C_0^2(\mathbb{R}\times\overline{\Omega}_0)$, we can extend this definition as follows, which is along the lines of [Cos90, Definition 2.17].

Definition III.4.1. *Let $u\in H^{1,\frac{1}{2}}(\mathbb{R}\times\Omega_0;\mathcal{L})$. Then, the Neumann trace operator $\gamma_1^{\mathrm{int}}u\in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_0)$ is the continuous linear form on $H^{\frac{1}{2},\frac{1}{2}}(\Sigma_0)$ defined by*

$$\gamma_1^{\mathrm{int}}u\colon \varphi\mapsto b(u,\mathcal{E}_0\varphi),$$

where $\mathcal{E}_0$ is the extension operator given in Lemma III.2.3.

Notice that we can also introduce the conormal derivative $\gamma_1^{\mathrm{int}}u\in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_0)$ as the unique solution of a variational problem, as it is done in [DNS19, Section 3.4]. This variational problem can for example be obtained by applying $\gamma_1^{\mathrm{int}}u$ to φ. According to [Cos90, Proposition 2.18], the Neumann trace has the following properties.

Lemma III.4.2. *(i) The map*

$$\gamma_1^{\mathrm{int}}\colon H^{1,\frac{1}{2}}(\mathbb{R}\times\Omega_0;\mathcal{L})\to H^{-\frac{1}{2},-\frac{1}{4}}(\mathbb{R}\times\Gamma_0)$$

is continuous and by restriction also the map

$$\gamma_1^{\mathrm{int}}\colon H^{1,\frac{1}{2}}(Q_0;\mathcal{L})\to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_0)$$

is continuous.

(ii) If $u\in C^2(\overline{Q}_0)$, then $\gamma_1^{\mathrm{int}}u = (\partial u/\partial\mathbf{n})|_{\Sigma_0}$ due to the Green formula.

III.4.2 Neumann trace operator on non-cylindrical domains

Having stated the Neumann trace operator on cylindrical domains, we are now in the position to introduce the Neumann trace operator on non-cylindrical domains. On time-dependent boundaries, one could consider the usual Neumann trace, as it is done for example in [DZ01, Section 6.1]. Instead, we follow here the idea of [Tau19] and employ a velocity corrected Neumann trace, which is motivated by the following so-called *Reynolds' transport theorem*, see e.g. [Gur81, p. 78] or [Hol00, Section 4.2].

Lemma III.4.3. *Let $f = f(t, \mathbf{x})$ be a C^1-function. Since Ω_t depends on time, integration over Ω_t and differentiation with respect to t do not commute. Instead, we have the relation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} f(t,\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_{\Omega_t} \frac{\partial f}{\partial t}(t,\mathbf{x})\,\mathrm{d}\mathbf{x} + \int_{\Gamma_t} f(t,\mathbf{x})\langle \mathbf{V}, \mathbf{n}\rangle\,\mathrm{d}\sigma.$$

The velocity of Γ_t in normal direction $\langle \mathbf{V}, \mathbf{n}\rangle$ will be treated in depth in Sections IV.1.1 and IV.1.2, see in particular (IV.1.3) and Lemma IV.1.4.

We first formally introduce this Neumann trace and afterwards characterize its properties rigorously.

Formal introduction of the Neumann trace

For a time dependent spatial surface, we define two Neumann trace operators

$$\gamma_1^{\pm}\varphi := \frac{\partial \varphi}{\partial \mathbf{n}_t} \mp \frac{1}{2}\langle \mathbf{V}, \mathbf{n}_t\rangle \varphi. \tag{III.4.1}$$

To motivate this definition, consider the boundary value problem

$$\begin{aligned} (\partial_t - \Delta)u &= f \qquad \text{in } Q_T,\\ \gamma_1 u &= g \qquad \text{on } \Sigma_T,\\ u(0,\cdot) &= 0 \qquad \text{in } \Omega_0, \end{aligned} \tag{III.4.2}$$

where we leave it a priori open what γ_1 means. Let us formally derive the weak formulation of the Neumann problem (III.4.2) by multiplying with a test function v satisfying $v(T,\cdot) = 0$ in Ω_T and using Reynolds' transport theorem (Lemma III.4.3)

$$\begin{aligned} \int_0^T\int_{\Omega_t} fv\,\mathrm{d}\mathbf{x}\mathrm{d}t &= \int_0^T\int_{\Omega_t}(\partial_t - \Delta)uv\,\mathrm{d}\mathbf{x}\mathrm{d}t\\ &= \int_0^T\int_{\Omega_t}\big\{\langle\nabla u, \nabla v\rangle + \partial_t(uv) - u\partial_t v\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t - \int_0^T\int_{\Gamma_t}\frac{\partial u}{\partial \mathbf{n}}v\,\mathrm{d}\sigma\mathrm{d}t\\ &= \int_0^T\int_{\Omega_t}\big\{\langle\nabla u, \nabla v\rangle - u\partial_t v\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} uv\,\mathrm{d}\mathbf{x}\mathrm{d}t\\ &\qquad - \int_0^T\int_{\Gamma_t}\left\{\frac{\partial u}{\partial \mathbf{n}}v + uv\langle\mathbf{V},\mathbf{n}\rangle\right\}\mathrm{d}\sigma\mathrm{d}t. \end{aligned}$$

Due to the fundamental theorem of calculus and the vanishing initial and end condition of u and v, respectively, we obtain the variational equation

$$a(u,v) = \int_0^T\int_{\Omega_t} fv\,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T\int_{\Gamma_t}\left\{\frac{\partial u}{\partial \mathbf{n}}v + \frac{1}{2}uv\langle\mathbf{V},\mathbf{n}\rangle\right\}\mathrm{d}\sigma\mathrm{d}t$$

with bilinear form

$$a(u,v) := \int_0^T\int_{\Omega_t}\big\{\langle\nabla u,\nabla v\rangle - u\partial_t v\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t - \frac{1}{2}\int_0^T\int_{\Gamma_t} uv\langle\mathbf{V},\mathbf{n}\rangle\,\mathrm{d}\sigma\mathrm{d}t.$$

Thus, if we set the previously unspecified trace in (III.4.2) as γ_1^-, we arrive at

$$a(u,v) = \int_0^T\int_{\Omega_t} fv\,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T\int_{\Gamma_t} gv\,\mathrm{d}\sigma\mathrm{d}t.$$

Rigorous introduction of the Neumann trace

We assume $\boldsymbol{\kappa}$ to be defined on $\mathbb{R}\times\mathbb{R}^d$ and not only on $[0,T]\times\mathbb{R}^d$. Moreover, for the sake of simplicity in representation, we always consider functions u and v throughout this section which satisfy

$$\int_{\mathbb{R}} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t} uv \,\mathrm{d}\mathbf{x}\mathrm{d}t = 0. \tag{III.4.3}$$

This assumption stems from the fact that we would like to integrate by parts in time. Later on, we will consider a finite time interval $(0,T)$ and equip u and v with the appropriate zero initial and end conditions. Extending u and v by zero for $t<0$ and $t>T$, respectively, leads then to the fulfilment of (III.4.3).

Let us define

$$d(u,v) := \int_{\mathbb{R}} \int_{\Omega_t} \partial_t uv \,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{1}{2}\int_{\mathbb{R}}\int_{\Gamma_t} \langle \mathbf{V},\mathbf{n}\rangle uv \,\mathrm{d}\sigma\mathrm{d}t. \tag{III.4.4}$$

Notice that the additional boundary term is a speciality of the time-dependent boundary. We shall first state the analogue of [Cos90, Lemma 2.6].

Lemma III.4.4. *The bilinear form $d(u,v)$ has a continuous extension from $C_0^\infty(\mathbb{R}^{1+d}) \times C_0^\infty(\mathbb{R}^{1+d})$ to $H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t)\big) \times H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t)\big)$, and it holds*

$$d(u,v) = -d(v,u). \tag{III.4.5}$$

Proof. The use of Reynolds' transport theorem (Lemma III.4.3) allows us to compute

$$\begin{aligned}
d(u,v) &= \int_{\mathbb{R}} \int_{\Omega_t} \partial_t uv \,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{1}{2}\int_{\mathbb{R}}\int_{\Gamma_t} \langle \mathbf{V},\mathbf{n}\rangle uv \,\mathrm{d}\sigma\mathrm{d}t \\
&= \int_{\mathbb{R}} \int_{\Omega_t} \big\{\partial_t(uv) - u\partial_t v\big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{1}{2}\int_{\mathbb{R}}\int_{\Gamma_t} \langle \mathbf{V},\mathbf{n}\rangle uv \,\mathrm{d}\sigma\mathrm{d}t \\
&= \int_{\mathbb{R}} \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} uv \,\mathrm{d}\mathbf{x}\mathrm{d}t - \int_{\mathbb{R}}\int_{\Omega_t} u\partial_t v \,\mathrm{d}\mathbf{x}\mathrm{d}t - \frac{1}{2}\int_{\mathbb{R}}\int_{\Gamma_t} \langle \mathbf{V},\mathbf{n}\rangle uv \,\mathrm{d}\sigma\mathrm{d}t.
\end{aligned}$$

The assumption (III.4.3) hence implies

$$d(u,v) = -\int_{\mathbb{R}}\int_{\Omega_t} u\partial_t v \,\mathrm{d}\mathbf{x}\mathrm{d}t - \frac{1}{2}\int_{\mathbb{R}}\int_{\Gamma_t} \langle \mathbf{V},\mathbf{n}\rangle uv \,\mathrm{d}\sigma\mathrm{d}t,$$

from where (III.4.5) follows immediately. The rest is in complete analogy to [Cos90, Lemma 2.6], but we need higher regularity in the spatial variable instead of just in $L^2(\Omega_0)$ as in [Cos90], because the boundary term in the definition of $d(u,v)$ has to be well-defined. □

As in Section III.4.1, we introduce the space

$$H^{1,\frac{1}{2}}(Q_T;\mathcal{L}) := \big\{u \in H^{1,\frac{1}{2}}(Q_T) \colon \mathcal{L}u \in L^2(Q_T)\big\},$$

where $\mathcal{L} := \partial_t - \Delta$ is the differential operator on the non-cylindrical domain. We state the analogue of [Cos90, Lemma 2.16] in the case of a non-cylindrical domain, the proof of which is obvious.

Lemma III.4.5. *The bilinear form*

$$b^-(u,v) := \int_0^T \int_{\Omega_t} \{\langle \nabla u, \nabla v\rangle - (\partial_t - \Delta)uv\} \,\mathrm{d}\mathbf{x}\mathrm{d}t + d(u,v)$$

with $d(u,v)$ being defined in (III.4.4) is continuous on $H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t);\partial_t-\Delta\big)\times H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t)\big)$. If $u,v\in C_0^2\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\overline{\Omega}_t)\big)$, we have

$$b^-(u,v) = \int_0^T \int_{\Gamma_t} \left\{\frac{\partial u}{\partial \mathbf{n}} v + \frac{1}{2}\langle \mathbf{V}, \mathbf{n}\rangle uv\right\} \mathrm{d}\sigma\mathrm{d}t$$

by means of Green's formula.

In complete analogy to the Neumann trace operator in the cylindrical case, we will define $\gamma_1^- u$, which is one of the two required Neumann trace operators.

Definition III.4.6. *Given $u\in H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t);\partial_t-\Delta\big)$, we denote by $\gamma_1^- u\in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ the continuous linear form on $H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ defined by*

$$\gamma_1^- u \colon \varphi \mapsto b^-(u, \mathcal{E}_0\varphi),$$

where $\mathcal{E}_0$ is the extension operator as mentioned in Section III.2.2.

The following lemma is the non-cylindrical equivalent to [Cos90, Proposition 2.18].

Lemma III.4.7. *The map*

$$\gamma_1^- : H^{1,\frac{1}{2}}\left(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t);\partial_t-\Delta\right) \to H^{-\frac{1}{2},-\frac{1}{4}}\left(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Gamma_t)\right)$$

is continuous and by restriction also the map

$$\gamma_1^- : H^{1,\frac{1}{2}}(Q_T;\partial_t-\Delta) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$$

is continuous. Moreover, if $u\in C^2(\overline{Q}_T)$, then it holds

$$\gamma_1^- u = \frac{\partial u}{\partial \mathbf{n}} + \frac{1}{2}\langle \mathbf{V}, \mathbf{n}\rangle u.$$

Proof. As in [Cos90], the continuity is a consequence of the continuity of the bilinear form $b(\cdot,\cdot)$ (cf. Lemma III.4.5). The second statement follows immediately from Green's first formula. □

Remark III.4.8. *In view of the reformulation of the heat equation in terms of boundary integral equations, we will moreover encounter a second Neumann trace operator, which we denote by γ_1^+. It can be introduced analogously to above by considering the differential operator $\partial_t+\Delta$ instead of $\partial_t-\Delta$. The former operator for example arises when considering a time reversal of the latter one. With*

$$b^+(u,v) := \int_0^T \int_{\Omega_t} \{\langle \nabla u, \nabla v\rangle + (\partial_t + \Delta)uv\} \,\mathrm{d}\mathbf{x}\mathrm{d}t - d(u,v),$$

we can state the analogue of Lemma III.4.5, namely the continuity of $b^+(\cdot,\cdot)$ *in the appropriate space and for* u *and* v *smooth enough, we have*

$$b^+(u,v) = \int_0^T \int_{\Gamma_t} \left\{ \frac{\partial u}{\partial \mathbf{n}} v - \frac{1}{2}\langle \mathbf{V}, \mathbf{n}\rangle uv \right\} \mathrm{d}\sigma \mathrm{d}t.$$

With this property at hand, we can define the trace operator γ_1^+ *in analogy to Definition III.4.6. For* u *smooth enough, it then holds*

$$\gamma_1^+ u = \frac{\partial u}{\partial \mathbf{n}} - \frac{1}{2}\langle \mathbf{V}, \mathbf{n}\rangle u.$$

The existence of two Neumann trace operators is a speciality of the time-dependent boundary.

To prove existence and uniqueness of the Neumann problem, we could apply Lions' projection theorem (see [Cos90, Lemma 2.1]). However, for the cylindrical case [Cos90, Lemma 2.21] states that this strategy does not yield satisfactory results, since one has to make stronger assumptions on the regularity of the input data. Therefore, as in [Cos90], we will proof the existence and uniqueness of solutions by using a boundary integral formulation (see Corollary III.6.18).

III.5 Green's formulas and combined trace maps

With the definition of the trace maps, we can now introduce Green's formulas and have a look at the mapping properties of the combined trace map (γ_0, γ_1^+).

Likewise to [Cos90, Formula (2.35)], given $u \in H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t); \partial_t - \Delta\big)$ and $v \in H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t)\big)$, we obtain Green's first formula

$$\int_{\mathbb{R}}\int_{\Omega_t} \langle \nabla u, \nabla v\rangle \,\mathrm{d}\mathbf{x}\mathrm{d}t + d(u,v) = \int_{\mathbb{R}}\int_{\Omega_t} (\partial_t - \Delta)uv \,\mathrm{d}\mathbf{x}\mathrm{d}t + \langle \gamma_1^- u, \gamma_0 v\rangle. \qquad \text{(III.5.1)}$$

By restriction, this formula also holds for $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta)$ and $v \in H^{1,\frac{1}{2}}_{;,0}(Q_T)$, but not, as was pointed out in [Cos90], when u, v are both in $H^{1,\frac{1}{2}}_{;0,}(Q_T)$.

In complete analogy, Green's formula for $u \in H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t); \partial_t + \Delta\big)$ and $v \in H^{1,\frac{1}{2}}\big(\bigcup_{t\in\mathbb{R}}(\{t\}\times\Omega_t)\big)$ reads

$$\int_{\mathbb{R}}\int_{\Omega_t} \langle \nabla u, \nabla v\rangle \,\mathrm{d}\mathbf{x}\mathrm{d}t - d(u,v) = \int_{\mathbb{R}}\int_{\Omega_t} (-\partial_t - \Delta)uv \,\mathrm{d}\mathbf{x}\mathrm{d}t + \langle \gamma_1^+ u, \gamma_0 v\rangle.$$

Again, by restriction, this formula also holds for $u \in H^{1,\frac{1}{2}}_{;,0}(Q_T; \partial_t + \Delta)$ and $v \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$.

We can now state Green's formulae for a finite time interval, the time-independent analogues of which are given in [Cos90, Proposition 2.19].

Notice that [Cos90] introduces a time reversal map. For a time-dependent domain, this approach does not make sense, since the integration over a time forward tube of a time reversed entity is not always well defined. Therefore, we choose a slightly different approach to obtain another Green's formula.

Lemma III.5.1.

(i) *Let* $u \in H^{1,\frac{1}{2}}_{;0,}\big(\bigcup_{t\in\mathbb{R}_+}(\{t\}\times\Omega_t);\partial_t-\Delta\big)$ *and* $v \in H^{1,\frac{1}{2}}_{;,0}\big(\bigcup_{-\infty<t<t_0}(\{t\}\times\Omega_t)\big)$. *Then, for* $t_0>0$*, there holds Green's first formula*

$$\int_0^{t_0}\int_{\Omega_t}\langle\nabla u,\nabla v\rangle\,\mathrm{d}\mathbf{x}\mathrm{d}t + d(u,v) = \int_0^{t_0}\int_{\Omega_t}(\partial_t-\Delta)uv\,\mathrm{d}\mathbf{x}\mathrm{d}t + \langle\gamma_1^- u,\gamma_0 v\rangle.$$

(ii) *Let* $u \in H^{1,\frac{1}{2}}_{;,0}\big(\bigcup_{-\infty<t<t_0}(\{t\}\times\Omega_t);\partial_t+\Delta\big)$ *and* $v \in H^{1,\frac{1}{2}}_{;0,}\big(\bigcup_{t\in\mathbb{R}_+}(\{t\}\times\Omega_t)\big)$. *Then, for* $t_0>0$*, there holds Green's alternative first formula*

$$\int_0^{t_0}\int_{\Omega_t}\langle\nabla u,\nabla v\rangle\,\mathrm{d}\mathbf{x}\mathrm{d}t - d(u,v) = \int_0^{t_0}\int_{\Omega_t}(-\partial_t-\Delta)uv\,\mathrm{d}\mathbf{x}\mathrm{d}t + \langle\gamma_1^+ u,\gamma_0 v\rangle.$$

(iii) *Let* $u \in H^{1,\frac{1}{2}}_{;0,}\big(\bigcup_{t\in\mathbb{R}_+}(\{t\}\times\Omega_t);\partial_t-\Delta\big)$ *and* $v \in H^{1,\frac{1}{2}}_{;,0}\big(\bigcup_{-\infty<t<t_0}(\{t\}\times\Omega_t);\partial_t+\Delta\big)$. *Then, for* $t_0>0$*, there holds Green's second formula*

$$\int_0^{t_0}\int_{\Omega_t}\big\{(\partial_t-\Delta)uv + u(\partial_t+\Delta)v\big\}\,\mathrm{d}\mathbf{x}\mathrm{d}t = \langle\gamma_0 u,\gamma_1^+ v\rangle - \langle\gamma_1^- u,\gamma_0 v\rangle.$$

Proof. Statements (i) and (ii) are clear. Statement (iii) follows then immediately from these by interchanging v and u in (ii) and using (III.4.5). ☐

We need the tube equivalent of [Cos90, Lemma 2.22]. In there, the space

$$\widetilde{C}^\infty(\overline{Q}_0) := C_0^\infty\big((0,T]\times\overline{\Omega}_0\big)$$

is defined as the space of the restrictions of functions in $C_0^\infty(\mathbb{R}_+\times\mathbb{R}^d)$ to $\overline{Q}_0$. This space $\widetilde{C}^\infty(\overline{Q}_0)$ is dense in $H^{1,\frac{1}{2}}_{;0,}(Q_0;\partial_t-\Delta)$ according to [Cos90, Lemma 2.22]. As we only consider a C^2-mapping between the reference cylinder and the tube, we will prove the analogue result only for C^2-functions.

Lemma III.5.2. *Let us define*

$$\widetilde{C}^2(\overline{Q}_T) := \Big\{u\colon u\circ\boldsymbol{\kappa}\in C_0^2\big((0,T]\times\overline{\Omega}_0\big)\Big\}.$$

Then, the space $\widetilde{C}^2(\overline{Q}_T)$ *is dense in* $H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t-\Delta)$.

Proof. We mimic the proof of [Cos90, Lemma 2.22], which is based on a proof of Grisvard in the elliptic case, see [Gri85, Lemma 1.5.3.9]. According to the proof of [Cos90, Lemma 2.22], we have that $C_0^\infty\big((0,T]\times\overline{\Omega}_0\big)$ is dense in $H^{1,\frac{1}{2}}_{;0,}(Q_0)$. Therefore, also $C_0^2\big((0,T]\times\overline{\Omega}_0\big)$ is dense in $H^{1,\frac{1}{2}}_{;0,}(Q_0)$. Due to the definition of the spaces on the tube via the mapping $\boldsymbol{\kappa}$ and the resulting equivalence of norms, we also obtain that $\widetilde{C}^2(\overline{Q}_T)$ is dense in $H^{1,\frac{1}{2}}_{;0,}(Q_T)$. Similarly, we obtain that

$$\widetilde{C}^2(Q_T) := \Big\{u\colon u\circ\boldsymbol{\kappa}\in C_0^2\big((0,T]\times\Omega_0\big)\Big\}$$

is dense in $H^{1,\frac{1}{2}}_{0;0,}(Q_T)$.

Let $\mathcal{P}$ be an extension operator from $H^{1,\frac{1}{2}}_{;0,}(Q_T)$ to $H^{1,\frac{1}{2}}(\mathbb{R}^{d+1})$. It thus holds $(\mathcal{P}u)|_{Q_T} = u$. As in [Cos90], let us choose $\mathcal{P}$ such that $\operatorname{supp}\mathcal{P} \subset [0,\infty)\times\mathbb{R}^d$.[1] In that way, we can identify $H^{1,\frac{1}{2}}_{;0,}(Q_T)$ with a closed subspace of $H^{1,\frac{1}{2}}_{;0,}(\mathbb{R}_+\times\mathbb{R}^d)$. The map $u \mapsto \big(\mathcal{P}u, (\partial_t - \Delta)u\big)$ identifies $H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t-\Delta)$ with a closed subspace of $H^{1,\frac{1}{2}}_{;0,}(\mathbb{R}_+\times\mathbb{R}^d)\times L^2(\mathbb{R}_+\times\mathbb{R}^d)$. Due to this identification, we find for every bounded linear functional $\ell : H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t-\Delta)\to\mathbb{R}$ some $f \in \big(H^{1,\frac{1}{2}}_{;0,}(\mathbb{R}_+\times\mathbb{R}^d)\big)' = H^{-1,-\frac{1}{2}}(\mathbb{R}_+\times\mathbb{R}^d)$ and $g \in L^2(\mathbb{R}_+\times\mathbb{R}^d)$ such that it holds

$$\langle \ell, u\rangle = \langle f, \mathcal{P}u\rangle + \int_{\mathbb{R}_+\times\mathbb{R}^d} g(\partial_t-\Delta)u \,\mathrm{d}(t,\mathbf{x})$$

for all $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t-\Delta)$. Since ℓ acts only on u, which is supported on $\overline{Q}_T$, we may assume that $\operatorname{supp} f \subset \overline{Q}_T$ and $\operatorname{supp} g\subset\overline{Q}_T$.

We shall suppose next that it holds $\langle \ell,\varphi\rangle = 0$ for all $\varphi \in \widetilde{C}^2(\overline{Q}_T)$. If we can show $\ell = 0$, we obtain the desired density result in accordance with [Wer18, Korollar III.1.9]. For all $\varphi \in C^2_0(\mathbb{R}_+\times\mathbb{R}^d)$, we conclude

$$\begin{aligned} 0 = \langle \ell,\varphi\rangle &= \langle f,\varphi\rangle + \int_{Q_T} g(\partial_t-\Delta)\varphi\,\mathrm{d}(t,\mathbf{x}) \\ &= \langle f,\varphi\rangle + \int_{\mathbb{R}_+\times\mathbb{R}^d} g(\partial_t-\Delta)\varphi\,\mathrm{d}(t,\mathbf{x}). \end{aligned}$$

This equation states that

$$f = (\partial_t + \Delta) g$$

holds on $\mathbb{R}_+\times\mathbb{R}^d$ in complete analogy to [Cos90]. Due to $f \in H^{-1,-\frac{1}{2}}(\mathbb{R}_+\times\mathbb{R}^d)$ and the mapping properties of the differential operator, we find $g \in H^{1,\frac{1}{2}}(\mathbb{R}_+\times\mathbb{R}^d)$ and, thus, $g|_{Q_T} \in H^{1,\frac{1}{2}}_{0;,0}(Q_T)$.

On a cylindrical domain, any function $h \in H^{1,\frac{1}{2}}_{0;,0}(Q_0)$ can be approximated by a series $h_n \in C^\infty_0\big((-\infty,T)\times\Omega_0\big)$ (see [Cos90, Proof of Lemma 2.22]). Hence, by choosing $h := g\circ\boldsymbol{\kappa}$ and setting $g_n := h_n\circ\boldsymbol{\kappa}^{-1}$, we can approximate $g|_{Q_T} \in H^{1,\frac{1}{2}}_{0;,0}(Q_T)$ by a series $g_n \in C^2_0\big(\bigcup_{-\infty<t<T}(\{t\}\times\Omega_t)\big)$ in the norm of $H^{1,\frac{1}{2}}\big(\bigcup_{0<t<\infty}(\{t\}\times\Omega_t)\big)$. Thus, denoting by $\hat{g}_n$ the extension of g_n by zero outside of Q_T, we find $(\partial_t+\Delta)\hat{g}_n \to f$ in $H^{-1,-\frac{1}{2}}(\mathbb{R}_+\times\mathbb{R}^d)$. We then conclude for any $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t-\Delta)$ that

$$\begin{aligned} \langle \ell,u\rangle &= \lim_{n\to\infty}\bigg[\big\langle(\partial_t+\Delta)\hat{g}_n,\mathcal{P}u\big\rangle + \int_{Q_T} g_n(\partial_t-\Delta)u\,\mathrm{d}(t,\mathbf{x})\bigg] \\ &= \lim_{n\to\infty}\bigg[\int_{Q_T}(\partial_t+\Delta)g_n u\,\mathrm{d}(t,\mathbf{x}) + \int_{Q_T} g_n(\partial_t-\Delta)u\,\mathrm{d}(t,\mathbf{x})\bigg] = 0. \end{aligned}$$

The expression above is equal to zero, because $u=0$ for $t=0$, $g_n = 0$ for $t=T$, and g_n has a zero boundary condition. $\square$

[1] Such an extension operator exists as it can be defined by $\mathcal{P}u = \big(\widetilde{\mathcal{P}}(u\circ\boldsymbol{\kappa})\big)\circ\boldsymbol{\kappa}^{-1}$ with $\widetilde{\mathcal{P}} : H^{1,\frac{1}{2}}_{;0,}(Q_0)\to H^{1,\frac{1}{2}}(\mathbb{R}_+\times\mathbb{R}^d)$ being the extension operator from [Cos90].

Remark III.5.3. *If we consider $t \mapsto T - t$ in Lemma III.5.2, we obtain that $\widehat{C}^2(\overline{Q}^T)$ is dense in $H^{1,\frac{1}{2}}_{;,0}(Q^T; -\partial_t - \Delta)$, where*

$$\widehat{C}^2(\overline{Q}_T) := \Big\{u\colon u \circ \boldsymbol{\kappa} \in C_0^2\big([0,T) \times \overline{\Omega}_0\big)\Big\}$$

and Q^T is the time-flipped Q_T. Since Q_T was arbitrary, we have $\widehat{C}^2(\overline{Q}_T)$ is dense in $H^{1,\frac{1}{2}}_{;,0}(Q_T; \partial_t + \Delta)$.

Next, we will introduce a lemma concerning the trace maps, which will be later used in the proof of the jump relations. It is the analogue of [Cos90, Lemma 2.23].

Lemma III.5.4. *The combined trace map $(\gamma_0, \gamma_1^+)\colon u \mapsto (\gamma_0 u, \gamma_1^+ u)$ maps $\widehat{C}^2(\overline{Q}_T)$ onto a dense subspace of $H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \times H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$.*

Proof. We again mimic the respective proof from [Cos90], but will not use a time reversal map. Let us assume a linear functional $(\chi, \psi) \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \times H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ that vanishes on the range of (γ_1^+, γ_0). We need to show that $(\chi, \psi) = (0, 0)$, since then the density follows by [Wer18, Korollar III.1.9]. To this end, assume

$$\langle \chi, \gamma_1^+ \varphi \rangle = \langle \psi, \gamma_0 \varphi \rangle \quad \text{for all } \varphi \in \widehat{C}^2(\overline{Q}_T). \tag{III.5.2}$$

Let

$$\mathcal{T} = (g \mapsto \mathcal{T}g)\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T)$$

be the solution operator (see Theorem III.3.5) of the Dirichlet problem

$$\begin{aligned} (\partial_t - \Delta)(\mathcal{T}g) &= 0 && \text{in } Q_T, \\ \gamma_0(\mathcal{T}g) &= g && \text{on } \Sigma_T. \end{aligned} \tag{III.5.3}$$

Moreover, let

$$\mathcal{S} = (f \mapsto \mathcal{S}f)\colon L^2(Q_T) \to H^{1,\frac{1}{2}}_{0;,0}(Q_T)$$

be the solution operator (see Theorem III.3.5 used for the substitution $t \mapsto T - t$) of the Dirichlet problem

$$\begin{aligned} (\partial_t + \Delta)(\mathcal{S}f) &= f && \text{in } Q_T, \\ \gamma_0(\mathcal{S}f) &= 0 && \text{on } \Sigma_T. \end{aligned}$$

We can apply Green's second formula from Lemma III.5.1 to $u := \mathcal{T}\chi$ and $v := \mathcal{S}f$ for any $f \in L^2(Q_T)$, since $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta)$ and $(\partial_t + \Delta)v \in L^2(Q_T)$. We obtain

$$\int_{Q_T} \big\{(\partial_t - \Delta)uv + u(\partial_t + \Delta)v\big\} \,\mathrm{d}(\mathbf{x}, t) = \langle \gamma_0 u, \gamma_1^+ v\rangle - \langle \gamma_1^- u, \gamma_0 v\rangle.$$

Since $\gamma_0 v = 0$ and $\gamma_0 u = \chi$, as well as $(\partial_t - \Delta)u = 0$ and $(\partial_t + \Delta)v = f$, we obtain

$$\int_{Q_T} uf \,\mathrm{d}(t, \mathbf{x}) = \langle \chi, \gamma_1^+ v\rangle.$$

Due to continuity and Remark III.5.3, (III.5.2) holds also for all $\varphi \in H^{1,\frac{1}{2}}_{;,0}(Q_T; \partial_t + \Delta)$ and, thus, also for $\varphi = \mathcal{S}f$. This implies

$$\langle \chi, \gamma_1^+ \mathcal{S}f\rangle = \langle \psi, \gamma_0 \mathcal{S}f\rangle.$$

Since $\gamma_0 \mathcal{S} f = 0$, we thus obtain $\int_{Q_T} uf \,\mathrm{d}(t, \mathbf{x}) = 0$ for all $f \in L^2(Q_T)$. Therefore, $0 = u = \mathcal{T}(\chi)$ and thus $\chi = \gamma_0 u = 0$. Looking again at (III.5.2) gives

$$\langle \psi, \gamma_0 \varphi \rangle = 0 \quad \text{for all } \varphi \in H^{1,\frac{1}{2}}_{;,0}(Q_T).$$

The trace map γ_0 is not only surjective for $\varphi \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ as shown in Section III.2.2, but also for $\varphi \in H^{1,\frac{1}{2}}_{;,0}(Q_T)$ if one considers the backward problem. We may hence conclude that $\psi = 0$. □

In the following, we state the analogue of [Cos90, Proposition 2.24].

Lemma III.5.5. *Green's first formula given in* (III.5.1) *holds for all* $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta)$ *and* $v \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$. *If also* $v \in H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta)$, *we can write the Green's formula as*

$$\begin{aligned} \int_{Q_T} \langle \nabla u, \nabla v \rangle \,\mathrm{d}(t, \mathbf{x}) - d(v, u) + \int_{\Omega_T} u(T, \mathbf{x}) v(T, \mathbf{x}) \,\mathrm{d}\mathbf{x} \\ = \langle \gamma_1^- u, \gamma_0 v \rangle + \int_{Q_T} (\partial_t - \Delta) uv \,\mathrm{d}(t, \mathbf{x}). \end{aligned} \tag{III.5.4}$$

Proof. We again mimic the proof of [Cos90, Proposition 2.24]. Given $u \in \widetilde{C}^2(\overline{Q}_T)$ and $v \in \widetilde{C}^1(\overline{Q}_T)$[2], we find

$$\begin{aligned} \int_{Q_T} \langle \nabla u, \nabla v \rangle \,\mathrm{d}(t, \mathbf{x}) + \int_{Q_T} \partial_t uv \,\mathrm{d}(t, \mathbf{x}) + \frac{1}{2} \int_0^T \int_{\Gamma_t} \langle \mathbf{V}, \mathbf{n} \rangle uv \,\mathrm{d}\sigma \mathrm{d}t \\ = \langle \gamma_1^- u, \gamma_0 v \rangle + \int_{Q_T} (\partial_t - \Delta) uv \,\mathrm{d}(t, \mathbf{x}). \end{aligned} \tag{III.5.5}$$

All terms are continuous with respect to v in the $H^{1,\frac{1}{2}}_{;0,}(Q_T)$-norm. Thus, by continuity, we can extend (III.5.5) to all $v \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$. Let $v \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ be fixed. Then, all terms in (III.5.5) except the term containing the $\partial_t u$ are obviously continuous with respect to u in the norm of $H^{1,\frac{1}{2}}_{;0,}(Q; \partial_t - \Delta)$. Therefore, also the term containing $\partial_t u$ is continuous. Lemma III.5.2 allows to extend (III.5.5) to all $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta)$. Thus, Green's first formula holds as claimed.

For $u, v \in \widetilde{C}^2(\overline{Q}_T)$, (III.5.4) holds. As in [Cos90], the term $\int_{\Omega_T} u(T, \mathbf{x}) v(T, \mathbf{x}) \,\mathrm{d}\mathbf{x}$ is continuous for u and v in the norm of $H^{1,\frac{1}{2}}_{;0,}(Q_T; \partial_t - \Delta) \subset \mathcal{V}(Q_T)$ and $\mathcal{V}(Q_T)$ consists of functions φ, which always satisfy $\varphi \circ \boldsymbol{\kappa} \in C\big([0, T]; L^2(\Omega_0)\big)$. From here, the second claim follows. □

III.6 The Calderón operator

In the following, we will establish the mapping properties of the layer potential operators used for the boundary element method.

[2] The space $\widetilde{C}^1(\overline{Q}_T)$ ist defined in complete analogy to $\widetilde{C}^2(\overline{Q}_T)$ via

$$\widetilde{C}^1(Q_T) := \big\{ u \colon u \circ \boldsymbol{\kappa} \in C^1_0\big((0, T] \times \Omega_0\big) \big\}$$

Let us first introduce the fundamental solution for the heat equation, which, in accordance with e.g. [Tau19], reads

$$G(t,\tau,\mathbf{x},\mathbf{y}) := \begin{cases} \frac{1}{(4\pi(t-\tau))^{\frac{d}{2}}} \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4(t-\tau)}\right), & \text{if } \tau < t, \\ 0, & \text{if } \tau \geq t, \end{cases}$$

Notice that this is equivalent to considering $\overline{G}(t-\tau,\mathbf{x},\mathbf{y})$, where $\overline{G}$ is given by

$$\overline{G}(\tau,\mathbf{x},\mathbf{y}) := \frac{1}{(4\pi\tau)^{\frac{d}{2}}} \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4\tau}\right) \frac{1}{2}(1+\operatorname{sign}\tau),$$

as introduced in [Cos90, Formula (2.39)]. Moreover, let us denote

$$\widetilde{G}(t,\mathbf{x}) = \begin{cases} \frac{1}{(4\pi t)^{\frac{d}{2}}} \exp\left(-\frac{\|\mathbf{x}\|^2}{4t}\right), & \text{if } t > 0, \\ 0, & \text{if } t \leq 0. \end{cases} \tag{III.6.1}$$

For $u \in C^2\big(\bigcup_{0<t<\infty}(\{t\}\times\overline{\Omega}_t)\big)$ with $u(0,\mathbf{x}) = 0$ on Ω_0, we have for $(t_0,\mathbf{x}_0) \in \bigcup_{0<t<\infty}(\{t\}\times\Omega_t)$ that

$$\begin{aligned} u(t_0,\mathbf{x}_0) = &\int_{Q_T} (\partial_t - \Delta)u(t,\mathbf{x})\widetilde{G}(t_0-t,\mathbf{x}_0-\mathbf{x})\,\mathrm{d}(t,\mathbf{x}) \\ &+ \int_0^T \int_{\Gamma_t} \widetilde{G}(t_0-t,\mathbf{x}_0-\mathbf{x})\frac{\partial u}{\partial \mathbf{n}}(t,\mathbf{x})\,\mathrm{d}\sigma_{\mathbf{x}}\mathrm{d}t \\ &- \int_0^T \int_{\Gamma_t} \frac{\partial \widetilde{G}}{\partial \mathbf{n}}(t_0-t,\mathbf{x}_0-\mathbf{x})u(t,\mathbf{x})\,\mathrm{d}\sigma_{\mathbf{x}}\mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} \widetilde{G}(t_0-t,\mathbf{x}_0-\mathbf{x})\langle \mathbf{V},\mathbf{n}\rangle(t,\mathbf{x})u(\mathbf{y},\tau)\,\mathrm{d}\sigma_{\mathbf{x}}\mathrm{d}t, \end{aligned}$$

as it can be seen from Lemma III.5.1 and the property of the fundamental solution. Moreover, we will only look at the case, for which $(\partial_t - \Delta)u = 0$ holds.

We introduce the single and double layer potentials as

$$\begin{aligned} \widetilde{\mathcal{V}}\varphi(t_0,\mathbf{x}_0) &:= \langle \varphi, \gamma_0 G\rangle = \int_0^T \int_{\Gamma_t} G(t_0,t,\mathbf{x}_0,\mathbf{y})\varphi(t,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau, \\ \widetilde{\mathcal{K}}w(t_0,\mathbf{x}_0) &:= \langle \gamma_1^+ G, w\rangle = \int_0^T \int_{\Gamma_t} \gamma^+_{1,(t,\mathbf{y})} G(t_0,t,\mathbf{x}_0,\mathbf{y})w(t,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau. \end{aligned}$$

Then, similarly to [Cos90, Theorem 2.20], we obtain the representation formula from [Tau19, Equation (6)] given in the following lemma.

Lemma III.6.1. *Let $u \in H^{1,\frac{1}{2}}(Q_T)$ with $(\partial_t - \Delta)u = 0$ in Q_T. Then, we have the representation formula*

$$u(t,\widetilde{\mathbf{x}}) = \widetilde{\mathcal{V}}\gamma_1^- u(t,\widetilde{\mathbf{x}}) - \widetilde{\mathcal{K}}u(t,\widetilde{\mathbf{x}}) \quad \textit{for all } (t,\widetilde{\mathbf{x}}) \in Q_T. \tag{III.6.2}$$

As in [Cos90, p. 514], we can rewrite the definition of the single layer potential by

$$\begin{aligned} \widetilde{\mathcal{V}}\varphi(t_0,\mathbf{x}_0) &= \big\langle \varphi, \gamma_0 G(t,t_0,\mathbf{x},\mathbf{x}_0)\big\rangle \\ &= \big\langle \gamma_0'\varphi, G(t,t_0,\mathbf{x},\mathbf{x}_0)\big\rangle \\ &= \widetilde{G} \star (\gamma_0'\varphi)(t_0,\mathbf{x}_0), \end{aligned} \tag{III.6.3}$$

where $\widetilde{G}$ is given in (III.6.1) and

$$\langle \gamma_0' \varphi, \chi \rangle = \langle \varphi, \gamma_0 \chi \rangle = \int_0^T \int_{\Gamma_t} \varphi \chi \, \mathrm{d}\sigma \mathrm{d}t \tag{III.6.4}$$

for all $\chi \in C_0^\infty(\mathbb{R}^{1+d})$. We will use this also for $\chi \in C_0^2(\mathbb{R}^{1+d})$.

We would like to find the mapping properties of the single and double layer potentials, which are the equivalent of the results given in [Cos90, Proposition 3.1, Remark 3.2, and Proposition 3.3].

Lemma III.6.2. *The mapping*

$$\widetilde{\mathcal{V}}\colon H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t - \Delta)$$

is continuous.

Proof. The proof follows as in [Cos90, p. 514–515] in the case of a cylindrical domain. In there, the claim is proven by considering the problem on $\mathbb{R}^{1+d}$ using Fourier techniques and then restricting it appropriately, which can also be done in the case of a non-cylindrical domain. □

Lemma III.6.3. *The mapping*

$$\widetilde{\mathcal{K}}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t - \Delta)$$

is continuous.

Proof. The proof is in complete analogy to [Cos90, p. 515], but we repeat it for the convenience of the reader. We consider the solution operator $\mathcal{T}$, which maps the Dirichlet data g to the solution $u := \mathcal{T}g$ of the partial differential equation (III.5.3). According to Theorem III.3.5, the solution operator $\mathcal{T}$ is a continuous mapping

$$\mathcal{T}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T;\partial_t - \Delta). \tag{III.6.5}$$

The representation formula (III.6.2) yields $u(t,\widetilde{\mathbf{x}}) = \widetilde{\mathcal{V}}\gamma_1^- u(t,\widetilde{\mathbf{x}}) - \widetilde{\mathcal{K}}u(t,\widetilde{\mathbf{x}})$ and thus $\mathcal{T}g = \widetilde{\mathcal{V}}\gamma_1^- \mathcal{T}g - \widetilde{\mathcal{K}}g$ for all $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$. Rearranging gives hence

$$\widetilde{\mathcal{K}} = \widetilde{\mathcal{V}}\gamma_1^- \mathcal{T} - \mathcal{T}.$$

The claim follows now by using the mapping property (III.6.5) of $\mathcal{T}$, $\widetilde{\mathcal{V}}$ (Lemma III.6.2), and γ_1^- (Lemma III.4.7). □

We can take the traces γ_0 of the single and double layer potential. Let the radius R be large enough such that the boundary Γ_t is contained in the ball $B_R := \{\mathbf{x} \in \mathbb{R}^d \colon \|\mathbf{x}\| < R\}$ and set $\Omega_t^c := B_R \backslash \overline{\Omega}_t$ and $Q_T^c := \bigcup_{-\infty<t<T} (\{t\} \times \Omega_t^c)$. Lemmata III.6.2 and III.6.3 provide also the continuity of the mappings

$$\widetilde{\mathcal{V}}\colon H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T^c;\partial_t - \Delta)$$

and

$$\widetilde{\mathcal{K}}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \to H^{1,\frac{1}{2}}_{;0,}(Q_T^c;\partial_t - \Delta).$$

In order to state the tube analogue of [Cos90, Theorem 3.4], we define the jumps as in [Cos90, Formula (3.16)] in accordance with

$$[\gamma_0 u] := \gamma_0(u|_{Q_T^c}) - \gamma_0(u|_{Q_T}), \quad [\gamma_1^{\pm} u] := \gamma_1^{\pm}(u|_{Q_T^c}) - \gamma_1^{\pm}(u|_{Q_T}).$$

We then have:

Lemma III.6.4. *For all $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ and all $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$, there hold the jump relations*

$$\begin{aligned} [\gamma_0 \widetilde{\mathcal{V}}\psi] &= 0, & [\gamma_1^- \widetilde{\mathcal{V}}\psi] &= -\psi, \\ [\gamma_0 \widetilde{\mathcal{K}} w] &= w, & [\gamma_1^- \widetilde{\mathcal{K}} w] &= 0. \end{aligned}$$

Proof. We mimic the proof of [Cos90, Theorem 3.4] without using the time reversal map. Let $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$. We set $u := \widetilde{\mathcal{V}}\psi$. Due to the mapping property of the single layer potential, we then have $u \in H^{1,\frac{1}{2}}_{;0,}\big((0,T) \times B_R(0)\big)$ and thus, by the trace lemma, we have $\gamma_0(u|_{Q_T}) = \gamma_0(u|_{Q_T^c})$.

Let us next consider the normal jump of $\widetilde{\mathcal{V}}$. From (III.6.3), we obtain by considering $u = \widetilde{\mathcal{V}}\psi$

$$(\partial_t - \Delta)u = \gamma_0'\psi$$

in $\mathbb{R}_+ \times \mathbb{R}^d$. We consider any test function $\varphi \in C_0^2\big((0,T) \times B_R\big)$ and obtain

$$\langle \psi, \gamma_0\varphi\rangle = \langle \gamma_0'\psi, \varphi\rangle = \big\langle (\partial_t - \Delta)u, \varphi\big\rangle = -\big\langle u, (\partial_t + \Delta)\varphi\big\rangle,$$

where the last equality holds due to the integration by parts on a cylindrical domain. We thus have

$$\langle \psi, \gamma_0\varphi\rangle = -\int_{(0,T)\times B_R} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}). \tag{III.6.6}$$

On the other hand, we can use Green's second formula, given in Lemma III.5.1 in Q_T and Q_T^c, where we use that $(\partial_t - \Delta)u = 0$ in $Q_T \cup Q_T^c$. This yields

$$\int_{Q_T} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}) = \langle \gamma_0 u, \gamma_1^+\varphi\rangle - \langle \gamma_1^- u, \gamma_0\varphi\rangle$$

and

$$\int_{Q_T^c} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}) = -\langle \gamma_0 u, \gamma_1^+\varphi\rangle + \langle \gamma_1^- u, \gamma_0\varphi\rangle.$$

Adding these two expressions yields

$$\int_{(0,T)\times B_R} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}) = \big\langle [\gamma_1^- u], \gamma_0\varphi\big\rangle, \tag{III.6.7}$$

where we used $[\gamma_0 u] = 0 = [\gamma_0\varphi] = [\gamma_1^+\varphi]$. Comparing (III.6.6) with (III.6.7) results in $[\gamma_1^- u] = -\psi$.

We are left with proving the jump relations for the double layer potential. To that end, we choose $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ and define $u := \widetilde{\mathcal{K}}w$. Let $\varphi \in C_0^\infty(\mathbb{R}_+ \times B_R)$ be a test function. As above, we obtain

$$\int_{(0,T)\times B_R} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}) = \big\langle [\gamma_1^- u], \gamma_0\varphi\big\rangle - \big\langle [\gamma_0 u], \gamma_1^+\varphi\big\rangle. \tag{III.6.8}$$

For $\widetilde{\mathcal{K}}$, we obtain $\widetilde{\mathcal{K}}w = \widetilde{G} \star \big((\gamma_1^+)'w\big)$ similar to (III.6.3). Therefore, we have $(\partial_t - \Delta)\widetilde{\mathcal{K}}w = (\gamma_1^+)'w$ in $\mathbb{R}_+ \times B_R$. From here, it follows that

$$-\int_{(0,T)\times B_R} (\partial_t + \Delta)\varphi u \,\mathrm{d}(t,\mathbf{x}) = \big\langle(\partial_t - \Delta)u, \varphi\big\rangle = \big\langle(\gamma_1^+)'w, \varphi\big\rangle = \langle w, \gamma_1^+\varphi\rangle. \quad \text{(III.6.9)}$$

Comparing (III.6.8) with (III.6.9) yields

$$\big\langle[\gamma_1^- u], \gamma_0\varphi\big\rangle = \big\langle[\gamma_0 u] - w, \gamma_1^+\varphi\big\rangle \quad \text{(III.6.10)}$$

for all $\varphi \in C_0^2(\mathbb{R}_+ \times B_R)$. Applying Lemma III.5.4 says that both sides of (III.6.10) have to vanish identically, from where $[\gamma_1^- u] = 0$ and $[\gamma_0 u] = w$ follows. $\square$

Now, as in [Cos90, Definition 3.5], we are in the position to define the boundary integral operators.

Definition III.6.5. *Let $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ and $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$. We can then define the single layer operator as*

$$\mathcal{V}\psi := \gamma_0\widetilde{\mathcal{V}}\psi,$$

the adjoint double layer operator as

$$\mathcal{K}'\psi := \frac{1}{2}\left(\gamma_1^-(\widetilde{\mathcal{V}}\psi)|_{Q_T} + \gamma_1^-(\widetilde{\mathcal{V}}\psi)|_{Q_T^c}\right),$$

the double layer operator as

$$\mathcal{K}w := \frac{1}{2}\left(\gamma_0(\widetilde{\mathcal{K}}w)|_{Q_T} + \gamma_0(\widetilde{\mathcal{K}}w)|_{Q_T^c}\right)$$

and the hypersingular operator as

$$\mathcal{D}w := -\gamma_1^-\widetilde{\mathcal{K}}w.$$

As in [Cos90, Theorem 3.7], we have the following mapping properties of these operators.

Theorem III.6.6. *The boundary integral operators from Definition III.6.5 are continuous mappings as follows*

$$\begin{aligned}
\mathcal{V}\colon H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) &\to H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T),\\
\mathcal{K}'\colon H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) &\to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T),\\
\mathcal{K}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) &\to H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T),\\
\mathcal{D}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) &\to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T).
\end{aligned}$$

Proof. The assertion follows immediately by using the mapping properties of the layer potentials from Lemma III.6.2 and Lemma III.6.3 as well as of the trace operators introduced in Section III.2.2 and from Lemma III.4.7. $\square$

We can state the analogue of [Cos90, Formulae (3.24)–(3.27)].

Lemma III.6.7. *It holds*

$$\begin{aligned}
\gamma_0(\widetilde{\mathcal{V}}\psi)|_{Q_T} &= \gamma_0(\widetilde{\mathcal{V}}\psi)|_{Q_T^c} = \mathcal{V}\psi,\\
\gamma_1^-(\widetilde{\mathcal{V}}\psi)|_{Q_T} &= \frac{1}{2}\psi + \mathcal{K}'\psi,\\
\gamma_1^-(\widetilde{\mathcal{V}}\psi)|_{Q_T^c} &= -\frac{1}{2}\psi + \mathcal{K}'\psi,\\
\gamma_0(\widetilde{\mathcal{K}}w)|_{Q_T} &= -\frac{1}{2}w + \mathcal{K}w,\\
\gamma_0(\widetilde{\mathcal{K}}w)|_{Q_T^c} &= \frac{1}{2}w + \mathcal{K}w,\\
\gamma_1^-(\widetilde{\mathcal{K}}w)|_{Q_T} &= \gamma_1^-(\mathcal{K}w)|_{Q_T^c} = -\mathcal{D}w.
\end{aligned}$$

Proof. We just prove the second statement, as the other statements follow similarly. According to Lemma III.6.4, we have

$$[\gamma_1^-\widetilde{\mathcal{V}}\psi] = \gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T^c} - \gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T} = -\psi.$$

Therefore,

$$\gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T} = \psi + \gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T^c}.$$

By Definition III.6.5, we have

$$\mathcal{K}'\psi := \frac{1}{2}\left(\gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T} + \gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T^c}\right).$$

Substituting this into the expression above yields

$$\gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T} = \psi + 2\mathcal{K}'\psi - \gamma_1^-\widetilde{\mathcal{V}}\psi|_{Q_T},$$

from where the claim follows immediately. □

Remark III.6.8. *Following [Tau19, Formulae (7)–(10)], the relations in the interior given in Lemma III.6.7 can also be written as*

$$\begin{aligned}
\gamma_0\widetilde{\mathcal{V}}\psi(t,\mathbf{x}) &= \int_0^T \int_{\Gamma_t} G(t,\tau,\mathbf{x},\mathbf{y})\psi(\tau,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau,\\
\gamma_1^-\widetilde{\mathcal{V}}\psi(t,\mathbf{x}) &= \frac{1}{2}\psi(t,\mathbf{x}) + \int_0^T \int_{\Gamma_t} \gamma_{1,(t,\mathbf{x})}^- G(t,\tau,\mathbf{x},\mathbf{y})\psi(\tau,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau,\\
\gamma_0\widetilde{\mathcal{K}}w(t,\mathbf{x}) &= -\frac{1}{2}w(t,\mathbf{x}) + \int_0^T \int_{\Gamma_t} \gamma_{1,(\tau,\mathbf{y})}^+ G(t,\tau,\mathbf{x},\mathbf{y})w(\tau,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau,\\
\gamma_1^-\widetilde{\mathcal{K}}w(t,\mathbf{x}) &= -\int_0^T \int_{\Gamma_t} \gamma_{1,(t,\mathbf{x})}^-\gamma_{1,(\tau,\mathbf{y})}^+ G(t,\tau,\mathbf{x},\mathbf{y})w(\tau,\mathbf{y})\,\mathrm{d}\sigma_{\mathbf{y}}\mathrm{d}\tau.
\end{aligned}$$

We can take the traces in the representation formula (III.6.2) to obtain the Dirichlet data and the Neumann data of the solution u of the homogeneous heat equation. This yields

$$\gamma_0 u = \frac{1}{2}\gamma_0 u - \mathcal{K}\gamma_0 u + \mathcal{V}\gamma_1^- u, \tag{III.6.11}$$

$$\gamma_1^- u = \mathcal{D}\gamma_0 u + \frac{1}{2}\gamma_1^- u + \mathcal{K}'\gamma_1^- u, \tag{III.6.12}$$

compare also [Tau19, Formulae (11) and (12)].

As in [Cos90, p. 518], we can define the Calderón projector and the associated involution $\mathcal{A}$ as

$$\mathcal{C}_{Q_T} := \frac{1}{2}\operatorname{id} + \mathcal{A} := \frac{1}{2}\operatorname{id} + \begin{bmatrix} -\mathcal{K} & \mathcal{V} \\ \mathcal{D} & \mathcal{K}' \end{bmatrix}.$$

We state next the analogue of [Cos90, Theorem 3.9].

Theorem III.6.9. *The operator $\mathcal{C}_{Q_T}$ is a projection operator in the space*

$$\mathcal{G} := H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \times H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T).$$

The following statements are equivalent for $(w, \psi) \in \mathcal{G}$:

(i) There is a $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ with $(\partial_t - \Delta)u = 0$ in Q_T and $w = \gamma_0 u$, $\psi = \gamma_1^- u$ on Σ_T.

(ii) It holds

$$\begin{bmatrix} w \\ \psi \end{bmatrix} = \mathcal{C}_{Q_T} \begin{bmatrix} w \\ \psi \end{bmatrix}.$$

Proof. We again follow the proof of [Cos90, Thereom 3.9].

(i) $\Rightarrow$ (ii) follows by the considerations above, especially in (III.6.11) and (III.6.12).

For the proof of (ii) $\Rightarrow$ (i), ψ and w are given and we define

$$u := \widetilde{\mathcal{V}}\psi - \widetilde{\mathcal{K}}w. \tag{III.6.13}$$

Using the mapping properties of the potentials implies that $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ and we obtain

$$\begin{bmatrix} \gamma_0 u \\ \gamma_1^- u \end{bmatrix} = \mathcal{C}_{Q_T} \begin{bmatrix} w \\ \psi \end{bmatrix}. \tag{III.6.14}$$

Since the right-hand side equals to $[w, \psi]^\intercal$ according to (ii), the claim follows immediately.

It remains to show the projection property of $\mathcal{C}_{Q_T}$. Because on the one hand $[\gamma_0 u, \gamma_1^- u]^\intercal = \mathcal{C}_{Q_T}[\gamma_0 u, \gamma_1^- u]^\intercal$ holds according to (III.6.11), (III.6.12) and on the other hand (III.6.14) holds for any $[w, \psi]^\intercal$ and u given by (III.6.13), we obtain $\mathcal{C}_{Q_T}[w, \psi]^\intercal = \mathcal{C}_{Q_T}^2[w, \psi]^\intercal$ for any $[w, \psi]^\intercal$ and thus

$$\mathcal{C}_{Q_T}^2 = \mathcal{C}_{Q_T}. \tag{III.6.15}$$

□

We can state the following corollary in analogy to [Cos90, Corollary 3.10].

Corollary III.6.10. *The operator $\mathcal{A}\colon \mathcal{G} \to \mathcal{G}$ is an isomorphism.*

Proof. We use the same argument as in the proof of [Cos90, Corollary 3.10]. Notice that we can reformulate (III.6.15) as follows:

$$\left(\frac{1}{2}\operatorname{id} + \mathcal{A}\right)^2 = \frac{1}{4}\operatorname{id} + \mathcal{A} + \mathcal{A}^2 = \frac{1}{2}\operatorname{id} + \mathcal{A}.$$

We hence conclude

$$\mathcal{A}^2 = \frac{1}{4}\,\mathrm{id}, \tag{III.6.16}$$

which is equivalent to

$$\mathcal{A}^{-1} = 4\mathcal{A}.$$

□

As in [Cos90], we can interchange the columns of the operator $\mathcal{A}$ to define the operator

$$A := \begin{bmatrix} \mathcal{V} & -\mathcal{K} \\ \mathcal{K}' & \mathcal{D} \end{bmatrix},$$

which is an isomorphism of the space

$$\mathcal{G}' := H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) \times H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$$

onto its dual space $\mathcal{G}$. Following [Cos90], we define the duality product between $\mathcal{G}'$ and $\mathcal{G}$ as

$$\left\langle \begin{bmatrix} \psi \\ w \end{bmatrix}, \begin{bmatrix} v \\ \varphi \end{bmatrix} \right\rangle := \langle \psi, v\rangle + \langle \varphi, w\rangle$$

for all v, $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ and φ, $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$. We are now in the position to state the analogue of [Cos90, Theorem 3.11], which is the positive definiteness of the operator A.

Theorem III.6.11. *There exists a constant $\alpha > 0$ such that*

$$\left\langle \begin{bmatrix} \psi \\ w \end{bmatrix}, A \begin{bmatrix} \psi \\ w \end{bmatrix} \right\rangle \geq \alpha \left(\|\psi\|^2_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)} + \|w\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)} \right)$$

for all $[\psi, w]^\intercal \in \mathcal{G}'$.

For the proof, we again mimic the proof of [Cos90, Theorem 3.11], which is based on the following lemma (see [Cos90, Lemma 3.12]). Its proof can be found in [Cos90].

Lemma III.6.12. *Let $A\colon X \to X'$ be a bounded linear operator, where X' is the dual space of the Hilbert space X. With a compact operator $T\colon X \to X'$ and a constant α, let A satisfy*

$$\big\langle (A + T)x, x \big\rangle \geq \alpha \|x\|^2_X \quad \text{for all } x \in X$$

and

$$\langle Ax, x\rangle > 0 \quad \text{for all } x \in X\backslash\{0\}. \tag{III.6.17}$$

Then, there exists a constant $\alpha_1 > 0$ such that

$$\langle Ax, x\rangle \geq \alpha_1 \|x\|^2_X \quad \text{for all } x \in X.$$

Moreover, we need the following analogue of [Cos90, Lemma 2.15].

Lemma III.6.13. *Let $u \in \mathcal{V}(Q_T)$ such that $(\partial_t - \Delta)u = 0$ in Q_T. Then, there exist constants m_1, m_2, and m_3 such that*

$$\|u\|_{H^{1,0}(Q_T)} \leq m_1 \|u\|_{H^{1,\frac{1}{2}}(Q_T)} \leq m_2 \|u\|_{\mathcal{V}(Q_T)} \leq m_3 \|u\|_{H^{1,0}(Q_T)}.$$

In other words, for functions $u \in \mathcal{V}(Q_T)$ satisfying the homogeneous heat equation, we have the equivalence of the norms in $\mathcal{V}(Q_T)$, $H^{1,0}(Q_T)$, and $H^{1,\frac{1}{2}}(Q_T)$.

Proof. The first and second inequality follow directly from the equivalence of norms on Q_T and Q_0, since the proof of [Cos90] is based on the definition of the norm for the first inequality and the interpolation result (III.1.7) for the second inequality. Nonetheless, we cannot apply the equivalence of norms on Q_T and norms on Q_0 directly for the third inequality, because we have $(\partial_t - \Delta)u = 0$ as an assumption, which is needed to show the third inequality. Mapping this differential operator from the tube onto the cylinder or vice versa will alter it. Therefore, we use the ideas of the proof of [Cos90, Lemma 2.15], but adapt them to our context.

Transforming the partial differential equation $(\partial_t - \Delta)u = 0$ from Q_T back to Q_0 via the weak formulation (see (III.3.4)) yields

$$\partial_t(u \circ \boldsymbol{\kappa}) - \mathcal{M}(u \circ \boldsymbol{\kappa}) = 0 \quad \text{in } Q_0,$$

where $\mathcal{M}$ is defined as

$$\begin{aligned}\mathcal{M}(u \circ \boldsymbol{\kappa}) := \operatorname{div}\Big((\mathrm{D}\boldsymbol{\kappa})^{-1}(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla(u \circ \boldsymbol{\kappa})\Big) + \big\langle(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla(u \circ \boldsymbol{\kappa}), \partial_t\boldsymbol{\kappa}\big\rangle \\ + \frac{1}{\det(\mathrm{D}\boldsymbol{\kappa})}\Big\langle\nabla\big(\det(\mathrm{D}\boldsymbol{\kappa})\big), (\mathrm{D}\boldsymbol{\kappa})^{-1}(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\nabla(u \circ \boldsymbol{\kappa})\Big\rangle.\end{aligned}$$

By the standard theory, for fixed $t \in (0,T)$, we have that $\mathcal{M}\colon H^1(\Omega_0) \to H^{-1}(\Omega_0)$ is bounded. Thus, for $u \in H^{1,0}(Q_0)$, we obtain $\mathcal{M}u \in L^2\big((0,T); H^{-1}(\Omega_0)\big)$ and we conclude

$$\begin{aligned}\|u\|^2_{\mathcal{V}(Q_T)} = \|u \circ \boldsymbol{\kappa}\|^2_{\mathcal{V}(Q_0)} &= \|u \circ \boldsymbol{\kappa}\|^2_{H^{1,0}(Q_0)} + \big\|\partial_t(u \circ \boldsymbol{\kappa})\big\|^2_{L^2((0,T);H^{-1}(\Omega_0))} \\ &= \|u \circ \boldsymbol{\kappa}\|^2_{H^{1,0}(Q_0)} + \big\|\mathcal{M}(u \circ \boldsymbol{\kappa})\big\|^2_{L^2((0,T);H^{-1}(\Omega_0))} \\ &\lesssim \|u \circ \boldsymbol{\kappa}\|^2_{H^{1,0}(Q_0)} \\ &= \|u\|^2_{H^{1,0}(Q_T)}.\end{aligned}$$

□

Proof of Theorem III.6.11. We follow the proof of [Cos90, Theorem 3.11]. As above, we let the radius $R > 0$ be big enough such that the ball B_R contains the boundary Γ_t for all t. We then write $\Omega^c_{t,R} = B_R \backslash \overline{\Omega}_t$ and $Q^c_{T,R} = \bigcup_{0<t<T}(\{t\} \times \Omega^c_{t,R})$.

Let $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ and $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$. Apart from the boundary Σ_T, we define

$$u := \widetilde{\mathcal{V}}\psi - \widetilde{\mathcal{K}}w. \tag{III.6.18}$$

From the jump relations (see Lemma III.6.4), we obtain

$$[\gamma_0 u] = -w, \quad [\gamma_1^- u] = -\psi. \tag{III.6.19}$$

Using Definition III.6.5 immediately yields

$$\frac{1}{2}\left(\begin{bmatrix}\gamma_0 u|_{Q_T} \\ \gamma_1^- u|_{Q_T}\end{bmatrix} + \begin{bmatrix}\gamma_0 u|_{Q^c_{T,R}} \\ \gamma_1^- u|_{Q^c_{T,R}}\end{bmatrix}\right) = A\begin{bmatrix}\psi \\ w\end{bmatrix}. \tag{III.6.20}$$

In view of (III.6.19) and (III.6.20), we can rewrite the bilinear form as

$$\begin{aligned}\left\langle\begin{bmatrix}\psi \\ w\end{bmatrix}, A\begin{bmatrix}\psi \\ w\end{bmatrix}\right\rangle &= \frac{1}{2}\left\langle\begin{bmatrix}\gamma_1^- u|_{Q_T} \\ \gamma_0 u|_{Q_T}\end{bmatrix} - \begin{bmatrix}\gamma_1^- u|_{Q^c_{T,R}} \\ \gamma_0 u|_{Q^c_{T,R}}\end{bmatrix}, \begin{bmatrix}\gamma_0 u|_{Q_T} \\ \gamma_1^- u|_{Q_T}\end{bmatrix} + \begin{bmatrix}\gamma_0 u|_{Q^c_{T,R}} \\ \gamma_1^- u_{Q^c_{T,R}}\end{bmatrix}\right\rangle \\ &= \langle\gamma_1^- u|_{Q_T}, \gamma_0 u|_{Q_T}\rangle - \langle\gamma_1^- u|_{Q^c_{T,R}}, \gamma_0 u|_{Q^c_{T,R}}\rangle,\end{aligned} \tag{III.6.21}$$

where we used (III.6.17).

Since u satisfies $(\partial_t - \Delta)u = 0$ in Q_T and also in $Q^c_{T,R}$, we apply Green's first formula (III.5.1) (see Lemma III.5.1) to obtain

$$\int_{Q_T} \|\nabla u\|^2 \, \mathrm{d}(\mathbf{x}, t) + d(u,u) = \langle \gamma_1^- u|_{Q_T}, \gamma_0 u|_{Q_T} \rangle,$$

while applying (III.5.4) (see Lemma III.5.5) yields

$$\int_{Q_T} \|\nabla u\|^2 \, \mathrm{d}(t, \mathbf{x}) - d(u,u) + \int_{\Omega_T} |u(T,\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} = \langle \gamma_1^- u|_{Q_T}, \gamma_0 u|_{Q_T} \rangle.$$

Adding the two expressions together gives[3]

$$\begin{aligned} \langle \gamma_1^- u|_{Q_T}, \gamma_0 u|_{Q_T} \rangle &= \int_{Q_T} \|\nabla u\|^2 \, \mathrm{d}(t, \mathbf{x}) + \frac{1}{2} \int_{\Omega_T} |u|^2 \, \mathrm{d}\mathbf{x} \\ &\geq \int_{Q_T} \|\nabla u\|^2 \, \mathrm{d}(t, \mathbf{x}). \end{aligned} \tag{III.6.22}$$

On $Q^c_{T,R}$, we obtain analogously

$$\begin{aligned} -\langle \gamma_1^- u|_{Q^c_{T,R}}, \gamma_0 u|_{Q^c_{T,R}} \rangle &= \int_{Q^c_{T,R}} \|\nabla u\|^2 \, \mathrm{d}(\mathbf{x}, t) \\ &\quad + \frac{1}{2} \int_{\Omega^c_{T,R}} |u(T,\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} - \int_0^T \int_{\partial B_R} u \partial_r u \, \mathrm{d}\sigma \mathrm{d}t, \end{aligned} \tag{III.6.23}$$

where $\partial_r u$ denotes the normal derivative of u at the boundary $(0,T) \times \partial B_R$. Inserting (III.6.22) and (III.6.23) into (III.6.21) yields

$$\left\langle \begin{bmatrix} \psi \\ w \end{bmatrix}, A \begin{bmatrix} \psi \\ w \end{bmatrix} \right\rangle \geq \int_{Q_T \cup Q^c_{T,R}} \|\nabla u\|^2 \, \mathrm{d}(\mathbf{x}, t) - \int_0^T \int_{\partial B_R} u \partial_r u \, \mathrm{d}\sigma \mathrm{d}t. \tag{III.6.24}$$

According to (III.6.18), $u|_{(0,T)\times\partial B_R}$ and $\partial_r u|_{(0,T)\times\partial B_R}$ are defined from $[w,\psi]^\intercal$ by the action of integral operators with smooth kernels. These integral operators as well as their adjoints are compact and therefore, using Young's inequality, there exists a compact operator $T_1 : \mathcal{G} \to \mathcal{G}$ such that

$$\left| \int_0^T \int_{\partial B_R} u \partial_r u \, \mathrm{d}\sigma \mathrm{d}t \right| \leq \left\langle \begin{bmatrix} \psi \\ w \end{bmatrix}, T_1 \begin{bmatrix} \psi \\ w \end{bmatrix} \right\rangle.$$

According to [Cos90], $H^{1,\frac{1}{2}}_{;0,}(Q_0)$ embeds compactly into $L^2(Q_0)$ and, therefore, also $H^{1,\frac{1}{2}}_{;0,}(Q_T)$ embeds compactly into $L^2(Q_T)$ due to the smooth mapping $\boldsymbol{\kappa}$. Then, in view of the mapping properties of $\widetilde{\mathcal{V}}$ and $\widetilde{\mathcal{K}}$ (see Lemma III.6.2 and Lemma III.6.3),

[3] At this point, it is crucial that we split the term $\langle \mathbf{V}, \mathbf{n} \rangle$ in (III.4.1) with the factor $\frac{1}{2}$. If we choose the factor differently, say λ and $1-\lambda$, we would obtain a boundary term involving $\int_0^T \int_{\Gamma_t} \langle \mathbf{V}, \mathbf{n} \rangle (\gamma_0^{\mathrm{int}} u)^2 \, \mathrm{d}\sigma \mathrm{d}t$, which would require an appropriate, not straight-forward treatment.

we obtain the existence of another compact operator $T_2\colon \mathcal{G} \to \mathcal{G}$, such that, due to the definition of the norm, we have

$$\begin{aligned}\int_{Q_T \cup Q^c_{T,R}} \|\nabla u\|^2 \,\mathrm{d}(t,\mathbf{x}) &= \|u|_{Q_T}\|^2_{H^{1,0}(Q_T)} + \|u|_{Q^c_{T,R}}\|^2_{H^{1,0}(Q^c_{T,R})} - \int_{Q_T \cup Q^c_{T,R}} |u|^2 \,\mathrm{d}(t,\mathbf{x}) \\ &= \|u|_{Q_T}\|^2_{H^{1,0}(Q_T)} + \|u|_{Q^c_{T,R}}\|^2_{H^{1,0}(Q^c_{T,R})} - \left\langle \begin{bmatrix}\psi\\ w\end{bmatrix}, T_2 \begin{bmatrix}\psi\\ w\end{bmatrix}\right\rangle.\end{aligned}$$

Due to Lemma III.6.13, the norms of $u|_{Q_T}$ in $H^{1,0}(Q_T)$ and $H^{1,\frac{1}{2}}(Q_T)$ are equivalent, and likewise those of $u|_{Q^c_{T,R}}$. Hence, (III.6.24) induces

$$\begin{aligned}\left\langle \begin{bmatrix}\psi\\ w\end{bmatrix}, A \begin{bmatrix}\psi\\ w\end{bmatrix}\right\rangle \geq \alpha \left(\|u|_{Q_T}\|^2_{H^{1,\frac{1}{2}}(Q_T)} + \|u|_{Q^c_{T,R}}\|^2_{H^{1,\frac{1}{2}}(Q^c_{T,R})} \right) \\ - \left\langle \begin{bmatrix}\psi\\ w\end{bmatrix}, (T_1 + T_2) \begin{bmatrix}\psi\\ w\end{bmatrix}\right\rangle.\end{aligned} \tag{III.6.25}$$

Using the jump relations (III.6.19) and then the trace lemmata (see Section III.2.2 and Lemma III.4.7) yields

$$\begin{aligned}\|w\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)} &= \left\|\gamma_0 u|_{Q_T} - \gamma_0 u|_{Q^c_{T,R}}\right\|_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)} \\ &\lesssim \left(\left\|u|_{Q_T}\right\|_{H^{1,\frac{1}{2}}(Q_T)} + \left\|u|_{Q^c_{T,R}}\right\|_{H^{1,\frac{1}{2}}(Q^c_{T,R})} \right)\end{aligned}$$

and similarly

$$\begin{aligned}\|\psi\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)} &= \left\|\gamma_1^- u|_{Q_T} - \gamma_1^- u|_{Q^c_{T,R}}\right\|_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)} \\ &\lesssim \left(\left\|u|_{Q_T}\right\|_{H^{1,\frac{1}{2}}(Q_T)} + \left\|u|_{Q^c_{T,R}}\right\|_{H^{1,\frac{1}{2}}(Q^c_{T,R})} \right).\end{aligned}$$

Looking at (III.6.25) we thus have the existence of a constant $\alpha > 0$ with

$$\left\langle \begin{bmatrix}\psi\\ w\end{bmatrix}, (A + T_1 + T_2) \begin{bmatrix}\psi\\ w\end{bmatrix}\right\rangle \geq \alpha \left(\|\psi\|^2_{H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)} + \|w\|^2_{H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)} \right),$$

which is the first assumption in Lemma III.6.12.

It remains to prove the positivity assumption in Lemma III.6.12. To that end, we show that the term $\int_0^T \int_{\partial B_R} u \partial_r u \,\mathrm{d}\sigma \mathrm{d}t$ in (III.6.24) goes to zero as $R \to \infty$. Let $0 < R_0 < R$ such that $\overline{\Omega}_t \subset B_{R_0}$ for all t and set $Q^c_{T,R_0} = (0,T) \times (B_{R_0} \backslash \overline{\Omega}_0)$. We can use Green's second formula from Lemma III.5.1 for $v = \widetilde{G}(T-t, \mathbf{x})$ with $(t_0, \mathbf{x}_0) \notin Q^c_{T,R_0}$. Thus, outside of Q^c_{T,R_0} for $\|\mathbf{x}\| > R_0$, the function u coincides with

$$u_0 := \widetilde{\mathcal{V}}\psi_0 - \widetilde{\mathcal{K}} w_0,$$

where the potentials take the densities on $\Sigma_{R_0} := (0,T) \times \partial B_{R_0}$ given by

$$w_0 := u|_{\Sigma_{R_0}}, \quad \psi_0 := \partial_r u|_{\Sigma_{R_0}}.$$

Since the singularity of u lies on the boundary Σ_T, the densities w_0 and ψ_0 are smooth and also the boundary Σ_{R_0} is smooth. Therefore, we can estimate

$u|_{\Sigma_R} = u_0|_{\Sigma_R}$ and $\partial_r u|_{\Sigma_R} = \partial_r u_0|_{\Sigma_R}$ for $R > R_0$ by looking at the behaviour of the fundamental solution G. Because the fundamental solution is the same for the cylindrical and the non-cylindrical case, we estimate

$$|G(t, \mathbf{x})| \leq C_\mu t^{-\mu} \|\mathbf{x}\|^{2\mu - d} \quad \text{for all } \mu \in \mathbb{R}$$

and we obtain a similar estimate for ∇G. Then, for finite T, we have

$$u = \mathcal{O}(R^{-d}), \quad \partial_r u = \mathcal{O}(R^{-d-1}) \quad \text{as } \|\mathbf{x}\| = R \to \infty.$$

Therefore, since the integrand is of order $\mathcal{O}(R^{-d-d-1})$ and the measure of the boundary ∂B_R is of order $\mathcal{O}(R^{d-1})$, we obtain

$$\int_0^T \int_{\partial B_R} u \partial_r u \, \mathrm{d}\sigma \mathrm{d}t = \mathcal{O}(R^{-d-2}) \to 0 \quad \text{as } \|\mathbf{x}\| = R \to \infty.$$

Since the left-hand side in (III.6.24) is independent of R, we can conclude that

$$\lim_{R \to \infty} \int_{Q^c_{T,R}} \|\nabla u\|^2 \, \mathrm{d}(t, \mathbf{x})$$

is finite and

$$\left\langle \begin{bmatrix} \psi \\ w \end{bmatrix}, A \begin{bmatrix} \psi \\ w \end{bmatrix} \right\rangle \geq \int_{(0,T) \times (\mathbb{R}^d \setminus \Gamma_t)} \|\nabla u\|^2 \, \mathrm{d}(t, \mathbf{x}).$$

Assume that the right-hand side vanishes. Then, since u is smooth enough, we obtain that $u(t, \cdot)$ is constant on Ω_t and $\mathbb{R}^d \setminus \overline{\Omega}_t$ for every $t \in (0, T)$. Since $u = 0$ on Ω_0, we thus obtain that $u \equiv 0$ on $(0, T) \times \mathbb{R}^d$. From the jump relations (III.6.19), we obtain $w = 0$ and $\psi = 0$. This implies the positivity assumption (III.6.17) of Lemma III.6.12 and the claim in the theorem follows immediately. □

Having the main result Theorem III.6.11 at hand, we can state a few corollaries along the lines of [Cos90, Corollary 3.13, Corollary 3.14, Remark 3.15, Corollary 3.16, Corollary 3.17].

Corollary III.6.14. *The single layer operator*

$$\mathcal{V} \colon H^{-\frac{1}{2}, -\frac{1}{4}}(\Sigma_T) \to H^{\frac{1}{2}, \frac{1}{4}}(\Sigma_T)$$

is an isomorphism and there exists $\alpha > 0$ such that

$$\langle \mathcal{V}\psi, \psi \rangle \geq \alpha \|\psi\|^2_{H^{-\frac{1}{2}, -\frac{1}{4}}(\Sigma_T)} \quad \textit{for all } \psi \in H^{-\frac{1}{2}, -\frac{1}{4}}(\Sigma_T). \tag{III.6.26}$$

The hypersingular operator

$$\mathcal{D} \colon H^{\frac{1}{2}, \frac{1}{4}}(\Sigma_T) \to H^{-\frac{1}{2}, -\frac{1}{4}}(\Sigma_T)$$

is an isomorphism and there exists $\alpha > 0$ such that

$$\langle \mathcal{D}w, w \rangle \geq \alpha \|w\|^2_{H^{\frac{1}{2}, \frac{1}{4}}(\Sigma_T)} \quad \textit{for all } w \in H^{\frac{1}{2}, \frac{1}{4}}(\Sigma_T). \tag{III.6.27}$$

Proof. As in the proof of [Cos90, Corollary 3.13], the coercivity estimates (III.6.26) and (III.6.27) result from Theorem III.6.11 by using the special cases $w = 0$ and $\psi = 0$, respectively. In view of the continuity of $\mathcal{V}$ and $\mathcal{D}$, this leads to the invertibility of the operators. □

Corollary III.6.15. *The operators*

$$\begin{aligned}\frac{1}{2}\operatorname{id}+\mathcal{K},\quad \frac{1}{2}\operatorname{id}-\mathcal{K}\colon H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T) \to H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T),\\ \frac{1}{2}\operatorname{id}+\mathcal{K}',\quad \frac{1}{2}\operatorname{id}-\mathcal{K}'\colon H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T) \to H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)\end{aligned}$$

are isomorphisms.

Proof. We again follow the proof of [Cos90, Corollary 3.14] directly. From the projection property (III.6.15), more specifically from (III.6.16), we obtain

$$\begin{aligned}\left(\frac{1}{2}\operatorname{id}+\mathcal{K}\right)\left(\frac{1}{2}\operatorname{id}-\mathcal{K}\right) &= \mathcal{V}\mathcal{D},\\ \left(\frac{1}{2}\operatorname{id}+\mathcal{K}'\right)\left(\frac{1}{2}\operatorname{id}-\mathcal{K}'\right) &= \mathcal{W}\mathcal{V}.\end{aligned}$$

Since the right-hand sides are isomorphisms, we immediately arrive at the claim. □

Remark III.6.16. *The other two relations gained from* (III.6.16) *lead to*

$$\mathcal{V}^{-1}\mathcal{K}\mathcal{V} = \mathcal{K}' = \mathcal{D}\mathcal{K}\mathcal{D}^{-1}.$$

Corollary III.6.17. *The unique solution $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ of the Dirichlet problem*

$$\begin{aligned}(\partial_t - \Delta)u &= 0 \qquad \text{in } Q_T,\\ \gamma_0 u &= g \qquad \text{on } \Sigma_T,\end{aligned}$$

with $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ can be represented

(i) as $u = \widetilde{\mathcal{V}}\psi - \widetilde{\mathcal{K}}g$, where $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ is the unique solution of the first kind integral equation

$$\mathcal{V}\psi = \left(\frac{1}{2}\operatorname{id}+\mathcal{K}\right)g.$$

(ii) as $u = \widetilde{\mathcal{V}}\psi - \widetilde{\mathcal{K}}g$, where $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ is the unique solution of the second kind integral equation

$$\left(\frac{1}{2}\operatorname{id}-\mathcal{K}'\right)\psi = \mathcal{D}g.$$

(iii) as $u = \widetilde{\mathcal{V}}\psi$, where $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ is the unique solution of the first kind integral equation

$$\mathcal{V}\psi = g.$$

(iv) as $u = \widetilde{\mathcal{K}}w$, where $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ is the unique solution of the second kind integral equation

$$\left(\frac{1}{2}\operatorname{id}-\mathcal{K}\right)w = -g.$$

In (i) and (ii), it particularly holds $\psi = \gamma_1^- u$ *on* Σ_T.

Proof. We can use directly the idea of the proof of [Cos90, Corollary 3.16], which are the uniqueness results from above and the jump relations given in Lemma III.6.7. □

Corollary III.6.18. *The unique solution* $u \in H^{1,\frac{1}{2}}_{;0,}(Q_T)$ *of the Neumann problem*

$$\begin{aligned} (\partial_t - \Delta)u &= 0 \qquad \text{in } Q_T, \\ \gamma_1^- u &= h \qquad \text{on } \Sigma_T, \end{aligned}$$

with $h \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ *can be represented*

(i) as $u = \widetilde{\mathcal{V}}h - \widetilde{\mathcal{K}}w$, *where* $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ *is the unique solution of the second kind integral equation*

$$\left(\frac{1}{2}\,\mathrm{id} + \mathcal{K}\right) w = \mathcal{V}h.$$

(ii) as $u = \widetilde{\mathcal{V}}h - \widetilde{\mathcal{K}}w$, *where* $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ *is the unique solution of the first kind integral equation*

$$\mathcal{D}w = \left(\frac{1}{2}\,\mathrm{id} - \mathcal{K}'\right) h.$$

(iii) as $u = \widetilde{\mathcal{V}}\psi$, *where* $\psi \in H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$ *is the unique solution of the second kind integral equation*

$$\left(\frac{1}{2}\,\mathrm{id} + \mathcal{K}'\right) \psi = h.$$

(iv) as $u = \widetilde{\mathcal{K}}w$, *where* $w \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma_T)$ *is the unique solution of the first kind integral equation*

$$\mathcal{D}w = -h.$$

In (i) and (ii), we have that $w = \gamma_0 u$ *on* Σ_T.

Proof. The proof follows by the same arguments as in the proof of [Cos90, Corollary 3.17], which is similar to the respective proof for the Dirichlet problem. □

III.7 Conclusion

We considered the heat equation on a time-varying (so-called non-cylindrical) domain. In contrast to the problem on a cylindrical domain, we used a modified Neumann trace operator containing a term which is dependent on the velocity of the moving surface. We were able to show the mapping properties of the layer operators by following the proofs of Costabel [Cos90]. To this end, we heavily used the fact that the non-cylindrical domain is a mapped cylindrical domain. Then, using mapped anisotropic Sobolev spaces, we obtain analogous mapping properties and are also able to prove existence and uniqueness of solutions of the Dirichlet and of the Neumann problem.

Chapter IV

Shape Calculus

In this chapter, we will discuss the *time-dependent* shape calculus. We recall preliminary theoretical results from the literature [DZ99b, DZ01, MZ06] and supplement some proofs which seem to be missing therein, need additional clarification or are valuable for the understanding. Moreover, we give some new general formulae which to the best of our knowledge cannot be found in the literature so far. As the literature is not concise when considering functionals over a boundary, we clarify upon this matter and present the appropriate formulae.

IV.1 Generation and perturbation of a tube

Recall from Section III.1, especially (III.1.1), that we consider a non-cylindrical domain Q_T, called tube, given by

$$Q_T = \bigcup_{0<t<T} (\{t\} \times \Omega_t),$$

where $\Omega_t \subset \mathbb{R}^d$ is a spatial domain at time t. Its lateral boundary is denoted by Σ_T, compare (III.1.2). It is reasonable to require certain properties of such a tube, such as the continuity of its lateral boundary. The precise requirements are discussed in the following. One of the difficulties during shape calculus, and later in shape optimization, is that we need an automated process for the generation of such tubes.

The generation of a tube can be accomplished from an Eulerian or a Lagrangian point of view. In the Eulerian setting, one considers a velocity field $\mathbf{V}$ generating the tube, while in the Lagrangian setting, one considers a parametrization of the tube. The framework of this section also allows the perturbation of tubes in both settings, which will enable us to compute directional derivatives, i.e., shape gradients. Notice that in the *time-independent* setting, the shape gradients are independent of the chosen paradigm, whereas the shape Hessians can differ, see [DZ91].

In the following, we will first introduce the two concepts, relate them and comment upon their use in numerical applications.

IV.1.1 Two paradigms to generate tubes

Let us recall that in the Reynolds' transport theorem, see Lemma III.4.3, a velocity field $\mathbf{V}$ in normal direction $\mathbf{n}$ appears. This velocity field can be used to describe how an individual particle gets moved throughout time when being exposed to $\mathbf{V}$. We call this movement the *pathline*. Hence, if we would inject a drop of dye at a certain point and time and do a time-lapse photography, we would see the pathline [SA08]. This relation is described by the ordinary differential equation, see [Zol79, p. 6],

$$\begin{aligned} \frac{\partial \mathbf{T}}{\partial t}(t,\mathbf{x}) &= \mathbf{V}\big(t,\mathbf{T}(t,\mathbf{x})\big) && \text{in } [0,T]\times\mathbb{R}^d, \\ \mathbf{T}(0,\mathbf{x}) &= \mathbf{x} && \text{in } \mathbb{R}^d, \end{aligned} \tag{IV.1.1}$$

which under certain smoothness assumptions has a unique solution, compare [DZ01, Proposition 2.1]. Its solution $\mathbf{T}(t,\cdot)\colon \mathbf{x}\mapsto \mathbf{x}_t = \mathbf{T}(t,\mathbf{x})$ describes the trajectory a fixed point $\mathbf{x}$ takes. The point $\mathbf{x}$ can be thought of as the Lagrangian (or material) coordinate, while $\mathbf{x}_t$ is the Eulerian (field) coordinate, see [SZ92, p. 49] and [OF03, Section 3.1]. Notice that for fixed t the homeomorphism

$$\mathbf{x}\mapsto \mathbf{T}(t,\mathbf{x})\colon \mathbb{R}^d\to\mathbb{R}^d$$

is an operator which maps the initial position to a position at a certain time t and is dependent on $\mathbf{V}$. To clarify this association, we also write $\mathbf{T}=\mathbf{T}_{\mathbf{V}}$.

From the considerations above we see that we can on the one hand start with a velocity field $\mathbf{V}$ and use it to generate a mapping $\mathbf{T}$. On the other hand, we can start with a mapping $\mathbf{T}$ from which a velocity field $\mathbf{V}$ can be computed. In the sequel, we make the relation between the two approaches more rigorous. For fixed t, let us denote by

$$\mathbf{x}_t\mapsto \mathbf{T}^{-1}(t,\mathbf{x}_t)\colon \mathbb{R}^d\to\mathbb{R}^d$$

the operator which maps the position at a time t to the initial position. We make the following assumption for the vector field $\mathbf{V}$.

Assumption IV.1.1. *We assume that for all $\mathbf{X}\in\mathbb{R}^d$ and $\mathbf{V}(\cdot,\mathbf{X})\in C^0\big([0,T];\mathbb{R}^d\big)$, there exists a $c>0$ such that for all $\mathbf{X},\mathbf{Y}\in\mathbb{R}^d$ it holds*

$$\|\mathbf{V}(\cdot,\mathbf{Y})-\mathbf{V}(\cdot,\mathbf{X})\|_{C^0\left([0,T];\mathbb{R}^d\right)}\le c\|\mathbf{Y}-\mathbf{X}\|.$$

We have the following equivalence result, see [DZ91, Theorem 2.1], [DZ92, Theorem 2.1] or [DZ11, Chapter 4, Theorem 4.1].

Theorem IV.1.2. *(i) Under Assumption IV.1.1 on $\mathbf{V}$, the map $\mathbf{T}$ from (IV.1.1) has the following three properties*

- *For all $\mathbf{x}\in\mathbb{R}^d$ it holds $\mathbf{T}(\cdot,\mathbf{x})\in C^1\big([0,T];\mathbb{R}^d\big)$. Moreover, there exists $c>0$, such that for all $\mathbf{x},\mathbf{y}\in\mathbb{R}^d$ it holds*

$$\|\mathbf{T}(\cdot,\mathbf{x})-\mathbf{T}(\cdot,\mathbf{y})\|_{C^1\left([0,T];\mathbb{R}^d\right)}\le c\|\mathbf{x}-\mathbf{y}\|.$$

- *For all $t\in[0,T]$ the map $\mathbf{x}\mapsto\mathbf{T}(t,\mathbf{x})\colon\mathbb{R}^d\to\mathbb{R}^d$ is bijective.*
- *For all $\mathbf{X}\in\mathbb{R}^d$ it holds $\mathbf{T}^{-1}(\cdot,\mathbf{X})\in C^0\big([0,T];\mathbb{R}^d\big)$. Moreover, there exists $c>0$ such that for all $\mathbf{X},\mathbf{Y}\in\mathbb{R}^d$ it holds*

$$\|\mathbf{T}^{-1}(\cdot,\mathbf{Y})-\mathbf{T}^{-1}(\cdot,\mathbf{X})\|_{C^0\left([0,T];\mathbb{R}^d\right)}\le c\|\mathbf{Y}-\mathbf{X}\|.$$

(ii) If there exists a $T \in \mathbb{R}$, $T > 0$, and a map $\mathbf{T}\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ satisfying the three properties in (i) above, then the map

$$(t, \mathbf{X}) \mapsto \mathbf{V}(t, \mathbf{X}) = \frac{\partial \mathbf{T}}{\partial t}\big(t, \mathbf{T}^{-1}(t, \mathbf{X})\big)\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d, \tag{IV.1.2}$$

satisfies Assumption IV.1.1. If additionally $\mathbf{T}(0,\cdot) = \mathrm{id}$, then $\mathbf{T}(\cdot, \mathbf{x})$ is the solution of (IV.1.1) for that $\mathbf{V}$.

Theorem IV.1.2 thus states that we can either consider velocity fields $\mathbf{V}$ satisfying Assumption IV.1.1 or transformations $\mathbf{T}$ satisfying the three properties mentioned in Theorem IV.1.2. When starting from $\mathbf{V}$, we obtain the *speed method* (also called *velocity method*), see Figure IV.2 on the top. The speed method allows for larger deformations and is favourable in an Eulerian setting. For a given initial domain Ω_0, we obtain a perturbed domain Ω_t by setting

$$\Omega_t = \mathbf{T}_{\mathbf{V}}(t, \Omega_0) = \big\{\mathbf{T}_{\mathbf{V}}(t, \mathbf{x})\colon \mathbf{x} \in \Omega_0\big\}.$$

When starting from $\mathbf{T}$, we actually consider a parametrization of the tube. In the following, we will thus retreat to the case where $\mathbf{T} = \boldsymbol{\kappa}$, where $\boldsymbol{\kappa}$ was introduced in Section III.1. The above description of generating a tube Q_T via a parametrization $\boldsymbol{\kappa}$ is displayed in Figure IV.1 on the top. We can associate to $\boldsymbol{\kappa}$ a velocity field $\mathbf{V}$ by considering (IV.1.2) for $\boldsymbol{\kappa}$ which in this case reads

$$\mathbf{V} = \partial_t \boldsymbol{\kappa} \circ \boldsymbol{\kappa}^{-1}. \tag{IV.1.3}$$

Remark IV.1.3. *We emphasize that the two paradigms of this section both correspond to a very specific setting for the description of the time-space domain. In particular, the space time domain always has the form (III.1.1), where Ω_t can be mapped to Ω_0 by a continuous homeomorphism.*

IV.1.2 Geometric properties of the tube

Let us denote the spatial normal to the domain $\Omega_t \subset \mathbb{R}^d$ by $\mathbf{n}$ and the time-space normal by $\boldsymbol{\nu}$. Moreover, by ∇, we denote the spatial gradient

$$\nabla = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_d}\right]^{\mathsf{T}},$$

while $\vec{\nabla}$ denotes the time-space nabla operator

$$\vec{\nabla} = \left[\frac{\partial}{\partial t}, \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_d}\right]^{\mathsf{T}}.$$

The time-space normal can be written as

$$\boldsymbol{\nu} = \frac{1}{\sqrt{1 + v_\nu^2}} \begin{bmatrix} v_\nu \\ \mathbf{n} \end{bmatrix} \tag{IV.1.4}$$

for some appropriate $v_\nu \in \mathbb{R}$. More precisely, there exists the following connection between v_ν and the vector field $\mathbf{V}$ generating the tube as described in Section IV.1.1, see [DZ99a, DZ99b, DZ01].

Lemma IV.1.4. *For the vector field* $\mathbf{V}$*, which generates the tube* Q_T*, it holds*

$$\langle \mathbf{V}, \mathbf{n} \rangle = -v_\nu,$$

where v_ν *is the temporal component of the unnormalized time-space normal* (IV.1.4).

Proof. Since to the best of our knowledge, no proof is given in the relevant literature, we show the claim in the following. Let us consider a parametrization $\vec{\boldsymbol{\kappa}}\colon \mathbb{R}^{1+d} \to \mathbb{R}^{1+d}$ of the tube Q_T given by

$$\vec{\boldsymbol{\kappa}}(t, \mathbf{u}) = \begin{bmatrix} t \\ \boldsymbol{\kappa}(t, \mathbf{u}) \end{bmatrix},$$

where $\boldsymbol{\kappa}\colon \mathbb{R}^d \to \mathbb{R}^d$ with $\boldsymbol{\kappa}(t, \Gamma_0) = \Gamma_t$, compare Section III.1 and Section IV.1. From Lemma II.2.7, we can write

$$\boldsymbol{\nu} \circ \vec{\boldsymbol{\kappa}} = \frac{(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0}{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|}, \tag{IV.1.5}$$

where $\boldsymbol{\nu}_0$ denotes the time-space normal on $\Sigma_0 = (0, T) \times \Gamma_0$ and thus corresponds to $\left[\begin{smallmatrix} 0 \\ \mathbf{n}_0 \end{smallmatrix}\right]$. In here, $\mathbf{n}_0$ is the spatial normal to Ω_0. Moreover, we have

$$\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}} = \begin{bmatrix} 1 & \mathbf{0}^\intercal \\ \partial_t \boldsymbol{\kappa} & \mathrm{D}\boldsymbol{\kappa} \end{bmatrix},$$

where $\mathbf{0}$ is the zero vector in $\mathbb{R}^d$. Inserting the inverse

$$(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-1} = \begin{bmatrix} 1 & \mathbf{0}^\intercal \\ -(\mathrm{D}\boldsymbol{\kappa})^{-1}\partial_t \boldsymbol{\kappa} & (\mathrm{D}\boldsymbol{\kappa})^{-1} \end{bmatrix}.$$

into (IV.1.5) yields

$$\boldsymbol{\nu} \circ \vec{\boldsymbol{\kappa}} = \frac{1}{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|} \begin{bmatrix} -(\partial_t \boldsymbol{\kappa})^\intercal (\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0 \\ (\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0 \end{bmatrix}.$$

From Lemma II.2.7, we obtain

$$(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0 = \mathbf{n} \circ \boldsymbol{\kappa} \big\|(\mathrm{D}\boldsymbol{\kappa})^{\intercal}\mathbf{n}_0\big\|,$$

and therefore

$$\boldsymbol{\nu}\big(t, \boldsymbol{\kappa}(\cdot,\cdot)\big) = \frac{\big\|(\mathrm{D}\,\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0\big\|}{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|} \begin{bmatrix} -(\partial_t \boldsymbol{\kappa})^\intercal \mathbf{n} \circ \boldsymbol{\kappa} \\ \mathbf{n} \circ \boldsymbol{\kappa} \end{bmatrix}.$$

Using (IV.1.3) and the fact that $\boldsymbol{\kappa}$ is bijective gives

$$\boldsymbol{\nu} = \frac{\big\|(\mathrm{D}\,\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0\big\|}{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|} \begin{bmatrix} -\langle \mathbf{V}, \mathbf{n} \rangle \\ \mathbf{n} \end{bmatrix} = \frac{1}{\sqrt{\langle \mathbf{V}, \mathbf{n} \rangle^2 + 1}} \begin{bmatrix} -\langle \mathbf{V}, \mathbf{n} \rangle \\ \mathbf{n} \end{bmatrix}, \tag{IV.1.6}$$

from where the claim follows directly by comparison with (IV.1.4). ☐

IV.1.3 Perturbation of a tube generated via a parametrization

As our goal in shape calculus is to compute directional derivatives, we need to perturb the tube in a certain direction. In a Lagrangian setting, where the tube is generated by the bijective mapping $\boldsymbol{\kappa}$ from (III.1.3), the perturbation of identity is the method of choice, see [MZ06]. The perturbation of identity yields a new tube (see Figure IV.1) via

$$Q_T^s = \bigcup_{0<t<T} \left(\{t\} \times (\mathrm{id} + s\mathbf{Z})(\Omega_t) \right)$$

for a vector field $\mathbf{Z}(t, \mathbf{x}) \in \mathbb{R}^d$ and s small enough. We denote $\Omega_{t,s} := (\mathrm{id} + s\mathbf{Z})(\Omega_t)$. Notice that the perturbations under consideration are horizontal, meaning that we consider perturbations of $(t, \boldsymbol{\kappa})$ in the direction $\left[\begin{smallmatrix} 0 \\ \mathbf{Z} \end{smallmatrix}\right]$, compare [MZ06]. Moreover, $\mathrm{id} + s\mathbf{Z}$ should satisfy a uniformity condition as in (III.1.4).

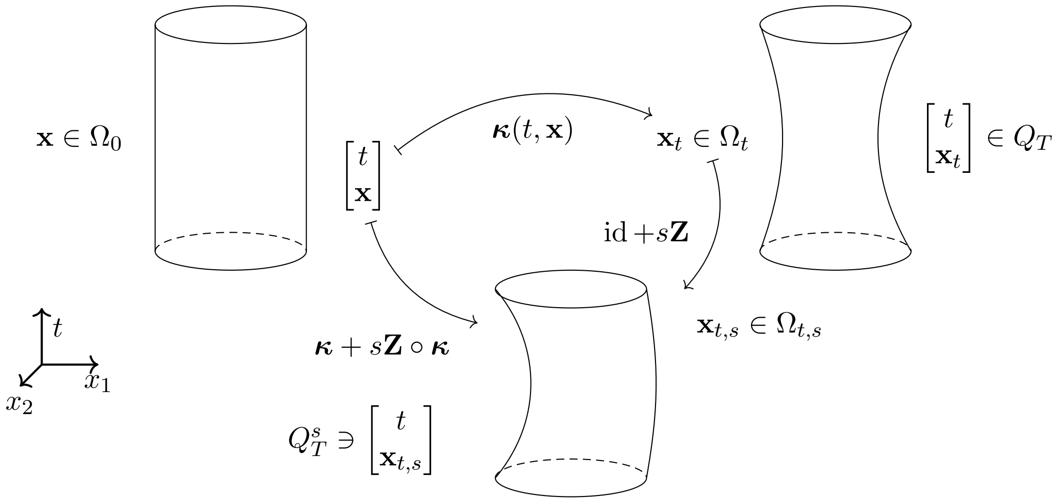


Figure IV.1: Perturbation of identity in the Lagrangian setting.

IV.1.4 Perturbation of a tube generated via the speed method

The shape calculus in the Eulerian setting is formulated for example in [DZ01] and [MZ06]. Let us consider a tube $Q_T^{\mathbf{V}}$ generated by a vector field $\mathbf{V}$. To obtain a perturbed tube $Q_T^{\mathbf{V}+s\mathbf{W}}$, we perturb the vector field $\mathbf{V}$ by considering $\mathbf{V} + s\mathbf{W}$. To that end, we consider for every point of time $t \in [0, T]$ and s small enough the domain

$$\Omega_{t,s} = \mathbf{T}_{\mathbf{V}+s\mathbf{W}}(t, \Omega_0),$$

see Figure IV.2. By setting

$$\boldsymbol{\mathcal{T}}_s = \mathbf{T}_{\mathbf{V}+s\mathbf{W}} \circ (\mathbf{T}_{\mathbf{V}})^{-1},$$

where the composition acts only on the spatial component, we can directly map Ω_t onto $\Omega_{t,s}$. We can again associate a vector field to this map by setting

$$\boldsymbol{\mathcal{Z}}_t(s, \cdot) = \left(\frac{\mathrm{d}}{\mathrm{d}s} \boldsymbol{\mathcal{T}}_s \right) \circ (\boldsymbol{\mathcal{T}}_s)^{-1}, \tag{IV.1.7}$$

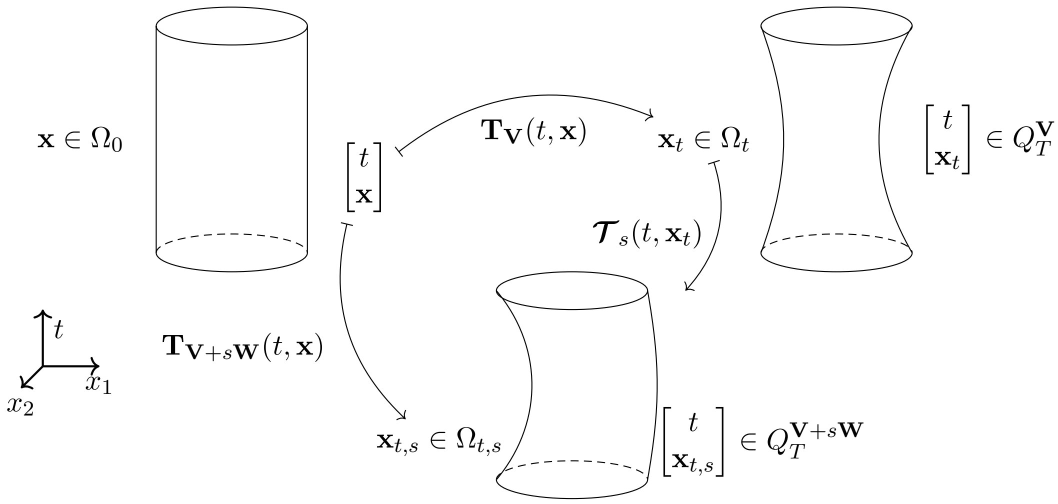


Figure IV.2: Perturbation of the tube in the Eulerian setting.

see Theorem IV.1.2. Since for the shape differentiability we consider $s \to 0$, we define $\mathbf{Z}(t, \mathbf{x}_t) = \boldsymbol{\mathcal{Z}}_t(0, \mathbf{x}_t)$. This vector field, called the transverse field, is characterized by the following differential equation, see [DZ01, Theorem 3.2],

$$\begin{aligned} \partial_t \mathbf{Z} + [\mathbf{Z}, \mathbf{V}] &= \mathbf{W} \qquad && \text{in } [0, T] \times D, \\ \mathbf{Z}(0, \cdot) &= 0 && \text{in } D, \end{aligned} \tag{IV.1.8}$$

where $[\cdot, \cdot]$ denote the Lie brackets $[\mathbf{Z}, \mathbf{V}] = \mathrm{D}\mathbf{Z}\mathbf{V} - \mathrm{D}\mathbf{V}\mathbf{Z}$ and $D \subset \mathbb{R}^d$ denotes the hold-all.

IV.2 Definitions of time-dependent shape calculus

In the following, we will focus on the case where the tube is generated by a parametrization and perturbed with a perturbation of identity. We comment in Section IV.4 on the case when the tube is generated by a vector field.

We define the space of admissible perturbation fields as

$$\mathcal{Z}_{\text{ad}} := \left\{ \mathbf{Z} \in C^2\big((0, T) \times D\big) \right\} \tag{IV.2.1}$$

and consider a perturbation field $\mathbf{Z} \in \mathcal{Z}_{\text{ad}}$. In here, D denotes the hold-all.

The Eulerian derivative of a functional $J(Q_T)$ in a direction $\mathbf{Z}$ is defined as follows, see [MZ06, p. 14] or [SZ92, Definition 2.19 and Definition 2.20, p. 54].

Definition IV.2.1. *The Eulerian derivative of a functional $J(Q_T)$ in a direction $\mathbf{Z} \in \mathcal{Z}_{ad}$ at Q_T is defined as*

$$\nabla J(Q_T)[\mathbf{Z}] := \lim_{s \searrow 0} \frac{J(Q_T^s) - J(Q_T)}{s}.$$

$J(Q_T)$ is called shape differentiable if the limit exists for all directions $\mathbf{Z} \in \mathcal{Z}_{ad}$ and if $\mathbf{Z} \mapsto \nabla J(Q_T)[\mathbf{Z}]$ is a linear and continuous mapping, thus in $\mathcal{Z}'_{ad}$.

Let $v_{t,s}$ denote a state computed on the perturbed domain Q_T^s and v_t the state computed on Q_T. Thus, the state inherently depends on the domain. According to [MZ06, Definition 6.1 and Definition 6.2, p. 166], we have the following two definitions of shape sensitivities.

Definition IV.2.2. *The* material derivative $\dot{v}[\mathbf{Z}]$ *at* $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ *in the direction* $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ *is defined as*

$$\dot{v}[\mathbf{Z}] = \lim_{s \searrow 0} \frac{v_{t,s} \circ (\mathrm{id} + s\mathbf{Z}) - v_t}{s}.$$

Definition IV.2.3. *The* local shape derivative *at* $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ *in the direction* $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ *is formally given by*

$$\delta v[\mathbf{Z}](t, \mathbf{x}) = \lim_{s \searrow 0} \frac{v_{t,s}(t, \mathbf{x}) - v_t(t, \mathbf{x})}{s}, \quad (t, \mathbf{x}) \in Q_T^s \cap Q_T.$$

Notice that the material derivative and the local shape derivative are connected via ([MZ06, Remark 6.2, p. 166])

$$\dot{u}[\mathbf{Z}] = \delta u[\mathbf{Z}] + \langle \nabla u, \mathbf{Z} \rangle, \tag{IV.2.2}$$

and thus the local shape derivative can also be defined rigorously by (IV.2.2).

Remark IV.2.4. *Since the local shape derivative acts only on the inherent dependency on the shape, it interchanges with coordinate derivatives in space and time. This is in contrast to the material derivative, which does not interchange with coordinate derivatives. More specifically, we have*

$$(\dot{\nabla u})[\mathbf{Z}] = \nabla\big(\dot{u}[\mathbf{Z}]\big) - (\mathrm{D}\mathbf{Z})^{\intercal} \nabla u, \tag{IV.2.3}$$

since with (IV.2.2) *we obtain*

$$(\dot{\nabla u})[\mathbf{Z}] = \delta(\nabla u)[\mathbf{Z}] + \mathrm{D}^2 u \mathbf{Z}$$

which yields together with the product rule

$$\nabla\big((\nabla u)^{\intercal} \mathbf{Z}\big) = \mathrm{D}^2 u \mathbf{Z} + (\mathrm{D}\mathbf{Z})^{\intercal} \nabla u$$

and interchanging of local and coordinate derivative the expression

$$(\dot{\nabla u})[\mathbf{Z}] = \nabla\big(\delta u[\mathbf{Z}]\big) + \nabla\big((\nabla u)^{\intercal} \mathbf{Z}\big) - (\mathrm{D}\mathbf{Z})^{\intercal} \nabla u$$

from where (IV.2.3) *follows by using again* (IV.2.2).

IV.3 Hadamard structure theorem

For the *time-independent* shape calculus, we have the so-called *Hadamard formula*, which states how the structure of the shape derivative of a functional J looks like. Its key message is that only boundary variations in normal direction are relevant for the shape gradient, see [MZ06, p. 15], [DZ11, Chapter 9, Corollary 1, p. 480] or [SZ92, Theorem 2.27, p. 59]. Intuitively this makes sense, since perturbations in tangential direction do not alter the shape. Let us consider a domain $\Omega \subset D$ with boundary Γ and normal $\mathbf{n}$, where D denotes the hold-all.

The following theorem gives the so-called *Hadamard formula*.

Theorem IV.3.1. *Let the functional $J(\Omega)$ be shape differentiable at every domain $\Omega \subset D$ of class C^{k+1}, $k \geq 0$. Suppose the shape gradient $\nabla J(\Omega)$ is in $\big(C_0^k(\Omega;\mathbb{R}^d)\big)'$. Then, there exists a scalar distribution $\mathfrak{g}(\Gamma) \in \big(C^k(\Gamma)\big)'$ such that the shape gradient in the direction $\mathbf{V}$ can be represented as*

$$\nabla J(\Omega)[\mathbf{V}] = \Big\langle \mathfrak{g}(\Gamma), \big\langle \gamma_0(\mathbf{V}), \mathbf{n} \big\rangle \Big\rangle_{(C^k(\Gamma))' \times C^k(\Gamma)}$$

for all $\mathbf{V} \in C_0^k(\overline{D};\mathbb{R}^d)$.

Remark IV.3.2. *If $\mathfrak{g}(\Gamma) \in L^1(\Gamma)$, then the directional derivative can be written as*

$$\nabla J(\Omega)[\mathbf{V}] = \int_\Gamma \mathfrak{g}(\Gamma) \big\langle \gamma_0(\mathbf{V}), \mathbf{n} \big\rangle \,\mathrm{d}\sigma.$$

In the *time-dependent* setting, we only consider horizontal perturbations of the form $\left[\begin{smallmatrix} 0 \\ \mathbf{Z} \end{smallmatrix}\right]$ and thus we do not perturb in time direction. Therefore, we can apply the Hadamard structure theorem for every point of time, given that we have a smooth spatial domain.

IV.4 Connection between the speed method and the perturbation of identity

For illustrative purposes, we recall how the speed method and the perturbation of identity are connected by following [MZ06, p. 175ff.]. Based on this comparison, we argue that the perturbation of identity is the more suitable setting for our numerical considerations, see Remark IV.4.3.

To elaborate the connection of the shape gradients for functionals depending on tubes generated by one of the two paradigms, let us consider a functional

$$\begin{aligned} J \colon \mathcal{A} &\to \mathbb{R}, \\ Q_T &\mapsto J(Q_T), \end{aligned}$$

where $\mathcal{A}$ is the space of admissible tubes. We parametrize the tube in a Lagrangian setting by using the parametrization $\boldsymbol{\kappa}$ (see Figure IV.1), thus we define $j_l = J \circ \boldsymbol{\kappa}$, and write $j_l(\boldsymbol{\kappa}) = J(Q_T)$. On the other hand, we can use velocity fields $\mathbf{V}$ to generate a tube via the associated mapping $\mathbf{T} = \mathbf{T_V}$ (see Figure IV.2), which we denote by $Q_T^{\mathbf{V}}$. We define $j_e = J \circ \mathbf{T_V}$, and write $j_e(\mathbf{V}) = J(Q_T^{\mathbf{V}})$, see [MZ06, p. 175ff.].

Remark IV.4.1. *Notice that we have in complete analogy to Definition IV.2.1*

$$\nabla J(Q_T^{\mathbf{V}})[\mathbf{W}] = \lim_{s \searrow 0} \frac{J(Q_T^{\mathbf{V}+s\mathbf{W}}) - J(Q_T^{\mathbf{V}})}{s},$$

where $Q_T^{\mathbf{V}}$ emphasizes that the tube is generated by the speed method by using the vector field $\mathbf{V}$ instead of a parametrization.

According to [MZ06, Theorem 6.4], the two points of view are related as follows.

Theorem IV.4.2. *The differentiability of the functional j_l at $\boldsymbol{\kappa}$ in the direction $\mathbf{Z} \circ \boldsymbol{\kappa}$ is equivalent to the differentiability of j_e at $\mathbf{V}$ in the direction $\mathbf{W}$ with $\mathbf{V} = \partial_t \boldsymbol{\kappa} \circ \boldsymbol{\kappa}^{-1}$, $\mathbf{W} = \partial_t(\mathbf{Z} \circ \boldsymbol{\kappa}) \circ \boldsymbol{\kappa}^{-1} - \mathrm{D}\mathbf{V}\mathbf{Z}$, and $\mathbf{Z}$ corresponding to the transverse field introduced in Section IV.1.4. The respective functional derivatives coincide, i.e. it holds*

$$\nabla J(\boldsymbol{\kappa})[\mathbf{Z} \circ \boldsymbol{\kappa}] =: \nabla j_l(\boldsymbol{\kappa})[\mathbf{Z} \circ \boldsymbol{\kappa}] = \nabla j_e(\mathbf{V})[\mathbf{W}].$$

Proof. We repeat the proof of [MZ06, Theorem 6.4] in the hope that the reader will benefit from a clearer structure and eliminated typos. As already stated in (IV.1.3), if we set $\mathbf{V} = \partial_t \boldsymbol{\kappa} \circ \boldsymbol{\kappa}^{-1}$, we have that $\boldsymbol{\kappa} = \mathbf{T}_{\mathbf{V}}$ (see also Lemma IV.1.2). We use the chain rule to compute

$$\begin{aligned}\nabla j_e(\mathbf{V})[\mathbf{W}] &= \nabla(J \circ \mathbf{T})(\mathbf{V})[\mathbf{W}] \\ &= \nabla J\big(\mathbf{T}(\mathbf{V})\big)\big[\nabla \mathbf{T}(\mathbf{V})[\mathbf{W}]\big].\end{aligned}$$

To arrive at the claim of the theorem, we would need

$$\nabla \mathbf{T}(\mathbf{V})[\mathbf{W}] = \mathbf{Z} \circ \mathbf{T}(\mathbf{V}).$$

We let $\mathbf{Z}$ coincide with the transverse field in the Eulerian setting, since from (IV.1.7) we have

$$\begin{aligned}\mathcal{Z}_t(0) &= \partial_s \mathbf{T}_{\mathbf{V}+s\mathbf{W}} \circ (\mathbf{T}_{\mathbf{V}})^{-1}|_{s=0} \\ &= \nabla \mathbf{T}(\mathbf{V})[\mathbf{W}] \circ \big(\mathbf{T}(\mathbf{V})\big)^{-1},\end{aligned}$$

and thus

$$\mathbf{Z} \circ \mathbf{T}(\mathbf{V}) = \nabla \mathbf{T}(\mathbf{V})[\mathbf{W}].$$

It remains to compute the expression for $\mathbf{W}$. In (IV.1.8), $\mathbf{Z}$ is characterized in terms of $\mathbf{W}$. We therefore have

$$\mathbf{W} = \partial_t \mathbf{Z} + \mathrm{D}\mathbf{Z}\mathbf{V} - \mathrm{D}\mathbf{V}\mathbf{Z}.$$

We can rewrite this by using the chain rule in the expression

$$\begin{aligned}\partial_t(\mathbf{Z} \circ \boldsymbol{\kappa}) \circ \boldsymbol{\kappa}^{-1} &= \partial_t \mathbf{Z} + \mathrm{D}\mathbf{Z}\partial_t \boldsymbol{\kappa} \circ \boldsymbol{\kappa}^{-1} \\ &= \partial_t \mathbf{Z} + \mathrm{D}\mathbf{Z}\mathbf{V}.\end{aligned}$$

Thus, we obtain as claimed

$$\mathbf{W} = \partial_t(\mathbf{Z} \circ \boldsymbol{\kappa}) \circ \boldsymbol{\kappa}^{-1} - \mathrm{D}\mathbf{V}\mathbf{Z}.$$

□

Remark IV.4.3. *Theorem IV.4.2 states that we analytically obtain the same shape gradient regardless of the choice of the generation and perturbation method. Nevertheless, for numerical considerations, one method might be more suitable than the other. As we are interested in the actual shape of the tube, a directly accessible and evaluable parametrization is clearly advantageous. In this respect, the perturbation of identity is the method of choice, because in the speed method one would have to solve the ordinary differential equation* (IV.1.1) *to obtain the shape of the tube. Moreover, we would also have to solve* (IV.1.8) *to obtain the correct perturbation field* $\mathbf{Z}$*. The situation might be different if one is interested in the flow velocity* $\mathbf{V}$*, for which the speed method appears to be more suitable.*

IV.5 Shape derivatives for functionals

Before stating the formulae for the shape derivative of a domain and of a boundary integral, we point out two different integral representations, which are canonical in the chosen setting. On the one hand, we can write a domain and surface integral as $\int_{Q_T} \cdot \,\mathrm{d}(t,\mathbf{x})$ and $\int_{\Sigma_T} \cdot \,\mathrm{d}\Sigma$, respectively. On the other hand, we can write them as a double integral in accordance with $\int_0^T \int_{\Omega_t} \cdot \,\mathrm{d}\mathbf{x}\mathrm{d}t$ and $\int_0^T \int_{\Gamma_t} \cdot \,\mathrm{d}\sigma\mathrm{d}t$, respectively, where Q_T, Ω_t, Σ_T and Γ_t are defined in (III.1.1) and (III.1.2). Since we cannot rewrite the integration domain as a product domain $(0,T)\times U$ for some appropriate U like in the cylindrical setting, we cannot apply Fubini's theorem. Therefore, we have to carefully analyse if the two representations are equal or not. This is done in the following two lemmata, for which we also give proofs as they seem to be missing in the literature.

IV.5.1 Integral representation

Lemma IV.5.1. *In the parametrization setting described in Section IV.1.1, it holds*

$$\mathrm{d}(t,\mathbf{x}) = \mathrm{d}\mathbf{x}\mathrm{d}t,$$

and therefore

$$\int_{Q_T} \cdot \,\mathrm{d}(t,\mathbf{x}) = \int_0^T \int_{\Omega_t} \cdot \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

Proof. We assume to have a parametrization $\vec{\boldsymbol{\kappa}}\colon \mathbb{R}^{1+d} \to \mathbb{R}^{1+d}$ with

$$\vec{\boldsymbol{\kappa}}(t,\mathbf{u}) = \begin{bmatrix} t \\ \boldsymbol{\kappa}(t,\mathbf{u}) \end{bmatrix},$$

where $\boldsymbol{\kappa}\colon \mathbb{R}^d \to \mathbb{R}^d$. Especially, we have $\vec{\boldsymbol{\kappa}}\big((0,T),\Omega_0\big) = Q_T$ and $\boldsymbol{\kappa}(t,\Omega_0) = \Omega_t$, see also Section III.1 and Section IV.1. Using Laplace's formula to compute the determinant along the first row of the Jacobian

$$\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}} = \begin{bmatrix} 1 & \mathbf{0}^\intercal \\ \partial_t\boldsymbol{\kappa} & \mathrm{D}\boldsymbol{\kappa} \end{bmatrix}$$

yields

$$\det(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}}) = \det(\mathrm{D}\boldsymbol{\kappa}). \tag{IV.5.1}$$

By applying Lemma II.2.5 and Fubini's theorem, we can compute for a smooth enough function f

$$\begin{aligned}
\int_{Q_T} f \,\mathrm{d}(t,\mathbf{x}) &= \int_{Q_0} f(\vec{\boldsymbol{\kappa}})\big|\det(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})\big| \,\mathrm{d}(t,\mathbf{x}) \\
&= \int_0^T \int_{\Omega_0} f(t,\boldsymbol{\kappa})\big|\det(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})\big| \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&= \int_0^T \int_{\Omega_0} f(t,\boldsymbol{\kappa})\big|\det(\mathrm{D}\boldsymbol{\kappa})\big| \,\mathrm{d}\mathbf{x}\mathrm{d}t \\
&= \int_0^T \int_{\Omega_t} f \,\mathrm{d}\mathbf{x}\mathrm{d}t,
\end{aligned}$$

where $Q_0 = (0,T)\times\Omega_0$. □

Thus, for domain integrals, it does not matter which of the two canonical representations we consider. This is in contrast to boundary integrals. The corresponding statement is already given in [MZ06, Remark 6.3, p. 167], but to the best of our knowledge no proof is given therein.

Lemma IV.5.2. *In the parametrization setting described Section IV.1.1, it holds*

$$\mathrm{d}\Sigma = \sqrt{1+v_\nu^2}\,\mathrm{d}\sigma\mathrm{d}t,$$

where v_ν is given in (IV.1.4). We therefore have

$$\int_{\Sigma_T} \cdot\,\mathrm{d}\Sigma = \int_0^T \int_{\Gamma_t} \cdot\,\sqrt{1+v_\nu^2}\,\mathrm{d}\sigma\mathrm{d}t.$$

Proof. As in the proof of Lemma IV.5.1, we consider a parametrization $\vec{\boldsymbol{\kappa}}\colon \mathbb{R}^{1+d} \to \mathbb{R}^{1+d}$ with

$$\vec{\boldsymbol{\kappa}}(t,\mathbf{u}) = \begin{bmatrix} t \\ \boldsymbol{\kappa}(t,\mathbf{u}) \end{bmatrix},$$

where $\boldsymbol{\kappa}\colon \mathbb{R}^d \to \mathbb{R}^d$ with $\boldsymbol{\kappa}(t,\Gamma_0) = \Gamma_t$, compare Section III.1. According to Lemma II.2.6 and Fubini's theorem, we compute for f smooth enough

$$\begin{aligned}\int_{\Sigma_T} f\,\mathrm{d}\Sigma &= \int_{\Sigma_0} f(\vec{\boldsymbol{\kappa}})\big|\det(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})\big|\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|\,\mathrm{d}\Sigma \\ &= \int_0^T \int_{\Gamma_0} f(t,\boldsymbol{\kappa})\big|\det(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})\big|\frac{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|}{\big\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0\big\|}\big\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0\big\|\,\mathrm{d}\sigma\mathrm{d}t.\end{aligned}$$

Here $\boldsymbol{\nu}_0$ denotes the time-space normal on $\Sigma_0 = (0,T)\times\Gamma_0$ and thus corresponds to $\left[\begin{smallmatrix}0\\ \mathbf{n}_0\end{smallmatrix}\right]$, where $\mathbf{n}_0$ is the spatial normal to Ω_0. If we show that

$$\frac{\big\|(\vec{\mathrm{D}}\vec{\boldsymbol{\kappa}})^{-\intercal}\boldsymbol{\nu}_0\big\|}{\big\|(\mathrm{D}\boldsymbol{\kappa})^{-\intercal}\mathbf{n}_0\big\|} = \sqrt{1+v_\nu^2}, \tag{IV.5.2}$$

the proof is complete by applying (IV.5.1) and Lemma II.2.6 in the inner integral. When using Lemma IV.1.4 to rewrite the expression in (IV.1.6) and comparing it to (IV.1.4), then (IV.5.2) follows at once.

□

IV.5.2 Shape derivative for domain integrals

This section is dedicated to the shape derivative of domain integrals, see for example [MZ06, Theorem 5.4]. We first consider the case, where the integrand corresponds to a function $u = u(Q_T)$. Proving the shape derivative of this functional illustrates the general procedure of such computations and reveals the underlying structure of the shape gradient. For the computations, we need the derivative of the determinant, which is stated in the following lemma, cf. [MN07, Theorem 1, p. 169].

Lemma IV.5.3. *The derivative of the determinant of a matrix $\mathbf{A}(s)$ is given by*

$$\frac{\partial\Big(\det\big(\mathbf{A}(s)\big)\Big)}{\partial s} = \operatorname{tr}\big(\mathbf{A}'(s)\mathbf{A}^{-1}(s)\big)\det\big(\mathbf{A}(s)\big).$$

Theorem IV.5.4. *Let us assume that $u = u(Q_T)$ admits a material and a local shape derivative for $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ and for any direction $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$. Assume that the map $s \mapsto J(Q_T^s)$ with*

$$J(Q_T) = \int_0^T \int_{\Omega_t} u \,\mathrm{d}\mathbf{x}\mathrm{d}t$$

is differentiable at $s = 0$. Then, the derivative of $J(Q_T)$ in the direction $\mathbf{Z}$ reads

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \delta u[\mathbf{Z}] \,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T \int_{\Gamma_t} u\langle \mathbf{Z}, \mathbf{n}\rangle \,\mathrm{d}\sigma\mathrm{d}t.$$

Proof. For the proof, we can proceed as in the time-independent case, see for example [DZ11, Chapter 9, Section 4.1]. As [MZ06, Theorem 5.4] lacks the proof, we present it here for the convenience of the reader. Let us consider the perturbed functional

$$J(Q_T^s) = \int_0^T \int_{\Omega_{t,s}} u_s \,\mathrm{d}\mathbf{x}\mathrm{d}t,$$

obtained by the perturbation of identity of the form $\mathrm{id} + s\mathbf{Z}$. The subscript s in u_s indicates that we consider $u = u(Q_T^s)$. Transforming the inner integral back to Ω_t yields according to Lemma II.2.5

$$J(Q_T^s) = \int_0^T \int_{\Omega_t} u_s \circ (\mathrm{id} + s\mathbf{Z}) \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

We can now compute the derivative with respect to s at $s = 0$. By the product rule and the Definition IV.2.2 of the material derivative, we obtain

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \left\{ \dot{u}[\mathbf{Z}] + u\partial_s\Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)\Big)|_{s=0} \right\} \mathrm{d}\mathbf{x}\mathrm{d}t.$$

Due to Lemma IV.5.3, it holds

$$\partial_s \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)|_{s=0} = \mathrm{tr}\left(\mathrm{D}\mathbf{Z}\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-1}\right) \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)\Big|_{s=0}$$

and therefore

$$\partial_s \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)|_{s=0} = \mathrm{tr}\big(\mathrm{D}\mathbf{Z}\big) = \mathrm{div}(\mathbf{Z}).$$

Inserting relation (IV.2.2) for the material derivative and applying the product rule yields

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \{\delta u[\mathbf{Z}] + \mathrm{div}(u\mathbf{Z})\} \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

The claim follows immediately by using the divergence theorem (Lemma II.2.14). □

The above theorem can be extended to a more general setting where the integrand is not just a function u, cf. [MZ06, Proposition 6.1, p. 171] for the statement without proof. In the following theorem, we additionally let the integrand depend on the gradient of u and therefore give the proof.

Theorem IV.5.5. *Let us assume that for $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ and for any direction $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ the following three statements hold:*

1. *j, u and ∇u admit a material derivative,*
2. *j, u and ∇u admit a local shape derivative,*
3. *the map $s \mapsto J(Q_T^s)$ is differentiable at $s = 0$, where*

$$J(Q_T) = \int_0^T \int_{\Omega_t} j(\Omega_t, u, \nabla u) \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

Then, the derivative in the direction $\mathbf{Z} \in \mathcal{Z}_{ad}$ of $J(Q_T)$ exists and reads

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \Big\{ &\dot{j}(\Omega_t, u, \nabla u)[\mathbf{Z}] + \partial_y j(\Omega_t, u, \nabla u)\dot{u}[\mathbf{Z}] \\ &+ \big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u), (\dot{\nabla u})[\mathbf{Z}] \big\rangle \\ &+ j(\Omega_t, u, \nabla u) \operatorname{div}(\mathbf{Z}) \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t,\end{aligned}$$

when using the material derivative, where we write $\partial_y j = \frac{\partial j}{\partial y}(\Omega_t, y, \mathbf{z}) \in \mathbb{R}$ and $\nabla_{\mathbf{z}} j = \frac{\partial j}{\partial \mathbf{z}}(\Omega_t, y, \mathbf{z}) \in \mathbb{R}^d$, as well as $u = (Q_T)$ and $\nabla u = \nabla u(Q_T)$. When using the local shape derivative, we obtain

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \Big\{ &\delta j(\Omega_t, u, \nabla u)[\mathbf{Z}] + \partial_y j(\Omega_t, u, \nabla u)\delta u[\mathbf{Z}] \\ &+ \big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u), \nabla \delta u[\mathbf{Z}] \big\rangle \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t \\ + \int_0^T \int_{\Gamma_t} &j(\Omega_t, u, \nabla u) \langle \mathbf{Z}, \mathbf{n} \rangle \,\mathrm{d}\sigma\mathrm{d}t.\end{aligned}$$

Proof. The expression containing the material derivative follows directly as in the proof of Theorem IV.5.4 by applying the multivariate chain rule to the perturbed functional

$$J(Q_T^s) = \int_0^T \int_{\Omega_{t,s}} j\big(\Omega_{t,s}, u_{t,s}, (\nabla u)_{t,s}\big) \,\mathrm{d}\mathbf{x}\mathrm{d}t,$$

where $u_{t,s}$ and $(\nabla u)_{t,s}$ denote u and ∇u computed on the perturbed domain Q_T^s.

To obtain the result expressed with the local shape derivative, we use (IV.2.2) and Remark IV.2.4 to obtain

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Omega_t} \Big\{ &\delta j(\Omega_t, u, \nabla u)[\mathbf{Z}] + \big\langle \nabla j(\Omega_t, u, \nabla u), \mathbf{Z} \big\rangle \\ &+ \partial_y j(\Omega_t, u, \nabla u)\delta u[\mathbf{Z}] + \big\langle \partial_y j(\Omega_t, u, \nabla u)\nabla u, \mathbf{Z} \big\rangle \\ &+ \Big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u), \nabla\big(\delta u[\mathbf{Z}]\big) + \mathrm{D}^2 u \mathbf{Z} \Big\rangle \\ &+ j(\Omega_t, u, \nabla u) \operatorname{div}(\mathbf{Z}) \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t.\end{aligned}$$

Due to the multivariate chain rule, we have

$$\begin{aligned}\operatorname{div}\big(j(\Omega_t, u, \nabla u)\mathbf{Z}\big) = \; &j(\Omega_t, u, \nabla u) \operatorname{div}(\mathbf{Z}) \\ &+ \big\langle \nabla j(\Omega_t, u, \nabla u), \mathbf{Z} \big\rangle \\ &+ \big\langle \partial_y j(\Omega_t, u, \nabla u)\nabla u, \mathbf{Z} \big\rangle \\ &+ \big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u), \mathrm{D}^2 u \mathbf{Z} \big\rangle,\end{aligned}$$

which can be inserted above. Applying the divergence theorem (Lemma II.2.14) yields the claim. ☐

IV.5.3 Shape derivative for boundary integrals

As in Section IV.5.2, we first consider a boundary functional with integrand $u = u(Q_T)$, which again illustrates the computations of the directional derivative. To that end, we need the derivative of the density term (compare (II.2.3))

$$\omega_s = \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)\Big\|\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-\intercal}\mathbf{n}\Big\|, \tag{IV.5.3}$$

which is stated in the following lemma, see [DZ11, p. 485] and [SZ92, Lemma 2.49].

Lemma IV.5.6. *The map $s \mapsto \omega_s$ with ω_s from (IV.5.3) is differentiable and it holds*

$$\partial_s \omega_s|_{s=0} = \lim_{s \searrow 0} \frac{\omega_s - \omega_0}{s} = \operatorname{div} \mathbf{Z} - \mathrm{D}\mathbf{Z}\mathbf{n} \cdot \mathbf{n} = \operatorname{div}_\Gamma \mathbf{Z}.$$

The following theorem states the shape gradient of a surface integral in the form $\int_0^T \int_{\Gamma_t} \cdot \,\mathrm{d}\sigma\mathrm{d}t$. It is the time-space analogue of [DZ11, Chapter 9, Theorem 4.3]. Notice that in [MZ06, Theorem 5.5] the shape gradient of a boundary functional only over Γ_t is stated without proof. Moreover, in [MZ06, Theorem 6.2] a functional over Σ_T is treated, but again without proof. As we will mention in Remark IV.5.8, we have to be careful with the choice of the boundary functional.

Theorem IV.5.7. *Let us assume that $u = u(Q_T)$ admits a material and a local shape derivative for $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ and for any direction $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$, and that the map $s \mapsto J(Q_T^s)$ is differentiable at $s = 0$, where*

$$J(Q_T) = \int_0^T \int_{\Gamma_t} u \,\mathrm{d}\sigma\mathrm{d}t.$$

Then, the derivative of $J(Q_T)$ in the direction $\mathbf{Z}$ reads

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \delta u[\mathbf{Z}] \,\mathrm{d}\sigma\mathrm{d}t + \int_0^T \int_{\Gamma_t} \left(\frac{\partial u}{\partial \mathbf{n}} + \mathcal{H}_{\mathbf{x}} u\right) \langle \mathbf{Z}, \mathbf{n}\rangle \,\mathrm{d}\sigma\mathrm{d}t,$$

where $\mathcal{H}_{\mathbf{x}}$ denotes the additive curvature in space at time t, compare Definition II.2.11.

Proof. We consider the perturbed functional

$$J(Q_T^s) = \int_0^T \int_{\Gamma_{t,s}} u_s \,\mathrm{d}\sigma\mathrm{d}t.$$

Transforming the inner integral back to Γ_t by using Lemma II.2.6 yields

$$J(Q_T^s) = \int_0^T \int_{\Gamma_t} u_s \circ (\mathrm{id} + s\mathbf{Z})\omega_s \,\mathrm{d}\sigma\mathrm{d}t,$$

where the density term is defined in (IV.5.3). Taking the derivative with respect to s evaluated at $s = 0$ gives with the aid of Lemma IV.5.6 and Definition II.2.12

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \big\{\dot{u}[\mathbf{Z}] + u \operatorname{div}_\Gamma \mathbf{Z}\big\} \,\mathrm{d}\sigma\mathrm{d}t.$$

Rewriting $\dot{u}[\mathbf{Z}]$ by (IV.2.2) and splitting ∇u into its tangential and normal contribution (see Definition II.2.12) leads to

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] &= \int_0^T \int_{\Gamma_t} \left\{\delta u[\mathbf{Z}] + \langle \nabla u, \mathbf{n}\rangle\langle \mathbf{n}, \mathbf{Z}\rangle + \langle \nabla_\Gamma u, \mathbf{Z}\rangle + u \operatorname{div}_\Gamma \mathbf{Z}\right\} \mathrm{d}\sigma \mathrm{d}t \\ &= \int_0^T \int_{\Gamma_t} \left\{\delta u[\mathbf{Z}] + \frac{\partial u}{\partial \mathbf{n}}\langle \mathbf{Z}, \mathbf{n}\rangle + \operatorname{div}_\Gamma(u\mathbf{Z})\right\} \mathrm{d}\sigma \mathrm{d}t.\end{aligned}$$

Applying the tangential Stokes formula (Lemma II.2.15) in the inner integral, while noticing that Γ_t is closed, proves the claim. □

Remark IV.5.8. *From this proof, we can see that it is crucial whether we consider a functional over Σ_T or over $(0, T)$ and Γ_t. Firstly, we see from Lemma IV.5.2 that we have to treat the surface measure carefully. Secondly, we use the tangential Stokes formula (Lemma II.2.15) to obtain the expression in Hadamard form. In our case, we assume the boundary Γ_t to be smooth and closed, therefore no extra terms appear. When having a functional over Σ_T and applying a time-space tangential Stokes formula, we would have to treat the bottom of the tube at $t = 0$ and the top of the tube at $t = T$ specifically, as Σ_T is not a closed surface. In particular, also the curvature appearing in the expression of the shape gradient would change from $\mathcal{H}_{\mathbf{x}}$ to $\mathcal{H}_{t,\mathbf{x}}$, which denotes the additive time-space curvature. Since in [MZ06] the proofs are omitted and it is not clear which curvature is meant in the formulae, we hope to have clarified this matter to the reader here.*

We would like to consider a boundary integral which, besides other terms, includes also the spatial normal, which obviously is dependent on the tube. This could for example appear when considering the derivative in normal direction of the solution of a partial differential equation. For the computations of the shape gradient, we need the material derivative and the local shape derivative of the normal, see [DZ11, p. 491].

Lemma IV.5.9. *The local shape derivative of $\boldsymbol{\mathcal{N}}$ (see Section II.2.4) in the direction $\mathbf{Z}$ reads*

$$\delta\boldsymbol{\mathcal{N}}[\mathbf{Z}]|_{\Gamma_t} = \langle \mathrm{D}\mathbf{Z}\mathbf{n}, \mathbf{n}\rangle\mathbf{n} - (\mathrm{D}\mathbf{Z})^\intercal\mathbf{n} - \boldsymbol{\mathcal{R}}\mathbf{Z}.$$

With relation (IV.2.2) *and* (II.2.4)*, the material derivative is given by*

$$\dot{\boldsymbol{\mathcal{N}}}[\mathbf{Z}]|_{\Gamma_t} = \langle \mathrm{D}\mathbf{Z}\mathbf{n}, \mathbf{n}\rangle\mathbf{n} - (\mathrm{D}\mathbf{Z})^\intercal\mathbf{n}.$$

For our computations, we rewrite the local shape derivative of the normal as follows. The result follows from considerations which are scattered over several pages of [DZ11, Chapter 9, Section 5], such that we provide a short proof for the convenience of the reader.

Lemma IV.5.10. *It holds*

$$\delta\boldsymbol{\mathcal{N}}[\mathbf{Z}]|_{\Gamma_t} = -\nabla_\Gamma\langle \mathbf{Z}, \mathbf{n}\rangle.$$

Proof. With (II.2.8), we can compute

$$\begin{aligned}\nabla_\Gamma\langle \mathbf{Z}, \mathbf{n}\rangle &= (\mathrm{D}_\Gamma\mathbf{Z})^\intercal\mathbf{n} + \mathrm{D}\boldsymbol{\mathcal{N}}\big(\mathbf{Z} - \langle \mathbf{Z}, \mathbf{n}\rangle\mathbf{n}\big) \\ &= (\mathrm{D}_\Gamma\mathbf{Z})^\intercal\mathbf{n} + \mathrm{D}\boldsymbol{\mathcal{N}}\mathbf{Z}\end{aligned}$$

due to (II.2.5). Rewriting the tangential Jacobian with the aid of (II.2.6) yields

$$\begin{aligned}\nabla_\Gamma \langle \mathbf{Z}, \mathbf{n} \rangle &= (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} - (\mathrm{D}\mathbf{Z}\mathbf{n}\mathbf{n}^\intercal)^\intercal \mathbf{n} + \mathrm{D}\boldsymbol{\mathcal{N}}\mathbf{Z}\\ &= (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} - \mathbf{n}\mathbf{n}^\intercal (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} + \mathrm{D}\boldsymbol{\mathcal{N}}\mathbf{Z},\end{aligned}$$

from which the claim follows with Lemma IV.5.9 and (II.2.4). □

Notice that in [MZ06, Proposition 6.1, p. 171] a result without proof for a functional over Σ_T is stated but without dependency of the integrand on the gradient and on the normal. In the time-independent case, [SS10b, Lemma 13] treats a similar integrand as the following theorem but lacking inherent dependency of the integrand upon the shape. Since both cases do not directly correspond to the case we consider here, we give the statement and prove it.

Theorem IV.5.11. *Let us assume that for $\boldsymbol{\kappa} \in \mathcal{Z}_{ad}$ and for any direction $\mathbf{Z} \circ \boldsymbol{\kappa} \in \mathcal{Z}_{ad}$, the following three statements hold:*

1. *j, u and ∇u admit a material derivative,*
2. *j, u and ∇u admit a local shape derivative,*
3. *the map $s \mapsto J(Q_T^s)$ is differentiable at $s = 0$, where*

$$J(Q_T) = \int_0^T \int_{\Gamma_t} j(\Omega_t, u, \nabla u, \mathbf{n}) \,\mathrm{d}\sigma \mathrm{d}t.$$

Moreover, we assume sufficient smoothness of the boundary such that there exists an extension of the normal which admits a material derivative and a local shape derivative for all t. Then, the derivative of $J(Q_T)$ in the direction $\mathbf{Z}$ exists and reads

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \Big\{ &\dot{j}(\Omega_t, u, \nabla u, \mathbf{n})[\mathbf{Z}] + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \dot{u}[\mathbf{Z}]\\ &+ \big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), (\dot{\nabla u})[\mathbf{Z}] \big\rangle\\ &+ \big\langle \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \langle \mathrm{D}\mathbf{Z}\mathbf{n}, \mathbf{n}\rangle \mathbf{n} - (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} \big\rangle\\ &+ j(\Omega_t, u, \nabla u, \mathbf{n}) \operatorname{div}_\Gamma \mathbf{Z} \Big\} \,\mathrm{d}\sigma \mathrm{d}t\end{aligned}$$

when using the material derivative, where we write $\partial_y j = \frac{\partial j}{\partial y}(\Omega_t, y, \mathbf{z}, \mathbf{w}) \in \mathbb{R}$, $\nabla_{\mathbf{z}} j = \frac{\partial j}{\partial \mathbf{z}}(\Omega_t, y, \mathbf{z}, \mathbf{w}) \in \mathbb{R}^d$ and $\nabla_{\mathbf{w}} j = \frac{\partial j}{\partial \mathbf{w}}(\Omega_t, y, \mathbf{z}, \mathbf{w}) \in \mathbb{R}^d$, as well as $u = u(Q_T)$ and $\nabla u = \nabla u(Q_T)$. Using the local shape derivative yields

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Gamma_t} \Big\{ \delta j(\Omega_t, u, \nabla u, \mathbf{n})[\mathbf{Z}] + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \delta u[\mathbf{Z}]\\ &\qquad + \Big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \nabla\big(\delta u[\mathbf{Z}]\big) \Big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t\\ &+ \int_0^T \int_{\Gamma_t} \Big\{ \frac{\partial j}{\partial \mathbf{n}}(\Omega_t, u, \nabla u, \mathbf{n}) + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}}\\ &\qquad + \big\langle \mathrm{D}^2 u \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{n} \big\rangle + \operatorname{div}_\Gamma \big(\nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n})\big)\\ &\qquad - \mathcal{H}_{\mathbf{x}} \big\langle \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{n} \big\rangle + \mathcal{H}_{\mathbf{x}} j(\Omega_t, u, \nabla u, \mathbf{n}) \Big\} \langle \mathbf{Z}, \mathbf{n} \rangle \,\mathrm{d}\sigma \mathrm{d}t.\end{aligned}$$

Proof. The claim expressed with the material derivative follows in complete analogy to the proof of Theorem IV.5.7 and by using Lemma IV.5.9.

To derive the formula expressed with the local shape derivative, we rewrite the material derivative with the aid of (IV.2.2) and Remark IV.2.4, yielding

$$
\begin{aligned}
\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \Big\{ & \delta j(\Omega_t, u, \nabla u, \mathbf{n})[\mathbf{Z}] + \big\langle \nabla j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{Z} \big\rangle \\
& + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \big(\delta u[\mathbf{Z}] + \langle \nabla u, \mathbf{Z} \rangle \big) \\
& + \Big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \nabla \big(\delta u[\mathbf{Z}] \big) + \mathrm{D}^2 u \mathbf{Z} \Big\rangle \\
& + \big\langle \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \langle \mathrm{D}\mathbf{Z}\mathbf{n}, \mathbf{n} \rangle \mathbf{n} - (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} \big\rangle \\
& + j(\Omega_t, u, \nabla u, \mathbf{n}) \operatorname{div}_\Gamma \mathbf{Z} \Big\} \,\mathrm{d}\sigma \mathrm{d}t.
\end{aligned}
$$

Inserting $\nabla_\Gamma(j)$ as a productive zero leads to

$$
\begin{aligned}
\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \Big\{ & \delta j(\Omega_t, u, \nabla u, \mathbf{n})[\mathbf{Z}] + \big\langle \nabla j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{Z} \big\rangle \\
& + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \big(\delta u[\mathbf{Z}] + \langle \nabla u, \mathbf{Z} \rangle \big) \\
& + \Big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \nabla \big(\delta u[\mathbf{Z}] \big) + \mathrm{D}^2 u \mathbf{Z} \Big\rangle \\
& + \big\langle \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \langle \mathrm{D}\mathbf{Z}\mathbf{n}, \mathbf{n} \rangle \mathbf{n} - (\mathrm{D}\mathbf{Z})^\intercal \mathbf{n} \big\rangle \\
& + j(\Omega_t, u, \nabla u, \mathbf{n}) \operatorname{div}_\Gamma \mathbf{Z} \Big\} \,\mathrm{d}\sigma \mathrm{d}t \\
+ \int_0^T \int_{\Gamma_t} \Big\{ & \Big\langle \nabla_\Gamma \big(j(\Omega_t, u, \nabla u, \mathbf{n}) \big), \mathbf{Z} \Big\rangle \\
& - \big\langle \nabla_\Gamma j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{Z} \big\rangle - \partial_y j(\Omega_t, u, \nabla u, \mathbf{n}) \big\langle \nabla_\Gamma u, \mathbf{Z} \big\rangle \\
& - \Big\langle \big(\mathrm{D}_\Gamma (\nabla u) \big)^\intercal \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{Z} \Big\rangle \\
& - \big\langle \big(\mathrm{D}_\Gamma \mathbf{n} \big)^\intercal \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{Z} \big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t.
\end{aligned}
$$

Using (II.2.6) to rewrite the tangential Jacobian gives, omitting the arguments of j and noticing the symmetry of $\mathrm{D}^2 u$,

$$
\big\langle (\mathrm{D}_\Gamma \nabla u)^\intercal \nabla_{\mathbf{z}} j, \mathbf{Z} \big\rangle = \big\langle (\mathrm{D}^2 u)^\intercal \nabla_{\mathbf{z}} j, \mathbf{Z} \big\rangle - \langle \mathbf{n}, \mathrm{D}^2 u \nabla_{\mathbf{z}} j \rangle \langle \mathbf{Z}, \mathbf{n} \rangle.
$$

Notice that, due to (II.2.5), we have $\mathrm{D}_\Gamma \mathbf{n} = \mathrm{D}\boldsymbol{\mathcal{N}}$. In the expression above, we recognize the local shape derivative $\delta\boldsymbol{\mathcal{N}}[\mathbf{Z}]$ (compare Lemma IV.5.9) and can therefore substitute it with the expression in Lemma IV.5.10. Moreover, inserting the rewritten tangential Jacobian, cancelling out the term $\langle \mathrm{D}^2 u \nabla_{\mathbf{z}} j, \mathbf{Z}\rangle$ and Definition II.2.12 yields

$$\begin{aligned}
\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \Big\{ & \delta j(\Omega_t, u, \nabla u, \mathbf{n})[\mathbf{Z}] + \frac{\partial j}{\partial \mathbf{n}}(\Omega_t, u, \nabla u, \mathbf{n})\langle \mathbf{Z}, \mathbf{n}\rangle \\
& + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n})\delta u[\mathbf{Z}] + \partial_y j(\Omega_t, u, \nabla u, \mathbf{n})\frac{\partial u}{\partial \mathbf{n}}\langle \mathbf{Z}, \mathbf{n}\rangle \\
& + \Big\langle \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \nabla\big(\delta u[\mathbf{Z}]\big)\Big\rangle \\
& + j(\Omega_t, u, \nabla u, \mathbf{n}) \operatorname{div}_\Gamma \mathbf{Z}\Big\} \,\mathrm{d}\sigma \mathrm{d}t \\
+ \int_0^T \int_{\Gamma_t} \Big\{ & \Big\langle \nabla_\Gamma\big(j(\Omega_t, u, \nabla u, \mathbf{n})\big), \mathbf{Z}\Big\rangle \\
& + \langle \mathbf{Z}, \mathbf{n}\rangle \big\langle \mathrm{D}^2 u \nabla_{\mathbf{z}} j(\Omega_t, u, \nabla u, \mathbf{n}), \mathbf{n}\big\rangle \\
& - \Big\langle \nabla_{\mathbf{w}} j(\Omega_t, u, \nabla u, \mathbf{n}), \nabla_\Gamma\big(\langle \mathbf{Z}, \mathbf{n}\rangle\big)\Big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t.
\end{aligned}$$

Applying the tangential Stokes formula in Lemma II.2.15 twice in the inner integral yields the claim. □

Remark IV.5.12. *If a quantity z is only defined on the boundary, we can still define a material derivative and a local shape derivative on the boundary, see [MZ06, Definition 6.3 and Definition 6.4, p. 168] or [SZ92, Definition 2.74 and Definition 2.88]. If we assume $z(\Sigma_T) = y(Q_T)|_{\Sigma_T}$, we obtain the relation*

$$\delta z(\Sigma_T)[\mathbf{Z}] = \delta y(Q_T)[\mathbf{Z}]|_{\Sigma_T} + \frac{\partial y}{\partial \mathbf{n}}\langle \mathbf{Z}, \mathbf{n}\rangle, \tag{IV.5.4}$$

compare [SZ92, p. 116] for the time-independent case. Thus, Theorem IV.5.11 above can also be formulated for quantities only defined on the boundary.

IV.6 Local shape derivative for a Dirichlet problem

In this section, we compute the local shape derivative of u, where u is the solution of a Dirichlet problem of the heat equation with homogeneous boundary conditions, i.e.

$$\begin{aligned}
(\partial_t - \Delta)u &= f && \text{in } Q_T, \\
\gamma_0 u &= 0 && \text{on } \Sigma_T, \\
u(0,\cdot) &= 0 && \text{in } \Omega_0.
\end{aligned} \tag{IV.6.1}$$

This corresponds to (III.3.7) with $g = 0$. The proof of the local shape derivative follows the lines of [CKY98], which treats the cylindrical case. We state the adjustment to the time-dependent setting and consider a slightly more general setting by letting the right-hand side f depend inherently on the domain, thus $f = f(Q_T)$. In order to compute the local shape derivative, we first characterize the material derivative.

Lemma IV.6.1. *Let us set $u^{t,s} := u_{t,s} \circ (\mathrm{id} + s\mathbf{Z})$ for $\mathbf{Z} \in \mathcal{Z}_{\mathrm{ad}}$, where $u_{t,s}$ is the state computed on Q_T^s, see also Section IV.2. The material derivative of* (IV.6.1)*, which is defined as the limit (see Definition IV.2.2)*

$$\dot{u}[\mathbf{Z}] := \lim_{s\to 0} \frac{u^{t,s} - u}{s},$$

exists in $H^{1,\frac{1}{2}}_{0;0,}(Q_T)$ *and satisfies*

$$S\big(\dot{u}[\mathbf{Z}],\varphi\big) = G(\varphi) \text{ for all } \varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q_T), \tag{IV.6.2}$$

where S *is given by* (III.3.8) *and*

$$\begin{aligned} G(\varphi) = \int_0^T \int_{\Omega_t} \Big\{ &\big\langle (\mathrm{D}\mathbf{Z} + \mathrm{D}\mathbf{Z}^\intercal)\nabla u, \nabla\varphi \big\rangle \\ &+ \varphi\big\langle \nabla(\operatorname{div}\mathbf{Z}), \nabla u\big\rangle + \langle \partial_t \mathbf{Z}, \nabla u\rangle \varphi + \dot{f}[\mathbf{Z}]\varphi \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t. \end{aligned} \tag{IV.6.3}$$

Proof. As an immediate consequence of [LSU68, Chapter IV, Theorem 9.1], the solution $u_{t,s}$ lies in $H^{2,1}_{;0,}(Q^s_T)$ under our smoothness assumptions. Notice that the increased regularity of the solution of the differential equation is needed for the boundary condition of the local shape derivative characterized later in (IV.6.7) and also for the adjoint problem we for example consider in Chapter V.

We have for the perturbed bilinear form

$$S_s(u_{t,s},\varphi) := \int_0^T \int_{\Omega_{t,s}} \big\{ \partial_t u_{t,s}\varphi + \langle \nabla u_{t,s}, \nabla\varphi\rangle \big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t \tag{IV.6.4}$$

that $S_s(u_{t,s},\varphi) = (f_{t,s},\varphi^s)_{L^2(Q^s_T)}$ for all $\varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q^s_T)$, where $f_{t,s}$ is the source term on the perturbed domain. The existence and uniqueness of a solution follows as in Theorem III.3.5 by using that the transformation $\boldsymbol{\kappa} + s\mathbf{Z}\circ\boldsymbol{\kappa}$ satisfies a uniformity condition as stated in (III.1.4). With similar computations as in the proof of Lemma III.3.1, when setting $\boldsymbol{\xi} = \mathrm{id} + s\mathbf{Z}$, $\Omega_\tau = \Omega_t$ and $\Omega_\varsigma = \Omega_{t,s}$, the transformation of the integral in (IV.6.4) back onto Ω_t reads

$$\begin{aligned} &S_s(u_{t,s},\varphi) \\ &\quad= \int_0^T \int_{\Omega_t} \det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big) \bigg[\Big\{ \partial_t u^{t,s} - \Big\langle \big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\intercal} \nabla u^{t,s}, \partial_t(\mathrm{id}+s\mathbf{Z}) \Big\rangle \Big\} \varphi^s \\ &\qquad\qquad + \Big\langle \big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\intercal}\nabla u^{t,s}, \big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\intercal}\nabla\varphi^s \Big\rangle \bigg] \,\mathrm{d}\mathbf{x}\mathrm{d}t, \end{aligned}$$

where we have set $u^{t,s} := u_{t,s}\circ(\mathrm{id}+s\mathbf{Z})$ and φ^s analogously. We define this bilinear form on the unperturbed domain as

$$\begin{aligned} S^s(w,\varphi) := \int_0^T \int_{\Omega_t} &\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big) \\ &\Big[\langle \mathbf{B}^s \nabla w, \nabla\varphi\rangle + \partial_t w\varphi - \Big\langle \big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\intercal}\nabla w, \partial_t(\mathrm{id}+s\mathbf{Z})\Big\rangle \varphi \Big] \,\mathrm{d}\mathbf{x}\mathrm{d}t, \end{aligned}$$

where

$$\mathbf{B}^s := \big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-1}\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\intercal}.$$

Note that the last term in the definition of $S^s(w,\varphi)$ is new in comparison with [CKY98].

We conclude the following statement:

$$S_s(u_{t,s},\varphi) = (f_{t,s},\varphi)_{L^2(Q^s_T)} \text{ for all } \varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q^s_T)$$

for $u_{t,s} \in H^{2,1}_{;0,}(Q^s_T)$ is equivalent to

$$S^s(u^{t,s}, \varphi) = \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) f^{t,s}, \varphi^s \Big)_{L^2(Q_T)} \quad \text{for all } \varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q_T) \tag{IV.6.5}$$

for $u^{t,s} \in H^{2,1}_{;0,}(Q_T)$. Integrating by parts, where we use the zero boundary values of the test function, and dividing by $\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)$ verifies that (IV.6.5) is equivalent to the formulation

$$\begin{aligned}
&\partial_t u^{t,s} - \Big\langle \big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-\mathsf{T}} \nabla u^{t,s}, \partial_t(\mathrm{id} + s\mathbf{Z}) \Big\rangle \\
&\qquad - \frac{1}{\det(\mathrm{D}(\mathrm{id} + s\mathbf{Z}))} \Big\langle \nabla \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)\Big), \mathbf{B}^s \nabla u^{t,s} \Big\rangle \\
&\qquad - \operatorname{div}(\mathbf{B}^s \nabla u^{t,s}) = f^{t,s} \qquad\qquad \text{in } \bigcup_{0<t<T} \big(\{t\} \times \Omega_t\big).
\end{aligned} \tag{IV.6.6}$$

Due to the considerations above, it holds

$$S(u^{t,s} - u, \varphi) = S(u^{t,s}, \varphi) - (f, \varphi)_{L^2(Q_T)} + \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) f^{t,s}, \varphi \Big)_{L^2(Q_T)} - S^s(u^{t,s}, \varphi).$$

We can therefore consider

$$\frac{1}{s} S(u^{t,s} - u, \varphi) = G_s(\varphi) \text{ for all } \varphi \in H^{1,\frac{1}{2}}_{0;,0}(Q_T)$$

for the computation of the material derivative, where

$$\begin{aligned}
G_s(\varphi) = \frac{1}{s} \int_0^T \int_{\Omega_t} \Big\{ &- \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \langle \mathbf{B}^s \nabla u^{t,s}, \nabla \varphi \rangle - \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \partial_t u^{t,s} \varphi \\
&+ \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \Big\langle \big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-\mathsf{T}} \nabla u^{t,s}, \partial_t(\mathrm{id} + s\mathbf{Z}) \Big\rangle \varphi \\
&+ \partial_t u^{t,s} \varphi + \langle \nabla u^{t,s}, \nabla \varphi \rangle + \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) f^{t,s} - f \Big) \varphi \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}$$

Herein, the second line and the terms with f are new in comparison with [CKY98].

We reformulate the expression for $G_s(\varphi)$ the same way as in [CKY98]. To that end, we first substitute $\partial_t u^{t,s}$ with the differential equation given in (IV.6.6) to arrive at

$$\begin{aligned}
G_s(\varphi) = \frac{1}{s} \int_0^T \int_{\Omega_t} \Big\{ &\Big\langle \Big[\mathbf{I} - \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \mathbf{B}^s \Big] \nabla u^{t,s}, \nabla \varphi \Big\rangle \\
&+ \Big[1 - \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \Big] \Big[f^{t,s} + \Big\langle \big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-\mathsf{T}} \nabla u^{t,s}, s\partial_t \mathbf{Z} \Big\rangle \\
&\qquad + \frac{1}{\det(\mathrm{D}(\mathrm{id} + s\mathbf{Z}))} \Big\langle \nabla \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)\Big), \mathbf{B}^s \nabla u^{t,s} \Big\rangle + \operatorname{div}(\mathbf{B}^s \nabla u^{t,s}) \Big] \varphi \\
&+ \det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) \Big\langle \big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big)^{-\mathsf{T}} \nabla u^{t,s}, s\partial_t \mathbf{Z} \Big\rangle \varphi \\
&+ \Big(\det\big(\mathrm{D}(\mathrm{id} + s\mathbf{Z})\big) f^{t,s} - f \Big) \varphi \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}$$

The term with $\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)f^{t,s}$ and a term with $\partial_t\mathbf{Z}$ cancel and this thus yields

$$
\begin{aligned}
G_s(\varphi) = \frac{1}{s}\int_0^T\int_{\Omega_t}\Bigg\{&\Big\langle\Big[\mathbf{I}-\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)\mathbf{B}^s\Big]\nabla u^{t,s},\nabla\varphi\Big\rangle\\
&+\Big[1-\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)\Big]\Bigg[\frac{1}{\det(\mathrm{D}(\mathrm{id}+s\mathbf{Z}))}\Big\langle\nabla\Big(\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)\Big),\mathbf{B}^s\nabla u^{t,s}\Big\rangle\\
&\qquad+\operatorname{div}(\mathbf{B}^s\nabla u^{t,s})\Bigg]\varphi\\
&+\Big\langle\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-\mathsf{T}}\nabla u^{t,s},s\partial_t\mathbf{Z}\Big\rangle\varphi\\
&+(f^{t,s}-f)\varphi\Bigg\}\,\mathrm{d}\mathbf{x}\mathrm{d}t.
\end{aligned}
$$

We use integration by parts on the divergence-term, which leads to

$$
\begin{aligned}
G_s(\varphi) = \frac{1}{s}\int_0^T\int_{\Omega_t}\Bigg\{&\langle[\mathbf{I}-\mathbf{B}^s]\nabla u^{t,s},\nabla\varphi\rangle\\
&+\frac{\varphi}{\det\big(\mathrm{D}(\mathbf{I}+s\mathbf{Z})\big)}\Big\langle\nabla\Big(\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)\Big),\mathbf{B}^s\nabla u^{t,s}\Big\rangle\Bigg\}\,\mathrm{d}\mathbf{x}\mathrm{d}t\\
+\frac{1}{s}\int_0^T\int_{\Omega_t}\Bigg\{&\Big\langle(\nabla u^{t,s})^{\mathsf{T}},\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-1}s\partial_t\mathbf{Z}\Big\rangle\varphi+(f^{t,s}-f)\varphi\Bigg\}\,\mathrm{d}\mathbf{x}\mathrm{d}t,
\end{aligned}
$$

where the last line is new in this time-dependent setting in comparison to the proof given in [CKY98]. We now need to show that G_s converges to G stated in (IV.6.3).

Clearly, $\varphi\mapsto G_s(\varphi)$ is a bounded linear functional on $H^{1,\frac{1}{2}}_{0;,0}(Q_T)$, i.e. $G_s\in\Big(H^{1,\frac{1}{2}}_{0;,0}(Q_T)\Big)'$. Therefore, we can interchange the integration and the limit $s\to 0$. Especially, as in [CKY98], we have

$$
\frac{1}{s}(\mathbf{I}-\mathbf{B}^s)\to\mathrm{D}\mathbf{Z}+\mathrm{D}\mathbf{Z}^{\mathsf{T}}
$$

and

$$
\frac{1}{s\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)}\nabla\Big(\det\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)\Big)\to\nabla\operatorname{div}\mathbf{Z}
$$

as $s\to 0$. Thus, it remains to compute

$$
\lim_{s\to 0}\frac{1}{s}\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-1}\partial_t(\mathrm{id}+s\mathbf{Z}).
$$

By using the Neumann series, we have

$$
\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-1}=\mathrm{id}-s\,\mathrm{D}\mathbf{Z}+o(s)
$$

and therefore

$$
\lim_{s\to 0}\frac{1}{s}\big(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\big)^{-1}\partial_t(\mathrm{id}+s\mathbf{Z})=\lim_{s\to 0}\frac{1}{s}\big(\mathrm{id}-s\,\mathrm{D}\mathbf{Z}+o(s)\big)s\partial_t\mathbf{Z}=\partial_t\mathbf{Z}.
$$

Moreover, it clearly holds

$$\left(\det\left(\mathrm{D}(\mathrm{id}+s\mathbf{Z})\right)\frac{f^{t,s}-f}{s},\varphi\right)_{L^2(Q_T)}\overset{s\to 0}{\longrightarrow}\left(\dot{f}[\mathbf{Z}],\varphi\right)_{L^2(Q_T)},$$

according to Definition IV.2.2.

In order to conclude the convergence $G_s \to G$ as $s \to 0$, we need that $u^{t,s}$ converges to u in $H^{1,0}(Q_T)$. To this end, we transform the equations for u and for $u^{t,s}$ to Q_0 by using the transformation $\boldsymbol{\kappa}$, yielding two differential equations similar to (IV.6.6). Applying [LSU68, Theorem 4.5 on p. 166] implies the convergence of $u_{t,s}\circ(\mathrm{id}+s\mathbf{Z})\circ\boldsymbol{\kappa}$ to $u\circ\boldsymbol{\kappa}$ and thus, with the uniformity condition (III.1.4), also $u^{t,s}$ converges to u. Therefore, we have convergence of $G_s \to G$ as $s\to 0$ in the dual space of $H^{1,\frac{1}{2}}_{0;,0}(Q_T)$ as in [CKY98], with $G(\varphi)$ as in (IV.6.3).

Now, we can argue as in [CKY98]: since the solution operator is an isomorphism from $H^{-1,-\frac{1}{2}}_{;0,}(Q_T)$ to $H^{1,\frac{1}{2}}_{0;0,}(Q_T)$ (see Theorem III.3.5), the statement in Lemma IV.6.1 is true. □

Having the material derivative for (IV.6.1) at hand, we are finally in the position to prove the local shape derivative posed in the following theorem. Notice that we consider $\mathbf{Z}\in\mathcal{Z}_{\mathrm{ad}}$ to ensure that the mapping $\mathrm{id}+s\mathbf{Z}$ and its inverse can satisfy a uniformity condition analogously to (III.1.4) for s small enough.

Theorem IV.6.2. *The local shape derivative of the state u of (IV.6.1) in the direction $\mathbf{Z}\in\mathcal{Z}_{\mathrm{ad}}$ can be computed as the solution of the partial differential equation*

$$\begin{aligned}
\partial_t\delta u[\mathbf{Z}]-\Delta\delta u[\mathbf{Z}]&=\delta f[\mathbf{Z}] && \text{in } Q_T,\\
\delta u[\mathbf{Z}]&=-\langle\mathbf{Z},\mathbf{n}\rangle\frac{\partial u}{\partial\mathbf{n}} && \text{on } \Sigma_T,\\
\delta u[\mathbf{Z}](0,\cdot)&=0 && \text{in } \Omega_0.
\end{aligned}\tag{IV.6.7}$$

Proof of Theorem IV.6.2. Starting from the material derivative, we would like to compute the local shape derivative $\delta u[\mathbf{Z}]$.

If we consider $u\in H^{2,1}_{;0,}(Q_T)$, we have $\nabla u\in H^{1,\frac{1}{2}}(Q_T)$ and $\Delta u\in L^2(Q_T)$ as in [CKY98]. This follows from $\boldsymbol{\kappa}$ being a diffeomorphism and from the time-independent case, compare also Remark III.1.1. Let us next introduce the test space

$$V(Q_0):=\left\{u=U|_{Q_0}\colon U\in C^2_0\big((-\infty,T)\times\Omega_0\big)\right\},$$

which is a dense subspace of $H^{1,\frac{1}{2}}_{0;,0}(Q_0)$, compare [CKY98] (for a C^∞-boundary, see for example [LM68, Remark 2.2 on p. 8]). Likewise to Section III.1, we define with its help the space $V(Q_T)$, which contains functions φ such that $\varphi\circ\boldsymbol{\kappa}\in V(Q_0)$. Then, for $\varphi\in V(Q_T)$, we have the same identity as in [CKY98, p. 859], namely

$$\begin{aligned}
\big\langle(\mathrm{D}\mathbf{Z}+\mathrm{D}\mathbf{Z}^{\intercal})\nabla u,\nabla\varphi\big\rangle+\varphi\big\langle\nabla(\operatorname{div}\mathbf{Z}),\nabla u\big\rangle&=\operatorname{div}\big(\operatorname{div}(\varphi\mathbf{Z})\nabla u-\langle\nabla u,\nabla\varphi\rangle\mathbf{Z}\big)\\
&\quad+\Big\langle\nabla\big(\langle\mathbf{Z},\nabla u\rangle\big),\nabla\varphi\Big\rangle-\operatorname{div}(\varphi\mathbf{Z})\Delta u.
\end{aligned}$$

Applying this identity and the divergence theorem (Lemma II.2.14) to (IV.6.3) yields

$$G(\varphi)=\int_0^T\int_{\Omega_t}\left\{\Big\langle\nabla\big(\langle\mathbf{Z},\nabla u\rangle\big),\nabla\varphi\Big\rangle-\operatorname{div}(\varphi\mathbf{Z})\underbrace{\Delta u}_{=\partial_t u-f}+\langle\nabla u,\partial_t\mathbf{Z}\rangle\varphi+\dot{f}[\mathbf{Z}]\varphi\right\}\mathrm{d}\mathbf{x}\mathrm{d}t,$$

where the boundary terms vanish due to the compact support of φ. Note that the last two terms of the integrand differ from the computations in [CKY98]. It holds

$$-\partial_t u \operatorname{div}(\mathbf{Z}\varphi) = -\operatorname{div}(\partial_t u \mathbf{Z}\varphi) + \big\langle \mathbf{Z}\varphi, \nabla(\partial_t u)\big\rangle$$

and, therefore, we can apply the divergence theorem again to get

$$G(\varphi) = \int_0^T \int_{\Omega_t} \Big\{ \Big\langle \nabla\big(\langle \mathbf{Z}, \nabla u\rangle\big), \nabla\varphi \Big\rangle \\ + \big\langle \mathbf{Z}\varphi, \nabla(\partial_t u)\big\rangle + \langle \nabla u, \partial_t \mathbf{Z}\rangle\varphi - \varphi\langle \mathbf{Z}, \nabla f\rangle + \dot{f}[\mathbf{Z}]\varphi \Big\} \,\mathrm{d}\mathbf{x}\mathrm{d}t.$$

Condensating the two time derivatives yields

$$G(\varphi) = \int_0^T \int_{\Omega_t} \Big\{ \partial_t\big(\langle \nabla u, \mathbf{Z}\rangle\big)\varphi + \Big\langle \nabla\big(\langle \mathbf{Z}, \nabla u\rangle\big), \nabla\varphi \Big\rangle - \varphi\langle \mathbf{Z}, \nabla f\rangle + \dot{f}[\mathbf{Z}]\varphi \Big\} \mathrm{d}\mathbf{x}\mathrm{d}t.$$

We rewrite $\dot{f}[\mathbf{Z}] = \delta f[\mathbf{Z}] + \langle \mathbf{Z}, \nabla f\rangle$ by using (IV.2.2) and arrive at

$$G(\varphi) = \int_0^T \int_{\Omega_t} \Big\{ \partial_t\big(\langle \nabla u, \mathbf{Z}\rangle\big)\varphi + \Big\langle \nabla\big(\langle \mathbf{Z}, \nabla u\rangle\big), \nabla\varphi \Big\rangle + \delta f[\mathbf{Z}]\varphi \Big\} \mathrm{d}\mathbf{x}\mathrm{d}t.$$

The integral on the right-hand side is the same expression as in [CKY98] with an additional last term. Therefore, we can use the identity (IV.2.2) and follow the rest of the proof in [CKY98, Theorem 2.1]. Thus, the local shape derivative satisfies the same partial differential equation as in [CKY98] except for being in a time-space tube Q_T instead a time-space cylinder Q_0 and an additional dependency of the source on the shape. □

Remark IV.6.3. *For an inhomogeneous initial condition $u(0,\cdot) = u_0$ in Ω_0, the proof can be modified straightforwardly if u_0 does not inherently depend on the domain. This leads to the same local shape derivative as given in Theorem IV.6.2.*

IV.7 Functionals dependent on a Dirichlet problem

To the best of our knowledge, no general formulae in Hadmard form for functionals dependent on the solution of a partial differential equation can be found in the literature for the time-dependent setting. Therefore, we state and prove such formulae for a domain and a boundary integral in the case of a Dirichlet problem for the heat equation with homogeneous Dirichlet data.

IV.7.1 Domain functional dependent on a Dirichlet problem

In this section, we consider the functional

$$J(Q_T) = \int_0^T \int_{\Omega_t} j(u, \nabla u)\,\mathrm{d}\mathbf{x}\mathrm{d}t, \tag{IV.7.1}$$

where u solves the state equation

$$\begin{aligned} (\partial_t - \Delta)u &= f && \text{in } Q_T,\\ \gamma_0 u &= 0 && \text{on } \Sigma_T,\\ u(0,\cdot) &= u_0 && \text{in } \Omega_0, \end{aligned} \tag{IV.7.2}$$

which corresponds to (III.3.11) with $g = 0$. We assume that f and u_0 have no inherent dependency on the domain. In particular, j is only dependent on the shape via the solution of the state equation u.

The local shape derivative of u is characterized by Theorem IV.6.2 and Remark IV.6.3. We should also introduce the adjoint problem, which is reverse in time,

$$\begin{aligned} \partial_t p + \Delta p &= \partial_y j(u, \nabla u) - \operatorname{div}\big(\nabla_{\mathbf{z}} j(u, \nabla u)\big) && \text{in } Q_T, \\ \gamma_0 p &= 0 && \text{on } \Sigma_T, \\ p(T, \cdot) &= 0 && \text{in } \Omega_T, \end{aligned} \tag{IV.7.3}$$

where $\partial_y j = \frac{\partial j}{\partial y}(y, \mathbf{z}) \in \mathbb{R}$ and $\nabla_{\mathbf{z}} j = \frac{\partial j}{\partial \mathbf{z}}(y, \mathbf{z}) \in \mathbb{R}^d$.

Theorem IV.7.1. *Under the smoothness assumptions of Theorem IV.5.5, the derivative of the functional (IV.7.1) in the direction $\mathbf{Z} \in \mathcal{Z}_{ad}$ can be written in the Hadamard form as*

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n} \rangle \Big[j(u, \nabla u) - \big\langle \nabla_{\mathbf{z}} j(u, \nabla u), \mathbf{n} \big\rangle \frac{\partial u}{\partial \mathbf{n}} - \frac{\partial p}{\partial \mathbf{n}} \frac{\partial u}{\partial \mathbf{n}} \Big] \,\mathrm{d}\sigma \mathrm{d}t.$$

Proof. Using Theorem IV.5.5 gives

$$\begin{aligned} \nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Omega_t} \Big\{ \partial_y j(u, \nabla u) \delta u[\mathbf{Z}] + \big\langle \nabla_{\mathbf{z}} j(u, \nabla u), \nabla \delta u[\mathbf{Z}] \big\rangle \Big\} \,\mathrm{d}\mathbf{x} \mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} j(u, \nabla u) \langle \mathbf{Z}, \mathbf{n} \rangle \,\mathrm{d}\sigma \mathrm{d}t. \end{aligned}$$

The divergence theorem (Lemma II.2.14) yields

$$\begin{aligned} \nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Omega_t} \Big\{ \partial_y j(u, \nabla u) \delta u[\mathbf{Z}] - \operatorname{div}\big(\nabla_{\mathbf{z}} j(u, \nabla u)\big) \delta u[\mathbf{Z}] \Big\} \,\mathrm{d}\mathbf{x} \mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} \Big\{ j(u, \nabla u) \langle \mathbf{Z}, \mathbf{n} \rangle + \delta u[\mathbf{Z}] \big\langle \nabla_{\mathbf{z}} j(u, \nabla u), \mathbf{n} \big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t. \end{aligned}$$

Inserting the differential equation for the adjoint p, given by (IV.7.3), leads to

$$\begin{aligned} \nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Omega_t} \big\{ \delta u[\mathbf{Z}] (\partial_t p + \Delta p) \big\} \,\mathrm{d}\mathbf{x} \mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} \Big\{ j(u, \nabla u) \langle \mathbf{Z}, \mathbf{n} \rangle + \delta u[\mathbf{Z}] \big\langle \nabla_{\mathbf{z}} j(u, \nabla u), \mathbf{n} \big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t. \end{aligned}$$

We can now apply Green's second formula from Lemma III.5.1 for $\delta u[\mathbf{Z}]$ and p to arrive at

$$\begin{aligned} \nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Gamma_t} \left\{ \frac{\partial p}{\partial \mathbf{n}} \delta u[\mathbf{Z}] - \frac{\partial \delta u[\mathbf{Z}]}{\partial \mathbf{n}} p - \delta u[\mathbf{Z}] p \langle \mathbf{V}, \mathbf{n} \rangle \right\} \mathrm{d}\sigma \mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} \Big\{ j(u, \nabla u) \langle \mathbf{Z}, \mathbf{n} \rangle + \delta u[\mathbf{Z}] \big\langle \nabla_{\mathbf{z}} j(u, \nabla u), \mathbf{n} \big\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t. \end{aligned}$$

Inserting the boundary conditions for p and $\delta u[\mathbf{Z}]$ finally leads to the claim. ☐

IV.7.2 Boundary functional dependent on a Dirichlet problem

In this section, we consider a boundary functional

$$J(\Sigma_T) = \int_0^T \int_{\Gamma_t} j(u, \nabla u, \mathbf{n}) \, \mathrm{d}\sigma \mathrm{d}t, \tag{IV.7.4}$$

where u solves as in Section IV.7.1 the state equation (IV.7.2) and the local shape derivative is again characterized by Theorem IV.6.2 and Remark IV.6.3. We deduce a general formula for the shape derivative of this boundary functional. To this end, we introduce the adjoint problem

$$\begin{aligned} \partial_t p + \Delta p &= 0 && \text{in } Q_T, \\ \gamma_0 p &= \langle \nabla_{\mathbf{z}} j, \mathbf{n} \rangle && \text{on } \Sigma_T, \\ p(T, \cdot) &= 0 && \text{in } \Omega_T, \end{aligned} \tag{IV.7.5}$$

where $\nabla_{\mathbf{z}} j = \frac{\partial j}{\partial \mathbf{z}}(y, \mathbf{z}, \mathbf{w})$. Then, we can prove the following theorem.

Theorem IV.7.2. *Under the smoothness assumptions of Theorem IV.5.11, the derivative of the functional (IV.7.4) in the direction $\mathbf{Z} \in \mathcal{Z}_{ad}$ can be written in the Hadamard form as*

$$\begin{aligned} \nabla J(\Gamma_t)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \bigg\{ & -\mathcal{H}_{\mathbf{x}} \frac{\partial u}{\partial \mathbf{n}} \langle \nabla_{\mathbf{z}} j(u, \nabla u, \mathbf{n}), \mathbf{n} \rangle + \operatorname{div}_\Gamma \big(\nabla_{\mathbf{z}} j(u, \nabla u, \mathbf{n}) \big) \frac{\partial u}{\partial \mathbf{n}} \\ & - \frac{\partial p}{\partial \mathbf{n}} \frac{\partial u}{\partial \mathbf{n}} + \frac{\partial u}{\partial \mathbf{n}} p \langle \mathbf{V}, \mathbf{n} \rangle + \Big\langle \mathrm{D}^2 u \nabla_{\mathbf{z}} j(u, \nabla u, \mathbf{n}), \mathbf{n} \Big\rangle \\ & + \operatorname{div}_\Gamma \Big(\nabla_{\mathbf{w}} j(u, \nabla u, \mathbf{n}) \Big) - \mathcal{H}_{\mathbf{x}} \Big\langle \nabla_{\mathbf{w}} j(u, \nabla u, \mathbf{n}), \mathbf{n} \Big\rangle \\ & + \mathcal{H}_{\mathbf{x}} j(u, \nabla u, \mathbf{n}) \bigg\} \langle \mathbf{Z}, \mathbf{n} \rangle \, \mathrm{d}\sigma \mathrm{d}t. \end{aligned}$$

Proof. According to Theorem IV.5.11, the directional derivative reads

$$\begin{aligned} \nabla J(\Gamma_t)[\mathbf{Z}] = & \int_0^T \int_{\Gamma_t} \Big\{ \partial_y j(u, \nabla u, \mathbf{n}) \delta u[\mathbf{Z}] + \Big\langle \nabla_{\mathbf{z}} j(u, \nabla u, \mathbf{n}), \nabla \big(\delta u[\mathbf{Z}] \big) \Big\rangle \Big\} \, \mathrm{d}\sigma \mathrm{d}t \\ & + \int_0^T \int_{\Gamma_t} \bigg\{ \partial_y j(u, \nabla u, \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}} + \Big\langle \mathrm{D}^2 u \nabla_{\mathbf{z}} j(u, \nabla u, \mathbf{n}), \mathbf{n} \Big\rangle \\ & \quad + \operatorname{div}_\Gamma \Big(\nabla_{\mathbf{w}} j(u, \nabla u, \mathbf{n}) \Big) - \mathcal{H}_{\mathbf{x}} \Big\langle \nabla_{\mathbf{w}} j(u, \nabla u, \mathbf{n}), \mathbf{n} \Big\rangle \\ & \quad + \mathcal{H}_{\mathbf{x}} j(u, \nabla u, \mathbf{n}) \bigg\} \langle \mathbf{Z}, \mathbf{n} \rangle \, \mathrm{d}\sigma \mathrm{d}t \end{aligned}$$

because j itself does not depend on the shape. We can rewrite the following term by using Definition II.2.12 as

$$\int_0^T \int_{\Gamma_t} \Big\langle \nabla_{\mathbf{z}} j, \nabla \big(\delta u[\mathbf{Z}] \big) \Big\rangle \, \mathrm{d}\sigma \mathrm{d}t = \int_0^T \int_{\Gamma_t} \Big\langle \nabla_{\mathbf{z}} j, \nabla_\Gamma \big(\delta u[\mathbf{Z}] \big) + \langle \nabla \delta u[\mathbf{Z}], \mathbf{n} \rangle \mathbf{n} \Big\rangle \, \mathrm{d}\sigma \mathrm{d}t,$$

where we omitted the arguments of j for ease of notation. Using the tangential Stokes formula (see Lemma II.2.15) then gives

$$\begin{aligned}\int_0^T \int_{\Gamma_t} \Big\langle \nabla_{\mathbf{Z}} j, \nabla\big(\delta u[\mathbf{Z}]\big)\Big\rangle \,\mathrm{d}\sigma \mathrm{d}t \\ = \int_0^T \int_{\Gamma_t} \Big\{ \mathcal{H}_{\mathbf{x}} \delta u[\mathbf{Z}] \langle \nabla_{\mathbf{Z}} j, \mathbf{n}\rangle - \operatorname{div}_\Gamma(\nabla_{\mathbf{Z}} j)\delta u[\mathbf{Z}] + \big\langle \nabla \delta u[\mathbf{Z}], \mathbf{n}\big\rangle \langle \nabla_{\mathbf{Z}} j, \mathbf{n}\rangle \Big\} \,\mathrm{d}\sigma \mathrm{d}t.\end{aligned}$$

In view of Green's second formula in Lemma III.5.1 for $\delta u[\mathbf{Z}]$ and p, it holds

$$\int_0^T \int_{\Gamma_t} \left\{ \frac{\partial p}{\partial \mathbf{n}} \delta u[\mathbf{Z}] - \frac{\partial \delta u[\mathbf{Z}]}{\partial \mathbf{n}} p - \delta u[\mathbf{Z}] p \langle \mathbf{V}, \mathbf{n}\rangle \right\} \mathrm{d}\sigma \mathrm{d}t = 0,$$

and we can thus conclude

$$\begin{aligned}\int_0^T \int_{\Gamma_t} \Big\langle \nabla_{\mathbf{Z}} j, \nabla\big(\delta u[\mathbf{Z}]\big)\Big\rangle \,\mathrm{d}\sigma \mathrm{d}t \\ = \int_0^T \int_{\Gamma_t} \left\{ \mathcal{H}_{\mathbf{x}} \delta u[\mathbf{Z}] \langle \nabla_{\mathbf{Z}} j, \mathbf{n}\rangle - \operatorname{div}_\Gamma(\nabla_{\mathbf{Z}} j)\delta u[\mathbf{Z}] + \frac{\partial p}{\partial \mathbf{n}} \delta u[\mathbf{Z}] - \delta u[\mathbf{Z}] p \langle \mathbf{V}, \mathbf{n}\rangle \right\} \mathrm{d}\sigma \mathrm{d}t.\end{aligned}$$

Inserting the boundary condition of $\delta u[\mathbf{Z}]$ and observing that the term involving $\partial_y j$ cancels then yields the claim. □

IV.8 Conclusion

The contribution of this chapter is threefold. Firstly, we organized and classified results from the literature. This includes how to generate and perturb a tube in a Lagrangian and Eulerian setting and how to use these tubes to perform shape calculus also with regard to numerical computations.

Secondly, we elaborated and clarified the crucial details when computing the shape gradient of a functional, which we could not find in the literature. This comprises in particular the choice of the boundary integral $\int_{\Sigma_T}$ or $\int_0^T \int_{\Gamma_t}$, which differ in the time-dependent case. We gave the proofs of the shape gradients of a domain and a boundary functional to have a comprehensible result, even though the techniques are similar to the time-independent shape calculus. Additionally, we computed the local shape derivative of a Dirichlet problem in a rigorous manner.

Thirdly, we derived some new general formulae for the shape gradient of functionals depending on a Dirichlet problem, which to the best of our knowledge cannot be found in the literature so far.

Chapter V

Detection of a time-dependent void

In this chapter, we apply the techniques of shape optimization to an inverse problem. The problem consists of identifying a void of zero temperature in a solid or liquid body by measuring the temperature and the transient heat flux on the accessible outer boundary.

V.1 Problem formulation

V.1.1 Model problem

Let $D \subset \mathbb{R}^d$ with $d = 2, 3$ be a simply connected, spatial domain with boundary $\Gamma^f = \partial D$. Moreover, we have a time component, and thus the domain $(0, T) \times D$ forms a cylindrical domain, called the time-space cylinder. At every time $t \in [0, T]$, a simply connected subdomain $S_t \subset D$ with boundary $\Gamma_t = \partial S_t$ lies inside D such that it holds $\operatorname{dist}(\Gamma^f, \Gamma_t) > 0$ for all t. The difference domain is called $\Omega_t := D \setminus \overline{S_t}$. Taking into account the time again, we thus consider tubes, which contain a void and are represented as

$$Q_T = \bigcup_{0<t<T} (\{t\} \times \Omega_t),$$

see (III.1.1), generated by $\boldsymbol{\kappa}$ as described in Sections III.1 and IV.1. The interior lateral boundary of the tube Q_T is called

$$\Sigma_T = \bigcup_{0<t<T} (\{t\} \times \Gamma_t),$$

see (III.1.2) and the exterior boundary of the tube is called $\Sigma^f = (0, T) \times \Gamma^f$. The topological setup is illustrated in Figure V.1. It is in analogy to [HT13], but we consider an interior boundary Γ_t which moves in time instead of a fixed interior boundary Γ_0.

We shall consider the following, overdetermined initial boundary value problem for the heat equation, where q and g are defined at the fixed exterior boundary Σ^f

$$\begin{aligned} \partial_t u &= \Delta u && \text{in } Q_T, \\ u &= 0 && \text{on } \Sigma_T, \\ u = q, \quad \frac{\partial u}{\partial \mathbf{n}} &= g && \text{on } \Sigma^f, \\ u(0, \cdot) &= 0 && \text{in } \Omega_0. \end{aligned} \tag{V.1.1}$$

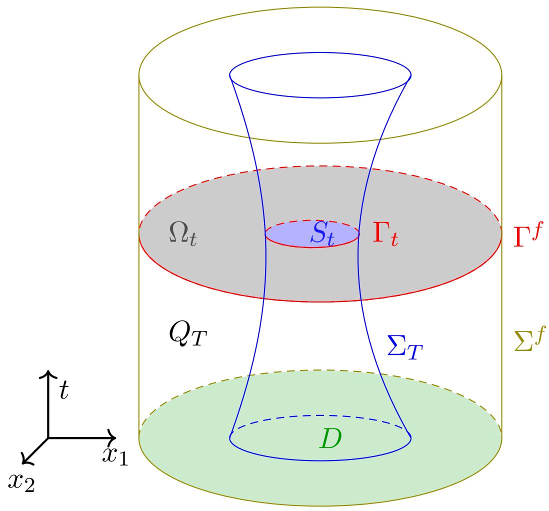


Figure V.1: The tube Q_T with the boundaries Σ_T and Σ^f for $d = 2$.

As introduced in Section III.1, $\mathbf{n}$ denotes the normal pointing outward of the domain Ω_t. In what follows, we assume that q vanishes for $t = 0$, which implies the compatibility with the initial condition. We then seek the free boundary Σ_T, such that the overdetermined problem (V.1.1) allows for a solution u. In [CKY98, Theorem 1.1], the uniqueness of such a boundary Σ_T is proven in the case of a time-independent boundary. The uniqueness in the time-dependent case of such an inverse problem is stated in [KT10, Proposition 3.1], subject to certain conditions on the sought-after domain.

V.1.2 Reformulation as a shape optimization problem

The task of finding the unknown boundary Σ_T, i.e. identifying the inclusion, is reformulated as a shape optimization problem by introducing the function v as the solution of the initial boundary value problem with Dirichlet boundary conditions for the heat equation

$$\begin{aligned} \partial_t v = \Delta v \quad & \text{in } Q_T, \\ v = 0 \quad & \text{on } \Sigma_T, \\ v = q \quad & \text{on } \Sigma^f, \\ v(0, \cdot) = 0 \quad & \text{in } \Omega_0. \end{aligned} \tag{V.1.2}$$

This problem has a unique solution $v \in H^{1,\frac{1}{2}}_{0;,}(Q_T)$ for $q \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma^f)$ according to Theorem III.3.5. According to Remark III.3.8, we also have higher regularity of the solution assuming that the data has higher regularity.

For the given state equation (V.1.2), we introduce the tracking-type functional for the Neumann data at the fixed boundary Σ^f

$$J(\Sigma_T) = \frac{1}{2} \int_0^T \int_{\Gamma^f} \left(\frac{\partial v}{\partial \mathbf{n}} - g \right)^2 \mathrm{d}\sigma \mathrm{d}t. \tag{V.1.3}$$

This objective functional should be minimized in the space of admissible boundaries Σ_T. It is non-negative, and it is zero and hence minimal if and only if $v = u$. The objective functional measures the L^2-error of the data mismatch and thus corresponds to the minimization in the least-squares sense. Notice that the existence of optimal solutions to the shape functional (V.1.3) can be proven by the techniques provided, for example, in [BB05, KS97].

V.2 Computation of the shape derivative

In order to minimize the objective functional (V.1.3), we apply a gradient-based optimization method. To this end, we shall compute the shape derivative of the functional with the techniques introduced in Chapter IV.

Notice that instead of considering the admissible perturbation fields as given in (IV.2.1), we only allow perturbation fields, which are zero on the outer boundary, thus

$$\mathcal{Z}_{\mathrm{ad}} := \Big\{\mathbf{Z} \in C^2\big((0,T)\times D\big) \text{ with } \mathbf{Z} = \mathbf{0} \text{ in a neighbourhood of } \Sigma^f\Big\}$$

and consider a perturbation field $\mathbf{Z} \in \mathcal{Z}_{\mathrm{ad}}$. This choice takes into account that the outer boundary Σ^f of the tube is fixed.

The local shape derivative of the state equation (V.1.2) can be computed with Theorem IV.6.2 reading

$$\begin{aligned} \partial_t \delta v[\mathbf{Z}] &= \Delta \delta v[\mathbf{Z}] && \text{in } Q_T,\\ \delta v[\mathbf{Z}] &= -\langle \mathbf{Z}, \mathbf{n}\rangle \frac{\partial v}{\partial \mathbf{n}} && \text{on } \Sigma_T,\\ \delta v[\mathbf{Z}] &= 0 && \text{on } \Sigma^f,\\ \delta v[\mathbf{Z}](0,\cdot) &= 0 && \text{in } \Omega_0. \end{aligned}$$

With the local shape derivative at hand, we can now derive the shape derivative of the objective functional (V.1.3).

Theorem V.2.1. *The shape derivative of the objective functional (V.1.3) in the direction $\mathbf{Z} \in \mathcal{Z}_{\mathrm{ad}}$ reads*

$$\nabla J(Q_T)[\mathbf{Z}] = -\int_0^T \int_{\Gamma_t} \frac{\partial p}{\partial \mathbf{n}} \frac{\partial v}{\partial \mathbf{n}} \langle \mathbf{Z}, \mathbf{n}\rangle \,\mathrm{d}\sigma \mathrm{d}t, \tag{V.2.1}$$

where the adjoint state p satisfies also the heat equation, but reversed in time:

$$\begin{aligned} -\partial_t p &= \Delta p && \text{in } Q_T,\\ p &= 0 && \text{on } \Sigma_T,\\ p &= \frac{\partial v}{\partial \mathbf{n}} - g && \text{on } \Sigma^f,\\ p(T,\cdot) &= 0 && \text{in } \Omega_T. \end{aligned} \tag{V.2.2}$$

Remark V.2.2. *According to Remark III.3.8, we have $\frac{\partial v}{\partial \mathbf{n}} \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma^f)$. Hence, assuming also that $g \in H^{\frac{1}{2},\frac{1}{4}}(\Sigma^f)$, the integrand of the functional (V.1.3) is well-defined and also the adjoint problem (V.2.2) is well-defined, allowing for a solution $p \in H^{1,\frac{1}{2}}_{;,0}(Q_T)$. Therefore, the Neumann trace $\frac{\partial p}{\partial \mathbf{n}}$ lies in $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma_T)$. Together with the smoothness of $\mathbf{Z}$ and the smoothness of the domain under consideration, this yields a well-defined shape derivative (V.2.1).*

Proof of Theorem V.2.1. Because we have two boundaries and the functional is over the fixed boundary, we state the proof here instead of applying the general formula given in Theorem IV.7.2. Due to $\mathbf{Z} = \mathbf{0}$ in a neighbourhood of Σ^f, we conclude

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma^f} \frac{\partial \delta v[\mathbf{Z}]}{\partial \mathbf{n}} \left(\frac{\partial v}{\partial \mathbf{n}} - g \right) \mathrm{d}\sigma \mathrm{d}t.$$

In view of the adjoint state equation (V.2.2), we can reformulate the derivative of J by

$$\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma^f} p \frac{\partial \delta v[\mathbf{Z}]}{\partial \mathbf{n}} \mathrm{d}\sigma \mathrm{d}t.$$

To derive (V.2.1), we apply Green's second formula given in Lemma III.5.1. This yields in view of the boundary conditions of p and $\delta v[\mathbf{Z}]$

$$\int_0^T \int_{\Gamma^f} \frac{\partial \delta v[\mathbf{Z}]}{\partial \mathbf{n}} p \, \mathrm{d}\sigma \mathrm{d}t = \int_0^T \int_{\Gamma_t} \frac{\partial p}{\partial \mathbf{n}} \delta v[\mathbf{Z}] \, \mathrm{d}\sigma \mathrm{d}t.$$

Hence, by inserting the boundary condition for $\delta v[\mathbf{Z}]$ as stated in (IV.6.7), we finally arrive at the desired result (V.2.1). □

Note that the tracking-type functional for the Dirichlet data has been considered in the setting of the speed method in [MZ06, pg. 36–46]. It also leads to the same local shape derivative and shape gradient as in the time-independent case derived in [HT13]. This is thus consistent with the formulae stated here in case of the tracking-type functional for the Neumann data.

Remark V.2.3. *As one can see from Theorem V.2.1, only the normal component of the perturbation field $\mathbf{Z}$ on Σ_T is relevant. Therefore, it suffices to consider only boundary perturbations $\mathbf{Z} \in C^2(\Sigma_T)$.*

Remark V.2.4. *Since the domain Q_T depends on the mapping $\boldsymbol{\kappa}$, we can also write $\nabla J(Q_T)[\mathbf{Z}] = \nabla J(\boldsymbol{\kappa})[\mathbf{Z}]$. Here, $\nabla J(\boldsymbol{\kappa})$ is obviously linear in $\mathbf{Z} \in \mathcal{Z}_{\mathrm{ad}}$ and one can verify that it is bounded. Thus, J is Gâteaux differentiable at $\boldsymbol{\kappa}$. In the same way, we can argue that J is Gâteaux differentiable in an open neighbourhood U of $\boldsymbol{\kappa}$. Moreover, one can prove that $\nabla J : U \to \mathcal{Z}_{\mathrm{ad}}'$ is continuous at $\boldsymbol{\kappa}$ by showing that $\|\nabla J(\boldsymbol{\kappa}) - \nabla J(\tilde{\boldsymbol{\kappa}})\| \to 0$ as $\boldsymbol{\kappa} \to \tilde{\boldsymbol{\kappa}}$. This can be done by transforming the problem onto the reference domain Q_0, using the convergence of $\tilde{\boldsymbol{\kappa}}$ to $\boldsymbol{\kappa}$ in $C^2\big([0,T] \times \mathbb{R}^d\big)$ and the convergence in $H^{1,0}(Q_0)$ of the solutions $p \circ \tilde{\boldsymbol{\kappa}}$ to $p \circ \boldsymbol{\kappa}$ and $v \circ \tilde{\boldsymbol{\kappa}}$ to $v \circ \boldsymbol{\kappa}$ according to [LSU68, Theorem 4.5 on p. 166]. Hence, by using Theorem II.1.31, we can conclude that J is also Fréchet differentiable at $\boldsymbol{\kappa}$ and, therefore, the application of a gradient-based method for the numerical computations in Section V.5 is justified (compare [HPUU08]).*

V.3 Discretization of the shape optimization problem

In order to solve the shape optimization problem under consideration numerically, we need a suitable discretization of the sought domain. It can for example be represented by level sets or by a parametrization of its boundary, where it suffices to consider only the interior boundary as the exterior boundary is fixed. We employ here the latter approach since we will apply a boundary element method to compute the state and its adjoint. By restriction to two spatial dimensions and C^2-smooth star-shaped voids, we can employ a parametrization in space which is based on a Fourier series for an unknown radial function, having time-dependent coefficients. Especially, we consider only boundary perturbation fields $\mathbf{Z} \in C^2(\Sigma_T)$, compare Remark V.2.3.

Our choice of parametrization of the interior moving boundary Σ_T of Q_T is

$$\Sigma_T = \left\{ \begin{bmatrix} t \\ \boldsymbol{\gamma}(t,\theta) \end{bmatrix} \in \mathbb{R}^3 \colon t \in [0,T],\ \theta \in [0,2\pi) \right\}, \tag{V.3.1}$$

where the time-dependent parametrization $\boldsymbol{\gamma}(t,\cdot)\colon [0,2\pi) \to \Gamma_t$ employs polar coordinates

$$\boldsymbol{\gamma}(t,\theta) = w(t,\theta) \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix}. \tag{V.3.2}$$

Here, $w(t,\theta)$ denotes the time- and angle-dependent radius, given by

$$\begin{aligned} w(t,\theta) := \sum_{\ell=0}^{N_L} L_\ell(t) \Bigg(& \alpha_{0,\ell} \\ & + \sum_{k=1}^{N_K-1} \left\{ \alpha_{k,\ell} \cos(k\theta) + \beta_{k,\ell} \sin(k\theta) \right\} + \alpha_{N_K,\ell} \cos(N_K\theta) \Bigg), \end{aligned} \tag{V.3.3}$$

with $L_\ell(t)$ being appropriate dilations and translations of the Legendre polynomials of degree ℓ.

Finding the optimal tube now corresponds to determining the unknown coefficients $\alpha_{k,\ell}$ and $\beta_{k,\ell}$ of the parametrization. Hence, we have the following finite dimensional problem:

$$\text{Seek } \boldsymbol{\gamma}^\star \in Z_N \text{ such that } \nabla J(\boldsymbol{\gamma}^\star)[\mathbf{Z}] = 0 \text{ for all } \mathbf{Z} \in Z_N.$$

Here, Z_N is the finite dimensional ansatz space of parametrizations. To compute the discrete shape gradient, we hence have to consider the directions

$$(\mathbf{Z} \circ \boldsymbol{\gamma})(t,\theta) = L_\ell(t) \cos(k\theta) \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix} \tag{V.3.4}$$

for all $\ell = 0, \ldots, N_L$ and $k = 0, \ldots, N_K$, and

$$(\mathbf{Z} \circ \boldsymbol{\gamma})(t,\theta) = L_\ell(t) \sin(k\theta) \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix} \tag{V.3.5}$$

for all $\ell = 0, \ldots, N_L$ and $k = 1, \ldots, N_K - 1$.

With the specific parametrization at hand, the discrete shape gradient with respect to the parameters t and θ reads

$$\begin{aligned} &\nabla J(Q_T)[\mathbf{Z} \circ \boldsymbol{\gamma}] \\ &= \int_0^T \int_0^{2\pi} \left(\frac{\partial p}{\partial \mathbf{n}} \circ \boldsymbol{\gamma} \right) \left(\frac{\partial v}{\partial \mathbf{n}} \circ \boldsymbol{\gamma} \right) \begin{bmatrix} L_1(t) \\ \vdots \\ L_{N_L}(t) \end{bmatrix} \otimes \begin{bmatrix} \sin\big((N_K-1)\theta\big) \\ \vdots \\ \sin(\theta) \\ 1 \\ \cos(\theta) \\ \vdots \\ \cos(N_K\theta) \end{bmatrix} w(t,\theta) \,\mathrm{d}\theta \mathrm{d}t, \end{aligned} \tag{V.3.6}$$

compare (V.2.1), where we plugged in the choices for the perturbation fields (V.3.4) and (V.3.5), respectively, and used the parametrization $\boldsymbol{\gamma}$ to compute the normal $\mathbf{n}$.

The integral in the shape gradient (V.2.1) is computed by using a trapezoidal rule in space and a trapezoidal rule in time. The Legendre polynomials are computed by using their three term recurrence formula as described in [PTVF92], and are normalized afterwards while the Fourier series is evaluated efficiently by the fast Fourier transform.

The gradient-based method of our choice is the quasi-Newton method, updated by the inverse BFGS rule without damping, cf. [GK99]. A second order line search is applied to find an appropriate step size in the quasi-Newton method. For an overview of possible other optimization algorithms, see [DS83, Fle80].

V.4 Solving parabolic boundary value problems

We shall describe the numerical method for solving the state and adjoint equation by using a boundary integral formulation. Since this is the approach that was already taken in [HT13] for a fixed boundary, we focus in this section on the changes for the time dependent-case.

Both, the state and the adjoint equation, are Dirichlet problems of the heat equation with homogeneous initial conditions. In the case of the adjoint equation this becomes apparent after the change of variables $t \mapsto T - t$.

The boundary integral approach has distinct advantages over domain based approaches, because it is not necessary to mesh a time-dependent domain or consider the transported problem in a cylindrical domain. Instead, we solve Green's integral equation. Recall from (III.6.11) that, for a time-dependent boundary, it has the form

$$\frac{1}{2}v(t,\mathbf{x}) = \mathcal{V}\gamma_1^- v(t,\mathbf{x}) - \mathcal{K}v(t,\mathbf{x}), \quad (t,\mathbf{x}) \in \Sigma_T \cup \Sigma^f. \tag{V.4.1}$$

Here, $\mathcal{V}$ and $\mathcal{K}$ are the thermal single and double layer operators, and v is a solution to the source-free heat equation with homogeneous initial conditions. The Neumann trace is introduced in Section III.4.2. Notice that, since Σ^f is fixed in time and thus has no normal velocity, (III.4.1) especially reads (see also [Tau19])

$$\gamma_1^\pm v := \begin{cases} \frac{\partial v}{\partial \mathbf{n}} \mp \frac{1}{2}\langle \mathbf{V}, \mathbf{n}\rangle v & \text{on } \Gamma_t, \\ \frac{\partial v}{\partial \mathbf{n}} & \text{on } \Gamma^f. \end{cases}$$

Here, $\langle \mathbf{V}, \mathbf{n}\rangle$ is the normal velocity, which can be computed analytically from the parametrization $\boldsymbol{\gamma}$ given in (V.3.2) as $\mathbf{V}(t,\theta) = \frac{\mathrm{d}}{\mathrm{d}t}\gamma(t,\theta)$, compare also (IV.1.3).

For the discretization of (V.4.1), it is desirable to have a method that can be easily adapted to time-dependent geometries, hence we use the Nyström discretization method of [Tau09, Tau19]. To that end, we write the thermal layer potentials of Definition III.6.5 by using Lemma III.6.7 and Remark III.6.8 in the form

$$\mathcal{V}\phi(t,\mathbf{x}) = \frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\sqrt{t-\tau}} V\phi(t,\tau,\mathbf{x})\,\mathrm{d}\tau, \tag{V.4.2}$$

$$\mathcal{K}\phi(t,\mathbf{x}) = \frac{1}{\sqrt{4\pi}} \int_0^t \frac{1}{\sqrt{t-\tau}} K\phi(t,\tau,\mathbf{x})\,\mathrm{d}\tau, \tag{V.4.3}$$

where

$$V\phi(t,\tau,\mathbf{x}) = \int\limits_{\Gamma_\tau\cup\Gamma^f} \frac{1}{(4\pi(t-\tau))^{\frac{d-1}{2}}} \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4(t-\tau)}\right)\phi(\mathbf{y},\tau)\,\mathrm{d}\sigma_{\mathbf{y}}, \tag{V.4.4}$$

$$K\phi(t,\tau,\mathbf{x}) = \int\limits_{\Gamma_\tau\cup\Gamma^f} \frac{1}{(4\pi(t-\tau))^{\frac{d-1}{2}}} \gamma_{1,\mathbf{y}}^{+}\left[\exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{4(t-\tau)}\right)\right]\phi(\mathbf{y},\tau)\,\mathrm{d}\sigma_{\mathbf{y}}, \tag{V.4.5}$$

and $\Gamma_\tau \cup \Gamma^f = \partial\Omega_\tau$, i.e., the union of the free and the fixed boundary. Here, $\gamma_{1,\mathbf{y}}^{+}$ is the normal trace (III.4.1) evaluated at $(\mathbf{y},\tau)$.

The kernel in the above time-dependent surface potentials is the Green's function of the $(d-1)$-dimensional heat equation. Thus, they may be regarded as Poisson-Weierstrass integrals defined on a surface instead of the usual plane. As in the planar case, these integrals are smooth functions in all variables when $0 \le \tau \le t$. The limiting behavior of these functions as $\tau \to t$ is

$$\begin{aligned} V\phi(t,\tau,\mathbf{x}) &= \phi(t,\tau,\mathbf{x}) + \mathcal{O}(t-\tau),\\ K\phi(t,\tau,\mathbf{x}) &= \overline{H}(t,\mathbf{x})\phi(\mathbf{x}) + \mathcal{O}(t-\tau), \end{aligned} \tag{V.4.6}$$

where $\overline{H}(\cdot)$ is the mean curvature (see Definition II.2.11) of the surface $\Gamma_t \cup \Gamma^f$, compare [Tau19].

Since the functions $V\phi$ and $K\phi$ are smooth, the integral operators in (V.4.2) and (V.4.3) have a $(t-\tau)^{-1/2}$- singularity, which suggests to use the trapezoidal rule with a singularity correction at the endpoint $t=\tau$. It is shown in [Tau09] that the rule

$$\mathcal{V}\phi(\mathbf{x},t_n) = \frac{h}{\sqrt{4\pi}}\sum_{j=0}^{n-1}{}' \frac{1}{\sqrt{t_n-t_j}} V(t_n,t_j)\phi(\mathbf{x},t_j) + \mu_n\psi(\mathbf{x},t_n) + \epsilon_h, \tag{V.4.7}$$

where h is the time step length, $t_j = hj$ and

$$\mu_n = \sqrt{\frac{t_n}{\pi}} - \frac{h}{\sqrt{4\pi}}\sum_{j=0}^{n-1}{}' \frac{1}{\sqrt{t_n-t_j}},$$

has a quadrature error of $\epsilon_h = \mathcal{O}(h^{3/2})$. Here, the prime at the summation sign indicates that the $j=0$ term in the sum is multiplied by the factor $1/2$. For the double layer, the analogous result holds when the μ_n-term is multiplied by the curvature.

A fully discrete version is obtained by approximating the surface integrals in (V.4.4) and (V.4.5) by a surface quadrature rule, usually a composite rule that integrates polynomials on triangular patches exactly. If the spatial mesh width h_s satisfies $\sqrt{h_s} \sim h$ and the spatial rule has at least degree of precision two then the quadrature error in (V.4.7) can be preserved, see [Tau09]. In the time-dependent case, these rules are constructed on $\Gamma_0 \cup \Gamma^f$ and then mapped to $\Gamma_t \cup \Gamma^f$.

For the state equation, the solution is smooth and the Nyström method based on the above quadrature is used to compute the normal trace of the solution. Thus, the Neumann data at the quadrature nodes are computed from (III.6.11) by substituting the given Dirichlet data of (V.1.2). This gives approximate values of the shape functional (V.1.3) and the boundary condition in the adjoint state (V.2.2).

The next task is to compute the Neumann data in the shape gradient (V.2.1) by solving the adjoint state. As already observed in [HT13], the adjoint equation (after time transformation $t \mapsto T - t$) has a singularity at $\tau = 0$ because the homogeneous initial condition is not compatible with the in general non-vanishing Dirichlet condition at $t = 0$.

It can be concluded from (V.4.6) and Green's integral equation that the Neumann data has a $t^{-1/2}$-singularity at $t = 0$. To preserve the $\mathcal{O}(h^{\frac{3}{2}})$ accuracy, the time quadrature rule (V.4.7) must be modified with singularity corrections on both endpoints. Since the normal velocity of the boundary does not appear in (V.4.6), the derivation and the weights of this rule are identical to the case of a steady boundary. Since this can be found in [HT13], it is not repeated here.

V.5 Numerical experiments

We shall present some numerical results in order to illustrate the approach. To this end, the exterior, fixed boundary of the space-time domain is chosen as the mantle of the cylinder with radius 1, where its height corresponds to the time interval $(0, T) = (0, 1)$. We choose $N_t = 90$ time intervals and, for every time step, $N_{\mathbf{x}} = 80$ spatial points. The void is depicted in Figure V.2. It has an explicit representation and is discretized by the same number of time intervals and spatial points as the exterior boundary.

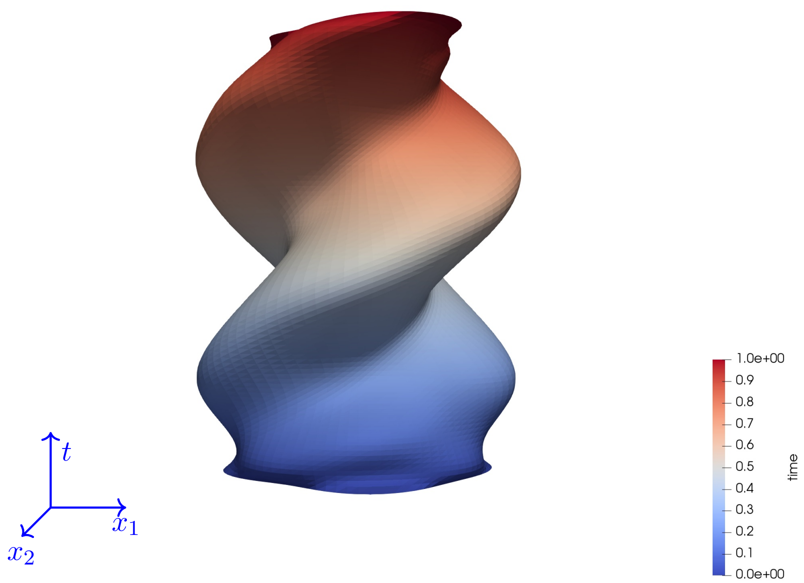


Figure V.2: First example: given inclusion in space and time.

We first solve the forward problem to construct the desired Neumann data g. We hence consider the desired shape found in Figure V.2 and choose the Dirichlet data $q(t, \cdot) = t$, which matches with the initial data $u(0, \cdot) = 0$ in Ω_0. In order to avoid an inverse crime, we use an indirect boundary element approach by solving the thermal single layer equation and then recover the Neumann data by applying the thermal adjoint operator. In addition, we add 1% random noise to the synthetic data.

Now, we can tackle the inverse problem. For the parametrization of the interior boundary, we choose 16 Fourier coefficients in space ($N_K = 8$) and 10 Legendre polynomials in time ($N_L = 9$), leading to 160 design parameters in total. As an initial guess for the free inner boundary, we choose the cylinder of radius 0.3. We perform 100 iterations in the optimization procedure and use a quasi-Newton method updated by the limited memory inverse BFGS rule, where 10 updates are stored, see [NW06] for example.

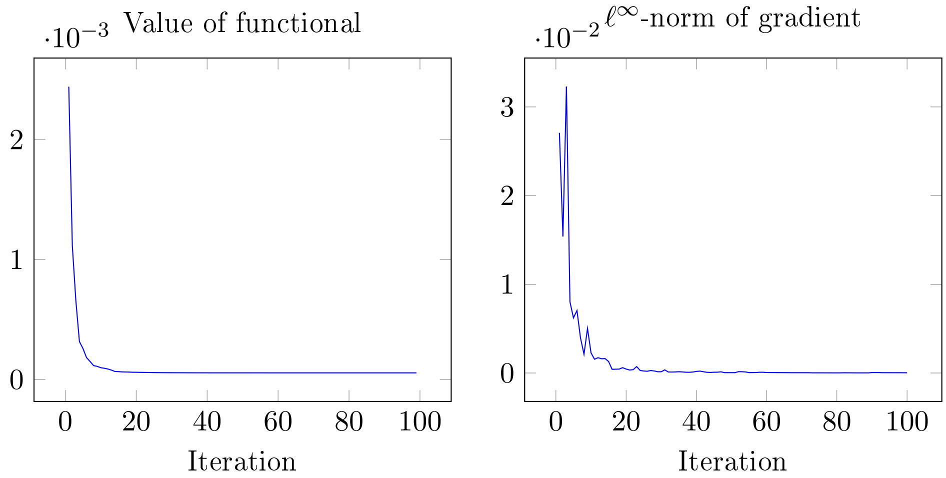


Figure V.3
First example: the histories of the functional (*left*) and of the shape gradient (*right*).

In Figure V.3 on the right, the evolution of the shape gradient during the course of the minimization algorithm is shown, while on the left the evolution of the functional is displayed. In Figure V.4, we can see the ℓ^2-error in the shape coefficients corresponding to the shape error. We clearly observe convergence of the minimization algorithm.

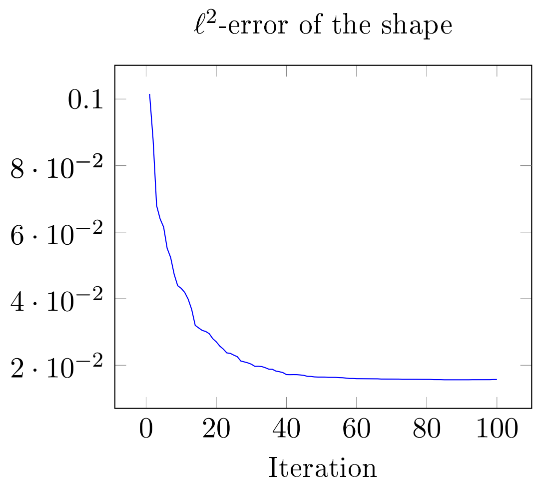
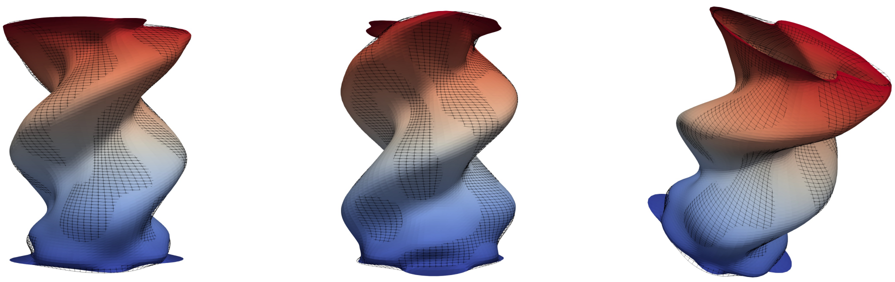


Figure V.4: First example: ℓ^2-error of the shape coefficients corresponding to the difference in the shapes.

In Figure V.5, we present the final reconstruction of the space-time shape, where the wireframe corresponds to the exact shape and the solid shape is its reconstruction. When looking at the time slices, one can observe that the spatial boundary Γ_t is very well reconstructed for the intermediate time slices with $0 < t < T$. Whereas, the reconstruction is not very good at the starting time $t = 0$ and the stopping time $T = 1$. Here, we have no measurement data either of the future or of the past which enter the shape functional (V.1.3). This makes the shape reconstruction more ill-posed in comparison to intermediate time slices.



(a) View with the x-axis in front.

(b) View with the x_2-axis in front.

(c) Three-dimensional view.

Figure V.5: First example: The desired shape as a wireframe together with the reconstructed shape in solid. The time corresponds to the z-axis.

To show the feasibility of our numerical computations, we reconstructed a second, non-symmetric inclusion (compare Figure V.6), using the same set-up and parameters as for the first inclusion.

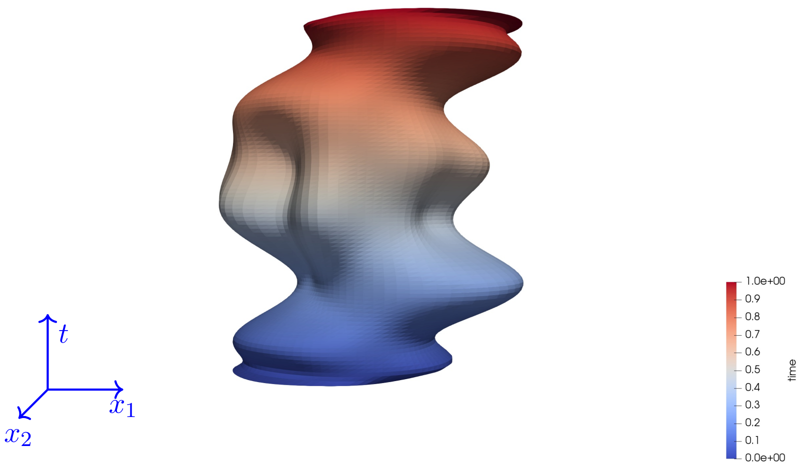
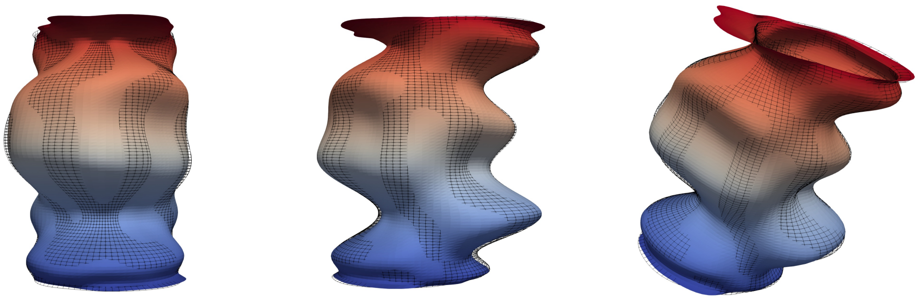


Figure V.6: Second example: given inclusion in space and time.

In Figure V.7, the final reconstruction is shown in solid and the desired shape in wireframe. As for the first numerical example, the reconstruction is fairly good for times away from the starting and ending time. Nonetheless, the reconstructed shape is a bit smoother compared to the desired shape. The value of the functional, the ℓ^∞-norm of the gradient, and the ℓ^2-error of the shape are not depicted since they evolve in a similar manner as in the first example shown in Figures V.3 and V.4.



(a) View with the x-axis in front.

(b) View with the x_2-axis in front.

(c) Three-dimensional view.

Figure V.7: Second example: The desired shape as a wireframe together with the reconstructed shape in solid. The time corresponds to the z-axis.

V.6 Conclusion

In this chapter, we solved a time-dependent shape reconstruction problem by means of shape optimization. We computed the shape derivative of the tracking-type functional for the Neumann data with the help of the perturbation of identity. It turned out that this shape derivative coincides with the one when the void is time-independent. We also demonstrated by numerical experiments that it is indeed possible to reconstruct a time-dependent shape by the proposed approach. By restricting to star-shaped voids, we have been able to compute the error between the desired shape and the reconstructed shape. The convergence of the minimization algorithm has clearly been observed.

Chapter VI

Stefan problem

In this chapter, we solve the multi-dimensional one-phase Stefan problem by applying tools from shape optimization. To that end, we rewrite the Stefan condition by using geometric properties of the tube and introduce a respective tracking-type functional.

VI.1 Problem formulation

VI.1.1 Classical one-phase Stefan problem

Let us consider the classical one-phase Stefan problem as described in [HS14, HS16]. This specific Stefan problem models the evolution of the solid-liquid phase interface. Thus, for every point of time $t \in [0, T]$, we have a time-dependent spatial domain which we denote by $\Omega_t \subset \mathbb{R}^d$, $d \geq 2$. This spatial domain has a time-dependent spatial boundary $\Gamma_t := \partial\Omega_t$. The setup is illustrated in Figure VI.1 for two spatial dimensions plus the temporal dimension. We again set

$$Q_T = \bigcup_{0<t<T} (\{t\} \times \Omega_t),$$

see (III.1.1), generated by $\boldsymbol{\kappa}$ as described in Sections III.1 and IV.1, with lateral boundary

$$\Sigma_T = \bigcup_{0<t<T} (\{t\} \times \Gamma_t),$$

see (III.1.2). Then, the temperature $u(t, \mathbf{x})$ of the liquid in Ω_t is described by the partial differential equation

$$\partial_t u - \Delta u = 0 \quad \text{in } \Omega_t, \tag{VI.1.1}$$

$$\langle \mathbf{V}, \mathbf{n} \rangle = -\frac{\partial u}{\partial \mathbf{n}} \quad \text{on } \Gamma_t, \tag{VI.1.2}$$

$$u = 0 \quad \text{on } \Gamma_t, \tag{VI.1.3}$$

$$u(0, \cdot) = u_0 \quad \text{in } \Omega_0 = \Omega. \tag{VI.1.4}$$

The domain Ω in (VI.1.4) is the initial shape of the liquid phase while condition (VI.1.2) is called the Stefan condition, compare [HS16]. The Stefan condition comes from the movement of the phase interface, see [Vis08, p. 387]. It expresses that the normal velocity $\langle \mathbf{V}, \mathbf{n} \rangle$ of the surface Γ_t equals the negative of the normal derivative

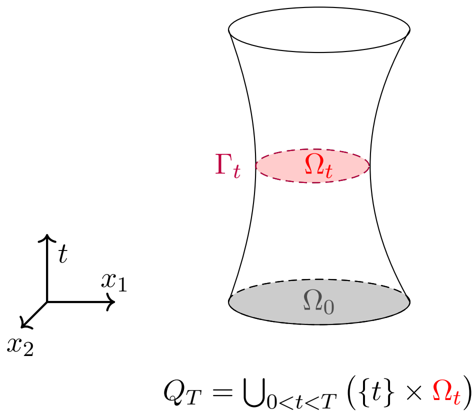


Figure VI.1: Setup of the Stefan problem.

of u at the boundary. We prescribe the initial position of the interface and the initial temperature distribution to make the problem meaningful. From this Stefan problem, we can see that the liquid freezes at zero temperature, cf. [HS14]. Notice that the one-phase Stefan problem is actually also a two-phase Stefan problem, but the temperature is only unknown in one region, while it is vanishing in the other region, compare [Vis08].

The domain Ω_t, thus the region which contains the liquid phase, is characterized by $\{\mathbf{x} \in \mathbb{R}^d : \ u(t, \mathbf{x}) > 0\}$ if we choose $u_0 > 0$ in Ω. Therefore, u can be interpreted as a level set function, see Section II.2.4. Due to (VI.1.1), the parabolic Hopf lemma (see e.g. [Fri58] for some remarks) implies $\partial u / \partial \mathbf{n} < 0$ on Γ_t for $t > 0$. Therefore, we obtain the so-called *Rayleigh-Taylor sign condition*

$$-\frac{\partial u_0}{\partial \mathbf{n}} \geq \lambda > 0 \text{ on } \Gamma_0,$$

which ensures the non-degeneracy in accordance with [HS14].

VI.1.2 Notation

Since we will switch back and forth between spatial and space-time considerations depending on what is more useful for the task at hand, we introduce some notation in this section to clarify the difference between the two.

Recall from Section IV.1.2 that for every point of time t we denote the spatial unit normal by $\mathbf{n} = \mathbf{n}_t$, which is thus normal to Ω_t. The time-space unit normal is denoted by $\boldsymbol{\nu}$, see (IV.1.4). Recall that by ∇ we denote the spatial gradient while $\vec{\nabla}$ denotes the time-space nabla operator. Notice that, for a time-space vector, the first entry always corresponds to the time component and the subsequent entries correspond to the spatial components. Thus, for the time-space normal, the time component is denoted by ν_1.

Moreover, we introduce the tangential gradient and denote it by ∇_Γ for space and $\vec{\nabla}_\Sigma$ for time-space, see Definition II.2.12. Accordingly, we denote the tangential divergence (see Definition II.2.12). The Jacobian matrix of a field $\mathbf{Z}$ is denoted by $\mathrm{D}\mathbf{Z}$ in space and for a time-space vector field $\vec{\mathbf{Z}}$ by $\vec{\mathrm{D}}\vec{\mathbf{Z}}$ in time-space.

VI.1.3 Rewriting the Stefan condition

Next, we intend to rewrite the Stefan condition (VI.1.2) into a form, which will be more useful for the reformulation of the Stefan problem as a shape optimization problem. To this end, we first consider the spatial normal and the time-space normal.

Since u can be interpreted as a level set function, applying [OF03, Formula (1.2) p. 9] implies that the outward pointing normal can be expressed as

$$\mathbf{n} = -\frac{\nabla u}{\|\nabla u\|} \tag{VI.1.5}$$

provided that $\nabla u \neq \mathbf{0}$. Notice that a priori the normal could have a plus or a minus sign. Taking the scalar product of (VI.1.5) with $\mathbf{n}$ yields

$$1 = -\frac{1}{\|\nabla u\|}\langle \nabla u, \mathbf{n}\rangle. \tag{VI.1.6}$$

Due to the parabolic Hopf lemma, we have $\partial u/\partial \mathbf{n} < 0$ on Γ_t and, therefore, the minus sign is the correct sign. Hence, from (VI.1.6), we can directly infer the following lemma.

Lemma VI.1.1. *It holds*

$$-\frac{\partial u}{\partial \mathbf{n}} = \|\nabla u\| \quad \text{on } \Gamma_t.$$

Lemma IV.1.4 allows us to rewrite the Stefan condition in a form, which is computable in our numerical setting as we can express it by means of the geometric quantity $\boldsymbol{\nu}$.

Lemma VI.1.2. *The left-hand side of the Stefan condition (VI.1.2) can be expressed as*

$$\langle \mathbf{V}, \mathbf{n}\rangle = -\frac{\nu_1}{\sqrt{1-\nu_1^2}},$$

where ν_1 denotes the first entry of the normalized time-space normal $\boldsymbol{\nu}$.

Proof. From the representation (IV.1.4) of $\boldsymbol{\nu}$, we infer that

$$\nu_1 = \frac{v_\nu}{\sqrt{1+v_\nu^2}}.$$

Taking the square and multiplying with the denominator gives

$$\nu_1^2(1+v_\nu^2) = v_\nu^2.$$

This expression can be solved for v_ν^2 by writing

$$\nu_1^2 = v_\nu^2(1-\nu_1^2),$$

and thus

$$v_\nu = \pm\frac{\nu_1}{\sqrt{1-\nu_1^2}}. \tag{VI.1.7}$$

The correct sign is the plus sign, because ν_1 and v_ν have the same sign. Employing Lemma IV.1.4 yields finally the claim. □

The velocity field in normal direction can also be written as stated in the following lemma, compare [Mei92, Chapter II, p. 37], and [Vis08, p. 387].

Lemma VI.1.3. *If $\nabla u \neq \mathbf{0}$, then it holds*

$$\langle \mathbf{V}, \mathbf{n} \rangle = \frac{\partial_t u}{\|\nabla u\|}.$$

Proof. Since u can be interpreted as a level set function, the interface is evolved by the convection equation, see [OF03, Formula (3.2), p. 26],

$$\partial_t u + \langle \mathbf{V}, \nabla u \rangle = 0, \tag{VI.1.8}$$

where $\mathbf{V}$ describes the velocity at every point of the implicit surface. In view of (VI.1.5), we can rewrite this expression to arrive at the claim. □

Remark VI.1.4. *Using Lemmata VI.1.1, VI.1.2, and VI.1.3, we immediately arrive at*

$$\partial_t u = \frac{\nu_1}{\sqrt{1-\nu_1^2}} \frac{\partial u}{\partial \mathbf{n}}. \tag{VI.1.9}$$

Moreover, from (IV.1.4)*, Lemma VI.1.2, and Lemma IV.1.4, we obtain*

$$\boldsymbol{\nu} = \begin{bmatrix} \nu_1 \\ \sqrt{1-\nu_1^2}\,\mathbf{n} \end{bmatrix} \in \mathbb{R}^{1+d}. \tag{VI.1.10}$$

VI.1.4 Reformulation as a shape optimization problem

We are now in the position to reformulate the Stefan problem (VI.1.1) to (VI.1.4) as a shape optimization problem. To that end, we consider the reduced Stefan problem

$$\begin{aligned} \partial_t u - \Delta u &= 0 && \text{in } \Omega_t, \\ u &= 0 && \text{on } \Gamma_t, \\ u(0,\cdot) &= u_0 && \text{in } \Omega_0 = \Omega. \end{aligned} \tag{VI.1.11}$$

This is a typical parabolic partial differential equation, where we assume that the boundary Γ_t is unknown. Notice that the solvability of the state equation follows from Theorem III.3.6. We would like to enforce the Stefan condition (VI.1.2) by introducing a tracking-type functional for the Stefan condition. Instead of tracking (VI.1.2), we will track the rewritten Stefan condition by using Lemma VI.1.2. Our choice of functional is hence

$$J(Q_T) = \frac{1}{2}\int_0^T \int_{\Gamma_t} \left(\frac{\partial u}{\partial \mathbf{n}} - \frac{\nu_1}{\sqrt{1-\nu_1^2}} \right)^2 \mathrm{d}\sigma \mathrm{d}t, \tag{VI.1.12}$$

where u denotes the solution of (VI.1.11) and ν_1 denotes the time component of the time-space normal $\boldsymbol{\nu}$, see (IV.1.4).

Since the integrand in the objective functional (VI.1.12) is non-negative, the objective functional is minimal if the Stefan condition (VI.1.2) is satisfied. This amounts to the shape optimization problem

minimize $J(Q_T)$ from (VI.1.12) over the class of admissible domains,
where u satisfies (VI.1.11).

Such problems can, for example, be numerically solved by applying a gradient-based method. Therefore, we shall compute the shape derivative of J in Section VI.2.

In order to perform shape calculus, we perturb the tube with a perturbation of identity, see Section IV.1. Our choice of the objective functional (see (VI.1.12)) is more suitable for the Lagrangian approach of shape optimization than tracking the L^2-error of the Stefan condition (VI.1.2) directly. This is due to the fact that the Stefan condition (VI.1.2) is posed in an Eulerian form, since it explicitly contains the vector field $\mathbf{V}$, which generates the tube.

VI.2 Computation of the shape derivative

VI.2.1 Ingredients for the shape derivative of the objective functional

To present the proof of the shape derivative of the objective functional in a clear manner, we shall provide some useful computations beforehand. Notice that the local shape derivative $\delta u[\mathbf{Z}]$ of the state (VI.1.11) can be characterized according to Theorem IV.6.2 and Remark IV.6.3.

Lemma VI.2.1. *It holds*

$$\delta\left(\frac{\partial u}{\partial \mathbf{n}}\right)[\mathbf{Z}] = \frac{\partial \delta u[\mathbf{Z}]}{\partial \mathbf{n}} \quad \textit{on } \Gamma_t,$$

where $\delta u[\mathbf{Z}]$ denotes the local shape derivative of (VI.1.11)*, see Definition IV.2.3.*

Proof. According to Lemma VI.1.1, we can compute

$$\delta\left(\frac{\partial u}{\partial \mathbf{n}}\right)[\mathbf{Z}] = -\delta\left(\|\nabla u\|\right)[\mathbf{Z}].$$

Thus, we have

$$\delta\left(\sqrt{\langle \nabla u, \nabla u\rangle}\right)[\mathbf{Z}] = \frac{\big\langle \nabla u, \nabla \delta u[\mathbf{Z}]\big\rangle}{\|\nabla u\|}$$

since spatial derivatives and the local shape derivative commute, see Remark IV.2.4. Using (VI.1.5) leads to the claim. □

Lemma VI.2.2. *The local shape derivative of $\nu_1/\sqrt{1-\nu_1^2}$ is given by*

$$\delta\left(\frac{\nu_1}{\sqrt{1-\nu_1^2}}\right)[\mathbf{Z}] = -\frac{1}{(1-\nu_1^2)^{\frac{3}{2}}}\langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \vec{z}_{\boldsymbol{\nu}}\rangle,$$

where $\vec{\mathbf{e}}_1 \in \mathbb{R}^{1+d}$ denotes the (first) canonical unit vector in $\mathbb{R}^{1+d}$, $\vec{\mathbf{Z}} = \left[\begin{smallmatrix} 0 \\ \mathbf{Z}\end{smallmatrix}\right]$ and $\vec{z}_{\boldsymbol{\nu}} := \langle \vec{\mathbf{Z}}, \boldsymbol{\nu}\rangle$.

Proof. With the chain rule and the quotient rule it follows

$$\delta\left(\frac{\nu_1}{\sqrt{1-\nu_1^2}}\right)[\mathbf{Z}] = \frac{1}{(1-\nu_1^2)^{\frac{3}{2}}}\delta\nu_1[\mathbf{Z}].$$

It remains to compute $\delta\nu_1[\mathbf{Z}]$. To this end, let us consider the whole time-space domain, which gets perturbed with the perturbation field $\vec{\mathbf{Z}}$ by applying the map

$\vec{\mathrm{id}} + s\vec{\mathbf{Z}}$. Due to the choice of $\vec{\mathbf{Z}}$, this corresponds to a horizontal perturbation, thus, a perturbation of the spatial component in the direction $\mathbf{Z}$. We can use Lemma IV.5.10 in the time-space setting and obtain the claim when looking at the first entry of the vector $\delta\boldsymbol{\nu}[\vec{\mathbf{Z}}]$.

□

Lemma VI.2.3. *There holds the identity*

$$\frac{\partial}{\partial \mathbf{n}}\langle \nabla u, \mathbf{n}\rangle = \langle \mathrm{D}^2 u\mathbf{n}, \mathbf{n}\rangle =: \frac{\partial^2 u}{\partial \mathbf{n}^2} \quad \text{on } \Gamma_t.$$

Proof. Due to (II.2.5), the claim follows from

$$\frac{\partial}{\partial \mathbf{n}}\langle \nabla u, \mathbf{n}\rangle = \big\langle \nabla\langle \nabla u, \mathbf{n}\rangle, \mathbf{n}\big\rangle = \langle \mathrm{D}^2 u\mathbf{n} + \boldsymbol{\mathcal{R}}\nabla u, \mathbf{n}\rangle.$$

□

To compute the second order normal derivative, we give the following lemma:

Lemma VI.2.4. *The second order normal derivative of u can be computed as*

$$\frac{\partial^2 u}{\partial \mathbf{n}^2} = \frac{\nu_1}{\sqrt{1-\nu_1^2}}\frac{\partial u}{\partial \mathbf{n}} - \overline{H}_{\mathbf{x}}\frac{\partial u}{\partial \mathbf{n}},$$

where $\overline{H}_{\mathbf{x}}$ denotes the spatial mean curvature, compare Definition II.2.11.

Proof. Let us consider a fixed point of time t. According to [SZ92, Proposition 2.68], for a smooth boundary Γ and function φ on Γ, it holds

$$\Delta\varphi = \Delta_\Gamma\varphi + \overline{H}_{\mathbf{x}}\frac{\partial \varphi}{\partial \mathbf{n}} + \frac{\partial^2\varphi}{\partial \mathbf{n}^2},$$

where Δ_Γ denotes the Laplace-Beltrami operator, defined as $\Delta_\Gamma\varphi := \mathrm{div}_\Gamma(\nabla_\Gamma\varphi)$, compare [DZ11, Chapter 9, Section 5.3]. Therefore, we can compute the second order normal derivative of u as

$$\frac{\partial^2 u}{\partial \mathbf{n}^2} = \Delta u - \overline{H}_{\mathbf{x}}\frac{\partial u}{\partial \mathbf{n}},$$

where we used that u vanishes on the boundary Γ_t and, thus, the tangential derivative equals to zero. Due to the state equation, we have that $\partial_t u = \Delta u$ and, therefore, we arrive at the claim by using (VI.1.9). □

The following lemma connects spatial and temporal derivatives of ν_1.

Lemma VI.2.5. *It holds*

$$\langle \nabla\nu_1, \mathbf{n}\rangle = -\partial_t\nu_1\frac{\nu_1}{\sqrt{1-\nu_1^2}}.$$

Proof. From (II.2.5) and the symmetry of the curvature operator, we have

$$\vec{\nabla}_{\boldsymbol{\nu}}\boldsymbol{\nu} = \vec{\boldsymbol{\mathcal{R}}}\boldsymbol{\nu} = \vec{\mathbf{0}},$$

where $\vec{\boldsymbol{\mathcal{R}}}$ denotes the time-space curvature operator. Looking at the first entry of $\vec{\boldsymbol{\mathcal{R}}}\boldsymbol{\nu}$ and using (VI.1.10) thus gives

$$\partial_t\nu_1\nu_1 + \langle \nabla\nu_1, \mathbf{n}\rangle\sqrt{1-\nu_1^2} = 0.$$

□

VI.2.2 Shape derivative of the objective functional

With the previous preparations at hand, we can compute the shape derivative

$$\nabla J(Q_T)[\mathbf{Z}] = \lim_{s\searrow 0} \frac{J(Q_T^s) - J(Q_T)}{s},$$

of the objective functional (VI.1.12), see Definition IV.2.1.

Theorem VI.2.6. *The shape derivative of the objective functional* (VI.1.12) *in the direction $\mathbf{Z} \in \mathcal{Z}_{ad}$ in Hadamard form reads*

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \Bigg\{ &- \frac{\partial p}{\partial \mathbf{n}} \frac{\partial u}{\partial \mathbf{n}} - \vec{\operatorname{div}}_\Sigma \left(p \frac{1}{1-\nu_1^2} \vec{\nabla}_\Sigma t \right) \\ &- p\overline{H}_{\mathbf{x}} \frac{\partial u}{\partial \mathbf{n}} + p \partial_t \nu_1 \frac{\nu_1}{(1-\nu_1^2)^2} + \frac{1}{2} \mathcal{H}_{\mathbf{x}} p^2 \Bigg\} \,\mathrm{d}\sigma \mathrm{d}t \\ &- \int_{\Gamma_0 \cup \Gamma_T} \frac{\tau_1}{\sqrt{1-\nu_1^2}} \langle \mathbf{Z}, \mathbf{n}\rangle p \,\mathrm{d}\sigma,\end{aligned}$$

Here, the adjoint state p satisfies the following backward heat equation

$$\begin{aligned} -\partial_t p - \Delta p &= 0 && \text{in } Q_T, \\ p &= \frac{\partial u}{\partial \mathbf{n}} - \frac{\nu_1}{\sqrt{1-\nu_1^2}} && \text{on } \Sigma_T, \\ p(T,\cdot) &= 0 && \text{on } \Omega_T, \end{aligned} \tag{VI.2.1}$$

$\mathcal{H}_{\mathbf{x}}$ denotes the spatial additive curvature of Γ_t (compare Definition II.2.11), and τ_1 is the first entry of $\boldsymbol{\tau}$ described in Lemma II.2.15.

Proof. Notice that we cannot employ the general Formula from Theorem IV.7.2 as we have an additional dependency on the geometry hidden in ν_1, which is not treated in the theorem. We therefore start from Theorem IV.5.7. This immediately yields

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] &= A + B + C \\ &:= \frac{1}{2} \int_0^T \int_{\Gamma_t} \delta \left(\left(\frac{\partial u}{\partial \mathbf{n}} - \frac{\nu_1}{\sqrt{1-\nu_1^2}} \right)^2 \right) [\mathbf{Z}] \,\mathrm{d}\sigma \mathrm{d}t \\ &\quad + \frac{1}{2} \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \frac{\partial}{\partial \mathbf{n}} \left(\left(\frac{\partial u}{\partial \mathbf{n}} - \frac{\nu_1}{\sqrt{1-\nu_1^2}} \right)^2 \right) \mathrm{d}\sigma \mathrm{d}t \\ &\quad + \frac{1}{2} \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \mathcal{H}_{\mathbf{x}} \left(\frac{\partial u}{\partial \mathbf{n}} - \frac{\nu_1}{\sqrt{1-\nu_1^2}} \right)^2 \mathrm{d}\sigma \mathrm{d}t. \end{aligned} \tag{VI.2.2}$$

While B and C are already in Hadamard form and only the normal derivative in B has to be treated, the integral A has to be brought into Hadamard form by using the adjoint problem. With the aid of the chain rule, Lemma VI.2.1, and Lemma VI.2.2, we compute A as

$$A = A_1 + A_2 = \int_0^T \int_{\Gamma_t} p \frac{\partial \delta u[\mathbf{Z}]}{\partial \mathbf{n}} \,\mathrm{d}\sigma \mathrm{d}t + \int_0^T \int_{\Gamma_t} p \frac{1}{(1-\nu_1^2)^{\frac{3}{2}}} \langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \vec{z}_{\boldsymbol{\nu}} \rangle \,\mathrm{d}\sigma \mathrm{d}t. \tag{VI.2.3}$$

The second term on the right-hand side is similar to [DZ11, p. 490 resp. 501], but since we only have the first component of the normal, we have the scalar product with $\vec{\mathbf{e}}_1$. To eliminate the Neumann derivative on $\delta u[\mathbf{Z}]$, we apply the Green's second identity from Lemma III.5.1 for p and $\delta u[\mathbf{Z}]$ yielding

$$A_1 = \int_0^T \int_{\Gamma_t} \left\{ \frac{\partial p}{\partial \mathbf{n}} \delta u[\mathbf{Z}] - p\delta u[\mathbf{Z}]\langle \mathbf{V}, \mathbf{n}\rangle \right\} \mathrm{d}\sigma \mathrm{d}t.$$

Applying Lemma VI.1.2 and inserting the boundary condition of $\delta u[\mathbf{Z}]$ leads finally to

$$A_1 = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \left\{ -\frac{\partial p}{\partial \mathbf{n}}\frac{\partial u}{\partial \mathbf{n}} - \frac{\partial u}{\partial \mathbf{n}} p \left(\frac{\nu_1}{\sqrt{1-\nu_1^2}} \right) \right\} \mathrm{d}\sigma \mathrm{d}t.$$

Let us next look at the term A_2. When inserting $\vec{\mathbf{e}}_1 = \vec{\nabla} t$, we get

$$A_2 = \int_0^T \int_{\Gamma_t} p \frac{1}{(1-\nu_1^2)^{\frac{3}{2}}} \langle \vec{\nabla} t, \vec{\nabla}_\Sigma \vec{z}_{\boldsymbol{\nu}} \rangle \,\mathrm{d}\sigma \mathrm{d}t.$$

We can split $\vec{\nabla} t$ in its tangential and normal component in time-space. The normal component vanishes within the scalar product due to (II.2.7). Using Lemma IV.5.2 together with (VI.1.7) gives

$$\mathrm{d}\Sigma = \frac{1}{\sqrt{1-\nu_1^2}} \mathrm{d}\sigma \mathrm{d}t. \tag{VI.2.4}$$

We therefore obtain

$$A_2 = \int_{\Sigma_T} p \frac{1}{1-\nu_1^2} \langle \vec{\nabla}_\Sigma t, \vec{\nabla}_\Sigma \vec{z}_{\boldsymbol{\nu}} \rangle \,\mathrm{d}\Sigma.$$

Following the ideas of [DZ11, Chapter 9, Section 5.7], we apply the product rule to get

$$A_2 = \int_{\Sigma_T} \left\{ \vec{\mathrm{div}}_\Sigma \left(p \frac{1}{1-\nu_1^2} \vec{\nabla}_\Sigma t \vec{z}_{\boldsymbol{\nu}} \right) - \vec{\mathrm{div}}_\Sigma \left(p \frac{1}{1-\nu_1^2} \vec{\nabla}_\Sigma t \right) \vec{z}_{\boldsymbol{\nu}} \right\} \mathrm{d}\Sigma.$$

Using Lemma II.2.15 then gives

$$\begin{aligned} A_2 = &\int_{\Sigma_T} \mathcal{H}_{t,\mathbf{x}} p \frac{1}{1-\nu_1^2} \langle \vec{\nabla}_\Sigma t, \boldsymbol{\nu} \rangle \vec{z}_{\boldsymbol{\nu}} \,\mathrm{d}\Sigma - \int_{\Gamma_0 \cup \Gamma_T} p \frac{1}{1-\nu_1^2} \langle \vec{\nabla}_\Sigma t, \boldsymbol{\tau} \rangle \vec{z}_{\boldsymbol{\nu}} \,\mathrm{d}\sigma \\ &- \int_{\Sigma_T} \vec{\mathrm{div}}_\Sigma \left(p \frac{1}{1-\nu_1^2} \vec{\nabla}_\Sigma t \right) \vec{z}_{\boldsymbol{\nu}} \,\mathrm{d}\Sigma. \end{aligned}$$

Herein, the first integral of the right-hand side vanishes due to $\langle \vec{\nabla}_\Sigma t, \boldsymbol{\nu} \rangle = 0$. In view of

$$\vec{\nabla}_\Sigma t = \vec{\mathbf{e}}_1 - \nu_1 \boldsymbol{\nu}, \tag{VI.2.5}$$

and $\langle \boldsymbol{\nu}, \boldsymbol{\tau} \rangle = 0$, the second integrand of the right-hand side reduces to $p\tau_1 \vec{z}_{\boldsymbol{\nu}}/(1-\nu_1^2)$, where τ_1 denotes the first coordinate of $\boldsymbol{\tau}$. By using (VI.1.10), $\vec{z}_{\boldsymbol{\nu}} = \sqrt{1-\nu_1^2}\langle \mathbf{Z}, \mathbf{n}\rangle$, and (VI.2.4), we thus have also A_2 in Hadamard form:

$$A_2 = -\int_{\Gamma_0 \cup \Gamma_T} p \frac{\tau_1}{\sqrt{1-\nu_1^2}} \langle \mathbf{Z}, \mathbf{n}\rangle \,\mathrm{d}\sigma - \int_0^T \int_{\Gamma_t} \vec{\mathrm{div}}_\Sigma \left(p \frac{1}{1-\nu_1^2} \vec{\nabla}_\Sigma t \right) \langle \mathbf{Z}, \mathbf{n}\rangle \,\mathrm{d}\sigma \mathrm{d}t.$$

Next, we shall treat the term B in (VI.2.2). It can be computed by using Lemma VI.2.3:

$$B = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n} \rangle p \left\{ \frac{\partial^2 u}{\partial \mathbf{n}^2} - \frac{\partial}{\partial \mathbf{n}} \left(\frac{\nu_1}{\sqrt{1-\nu_1^2}} \right) \right\} \mathrm{d}\sigma \mathrm{d}t.$$

In view of Lemma VI.2.4, we can eliminate the second order normal derivative. Moreover, the second term can be treated by using the quotient rule, resulting in

$$\frac{\partial}{\partial \mathbf{n}} \left(\frac{\nu_1}{\sqrt{1-\nu_1^2}} \right) = \frac{1}{(1-\nu_1^2)^{\frac{3}{2}}} \langle \nabla \nu_1, \mathbf{n} \rangle.$$

Application of Lemma VI.2.5 yields finally

$$B = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n} \rangle p \left\{ \frac{\nu_1}{\sqrt{1-\nu_1^2}} \frac{\partial u}{\partial \mathbf{n}} - \overline{H}_{\mathbf{x}} \frac{\partial u}{\partial \mathbf{n}} + \partial_t \nu_1 \frac{\nu_1}{(1-\nu_1^2)^2} \right\} \mathrm{d}\sigma \mathrm{d}t.$$

The claim follows when taking finally into account that

$$C = \frac{1}{2} \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n} \rangle \mathcal{H}_{\mathbf{x}} p^2 \, \mathrm{d}\sigma \mathrm{d}t$$

and computing $A_1 + A_2 + B + C$. □

VI.2.3 Shape derivative for the numerical computations

The shape gradient of the objective functional given in Theorem VI.2.6 is in Hadamard form. Nevertheless, for numerical computations, we need to rewrite the term containing the surface divergence to make it computable. Two approaches can be chosen: On the one hand, we can compute the surface divergence directly by using the product rule, treating the three terms separately and try to reformulate them into computable terms. Especially, one would have to reformulate the surface gradient of the adjoint problem. On the other hand, we could stop the manipulations of the term A_2 in the proof of Theorem VI.2.6 at (VI.2.3) in order to avoid the computation of the surface divergence of several other terms. We then have to compute the surface gradient of the perturbation field in normal direction. Since we choose a smooth setting for our numerical computations, we pursue this approach.

In view of the definition of A_2 in (VI.2.3), we compute

$$\langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \langle \vec{\mathbf{Z}}, \boldsymbol{\nu} \rangle \rangle = \sqrt{1-\nu_1^2} \langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \langle \mathbf{Z}, \mathbf{n} \rangle \rangle - \langle \mathbf{Z}, \mathbf{n} \rangle \frac{\nu_1}{\sqrt{1-\nu_1^2}} \langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \nu_1 \rangle.$$

The term $\langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma \nu_1 \rangle$ corresponds to an entry in the time-space curvature operator, namely $\partial_t \nu_1$. Adding the terms A_1, B, and C from the proof of Theorem VI.2.6 to the so computed expression of A_2 yields

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = \int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \bigg\{ &- \frac{\partial u}{\partial \mathbf{n}}\frac{\partial p}{\partial \mathbf{n}} - p\frac{\partial u}{\partial \mathbf{n}}\frac{\nu_1}{\sqrt{1-\nu_1^2}}\bigg\} \\ &+ p\frac{1}{1-\nu_1^2}\big\langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma\langle \mathbf{Z}, \mathbf{n}\rangle\big\rangle - \langle \mathbf{Z}, \mathbf{n}\rangle p \frac{\nu_1}{(1-\nu_1^2)^2}\partial_t \nu_1 \\ &+ \langle \mathbf{Z}, \mathbf{n}\rangle \bigg\{ p\bigg(\frac{\nu_1}{\sqrt{1-\nu_1^2}}\frac{\partial u}{\partial \mathbf{n}} - \overline{H}_{\mathbf{x}}\frac{\partial u}{\partial \mathbf{n}} + \partial_t \nu_1 \frac{\nu_1}{(1-\nu_1^2)^2}\bigg) \\ &\qquad + \frac{1}{2}\mathcal{H}_{\mathbf{x}} p^2\bigg\} \,\mathrm{d}\sigma \mathrm{d}t.\end{aligned}$$

Two terms cancel out and we therefore arrive at

$$\begin{aligned}\nabla J(Q_T)[\mathbf{Z}] = &\int_0^T \int_{\Gamma_t} \langle \mathbf{Z}, \mathbf{n}\rangle \bigg\{ - \frac{\partial u}{\partial \mathbf{n}}\frac{\partial p}{\partial \mathbf{n}} - \overline{H}_{\mathbf{x}} p \frac{\partial u}{\partial \mathbf{n}} + \frac{1}{2}\mathcal{H}_{\mathbf{x}} p^2\bigg\} \,\mathrm{d}\sigma \mathrm{d}t \\ &+ \int_0^T \int_{\Gamma_t} p\frac{1}{1-\nu_1^2}\big\langle \vec{\mathbf{e}}_1, \vec{\nabla}_\Sigma\langle \mathbf{Z}, \mathbf{n}\rangle\big\rangle \,\mathrm{d}\sigma \mathrm{d}t.\end{aligned} \tag{VI.2.6}$$

We use this form of the shape gradient for our numerical computations.

VI.3 Numerical experiment

In this section, we indicate how we solve the optimization problem. The example serves as a proof of concept, and is therefore intentionally kept simple.

VI.3.1 Parametrization of the shape optimization problem

To numerically solve the Stefan problem, reformulated as a shape optimization problem, we restrict ourselves again to a star-shaped spatial domain $\Omega_t \subset \mathbb{R}^2$ for every point of time t (compare Section V.3). Thus, the boundary Σ_T is represented by (V.3.1) and the time-dependent parametrization $\boldsymbol{\gamma}(t,\cdot) : [0, 2\pi) \to \Gamma_t$ employs again polar coordinates, see (V.3.2). Instead of considering the time- and angle-dependent radius with an even number of Fourier coefficients in space as it is done in (V.3.3), we set

$$w(t,\theta) := \sum_{\ell=0}^{N_L} L_\ell(t)\bigg(\alpha_{0,\ell} + \sum_{k=1}^{N_K}\big\{\alpha_{k,\ell}\cos(k\theta) + \beta_{k,\ell}\sin(k\theta)\big\}\bigg),$$

with $L_\ell(t)$ being appropriate dilations and translations of the Legendre polynomials of degree ℓ. Consequently, we obtain an L^2-orthogonal basis for the shape representation which ensures numerical stability of the boundary discretization. Especially, it corresponds to a p-method, meaning that the boundary is approximated exponentially in N_L and N_T when Σ_T is smooth, provided that $N_L \sim N_T$ is chosen proportionally.

Finding the optimal tube now corresponds to determining the unknown coefficients $\alpha_{k,\ell}$ and $\beta_{k,\ell}$ of the parametrization. Hence, we have the following finite dimensional problem:

$$\text{Seek } \boldsymbol{\gamma}^\star \in Z_N \text{ such that } \nabla J(\boldsymbol{\gamma}^\star)[\mathbf{Z}] = 0 \text{ for all } \mathbf{Z} \in Z_N.$$

Here, Z_N is the finite dimensional ansatz space of parametrizations. To compute the discrete shape gradient, we hence have to consider the directions

$$(\mathbf{Z} \circ \boldsymbol{\gamma})(t, \theta) = L_\ell(t) \cos(k\theta) \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix}$$

for all $\ell = 1, \dots, N_L$ and $k = 0, \dots, N_K$, and

$$(\mathbf{Z} \circ \boldsymbol{\gamma})(t, \theta) = L_\ell(t) \sin(k\theta) \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix}$$

for all $\ell = 1, \dots, N_L$ and $k = 1, \dots, N_K$. Notice that, since the initial domain Ω_0 has to remain fixed, we do not wobble at the shape parameters $\alpha_{k,0}$ and $\beta_{k,0}$.

VI.3.2 Implementation of the shape gradient

With the parametrization of the boundary at hand, we shall next explain how to implement the shape gradient (VI.2.6).

We first need to compute the solutions u of the state equation (VI.1.11) and p of the adjoint equation (VI.2.1). Although we only need the Neumann data on the boundary, we cannot apply the boundary element method easily as we have a non-trivial initial condition $u = u_0$ for $t = 0$. Therefore, we employ the finite element method in space and couple it with the theta-scheme to solve the parabolic equation.

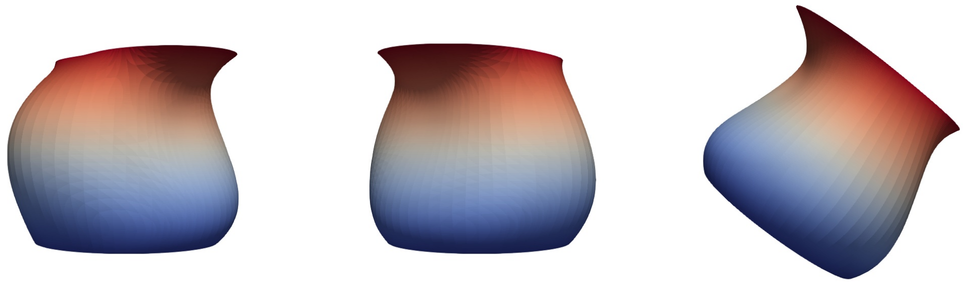
We use the space-time cylinder as reference domain, which means that we need to introduce a finite element mesh of the unit circle. This mesh then gets mapped onto the spatial domain Ω_t described by the parametrization for every point of time t, similarly as in [Har08]. Then, standard piecewise linear finite elements can be used to solve the partial differential equation for every time step, when mapping the weak formulation back to the reference domain. For the time discretization, we use the theta-scheme on the reference domain, including the inhomogeneous Dirichlet data, see [Tra13, Section 8.2.1] for example.

For the mapping of the domain onto the reference domain, we need to evaluate the Legendre polynomials in the parametrization, which can be done by using their three-term recurrence formula as described in [PTVF92].

From the finite element approximation of the state, the Neumann data can be computed, which are piecewise constant. The approximate Neumann data are then projected onto the space of piecewise linear functions as they enter the Dirichlet data of the adjoint state. Notice that the adjoint problem has a singularity at $t = T$. We do not treat this singularity specifically, but need to perform our computations on a fine level to resolve this singularity.

Another component for the shape gradient (VI.2.6) is the additive curvature and the mean curvature in space. Since we consider a two-dimensional setting, both coincide and can be computed from the parametrization, see [DC93, pg. 21]. Finally, the surface gradient of $\langle \mathbf{Z}, \mathbf{n} \rangle$ can be computed as explained in [CK92] or [Har01, Section C.1] by using the parametrization at hand.

We have now all the components to compute the integrand of the shape gradient in (VI.2.6). The integral is computed by using a trapezoidal rule in space and a trapezoidal rule in time on the reference cylindrical domain.



(a) View with the x_1-axis in front.

(b) View with the x_2-axis in front.

(c) Three-dimensional view.

Figure VI.2: Initial guess of the shape optimization problem. The colours correspond to the time slices.

VI.3.3 Numerical results

For the parametrization of the boundary, we choose 15 Fourier coefficients in space ($N_K = 7$) and 10 Legendre polynomials in time ($N_L = 9$), leading to 150 design parameters in total, from which 135 are unknown as we let Ω_0 be fixed. We choose Ω_0 as the unit circle of radius 1. We set $u_0 = J_0\big(\|\mathbf{x}\|\lambda_0\big)$, where J_0 denotes the Bessel function of the first kind and λ_0 is its smallest positive root. In every time-step, we use 163'840 finite elements. We choose $T = 0.2$ and a time step size of $\Delta_t = 0.0005$. We perform 50 iterations in the optimization procedure and use a quasi-Newton method updated by the limited memory inverse BFGS rule, where 10 updates are stored, see [NW06] for example. A second order line search is applied to find an appropriate step size in the quasi-Newton method. The optimization algorithm is started with the initial shape displayed in Figure VI.2.

In Figure VI.3 on the right, the evolution of the ℓ^∞-norm of the shape gradient is displayed during the course of the minimization algorithm, while on the left the evolution of the functional is shown.

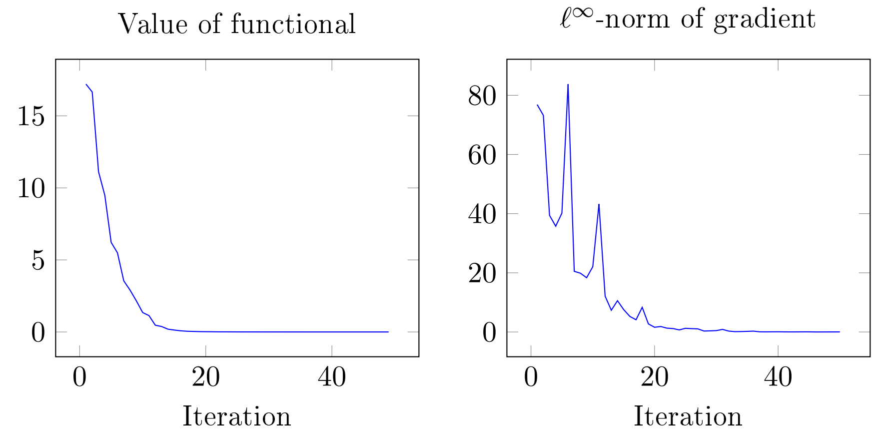


Figure VI.3: The histories of the functional (*left*) and of the shape gradient (*right*).

We clearly observe that these two values tend to zero, thus we have convergence of the minimization algorithm. Figure VI.4 shows the terminal shape at the end of the optimization process. It is a truncated cone. This solution corresponds to the intuition we have for the solution of the Stefan problem, as we would expect the initial circle to grow uniformly throughout time.

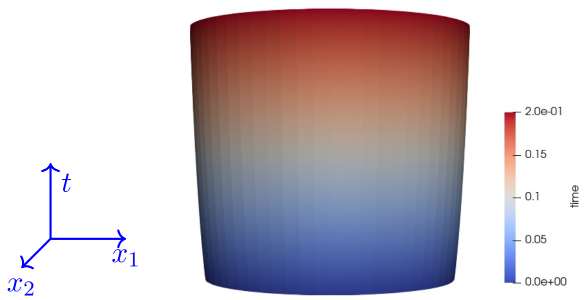


Figure VI.4: Terminal shape of the shape optimization problem.

VI.4 Conclusion

In this chapter, we reformulated the Stefan problem as a shape optimization problem by introducing a shape functional subject to a differential equation. Bearing in mind that we would like to apply a gradient-based optimization algorithm, we computed the directional derivative of the shape functional after rewriting the so-called Stefan condition in a suitable form. Using a parametrization of the boundary by means of a Fourier series allows for computing all terms of the discrete shape gradient. The theoretical results are supported by a numerical experiment, which serves as a proof of concept.

Chapter VII

Final Remarks

In this thesis, we extended the solution theory of parabolic boundary equations in the canonical Sobolev spaces, which are also suitable for time-space boundary element method, to non-cylindrical domains. We further covered the theory of shape optimization for tubes in a way that can be used for numerical experiments, gave some general formulae and clarified the treatment of boundary functionals. This allowed us to treat two numerical examples, namely an inverse problem and a forward Stefan problem.

More specifically, we discussed anisotropic Sobolev spaces on non-cylindrical domains and introduced a velocity corrected Neumann trace. We then adapted the proofs from the cylindrical case in [Cos90] to the non-cylindrical case, and provided the corresponding mapping properties of the boundary integral operators. These are then used to establish existence and uniqueness of solutions of the heat equation on non-cylindrical domains with Dirichlet or Neumann boundary conditions.

Moreover, we covered the theory of shape optimization for tubes in a way that can be used for numerical experiments by elaborating on the difference between the perturbation of identity and the speed method. We stated the seemingly missing proofs for the general formulae of shape derivatives of domain and boundary functionals and especially noticed that one has to be careful when considering boundary functionals on time-dependent boundaries. Additionally, we rigorously computed the local shape derivative of the Dirichlet problem.

Focussing on the perturbation of identity rather than on the speed method for our numerical examples, we illustrated our theory with an inverse problem and with solving a Stefan problem in two time-dependent spatial dimensions.

In the first example, we solved a time-dependent shape reconstruction problem by means of shape optimization. We computed the shape derivative of the tracking-type functional for the Neumann data. It turned out that this shape derivative coincides with the one when the void is time-independent. We also demonstrated by numerical experiments that it is indeed possible to reconstruct a time-dependent shape by the proposed approach and convergence of the minimization algorithm has clearly been observed.

In the second example, the Stefan problem was reformulated as a shape optimization problem by introducing again a tracking-type functional for the Stefan condition subject to a differential equation. Notice that we had to rewrite the so-called Stefan condition in a suitable form and that the shape optimization theory for this problem is now available for more than only one spatial dimension. Again, we were able to support our theoretical findings by a numerical example.

Although some theoretical gaps were closed with the newly developed theory in this thesis, there exist still some open points. We focussed on the heat equation with Dirichlet boundary conditions and gave a proof for its local shape derivative. The same could be done for the Neumann problem by performing a proof analogously to [CKY99]. To that end, one would need the correct function spaces and, in analogy to the Dirichlet problem, an additional result for the existence and uniqueness of solutions of the Neumann problem for higher regularity, such that the local shape derivative is well-defined. A respective result might be obtained by using a bootstrapping argument, for example similarly to [Eva10]. It should also be discussed, which Neumann trace is the physically correct one: the one where the Neumann trace has an additional velocity correction term as introduced in Chapter III or the one which simply takes the normal derivative, as it was considered in [DZ01, Section 6.1].

The theory and algorithmic framework of the numerical examples should be easily adjustable to other examples, such as the inverse problem of identifying a source in analogy to [HT11]. On the algorithmic side, one could treat three spatial dimensions by using spherical harmonics as a basis for the parametrization. On the other hand, one could perform numerical experiments in the setting of the speed method. Instead of choosing a parametrization of the domain, one would have to consider the velocity fields as the unknowns. Reconstructing the domain would then involve solving an additional differential equation, compare Section IV.1, but this approach would make sense, if one is only interested in the velocity field.

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