Technical University of Munich

DEPARTMENT OF MATHEMATICS

FEM error analysis of
parabolic shape gradients

Master's Thesis

von

Leonardo Mutti

Supervisor: Prof. Dr. Michael Ulbrich
Advisor: Prof. Dr. Michael Ulbrich
Submission Date: [Day. Month. Year]

I hereby declare that this thesis is my own work and that no other sources have been used except those clearly indicated and referenced.

Place, Date
original, hand-written signature

Acknowledgements

First and foremost, I would like to express my gratitude to my supervisor Michael Ulbrich. Apart from suggesting this fascinating topic and providing me with his feedback and advice, he was encouraging, never pressuring me, which helped to put me in the right mindset.

No matter the outcome, conducting this thesis from start to finish was a personal success. Because parents and family play a substantial role in one's development, they must share the biggest part of my success today: they too should be proud of themselves.

To my friends and to Anna, one way or another you helped shaping me into the person who made it to here: thank you.

Abstract

In the context of elliptic, PDE constrained shape optimization, it has already been noted that a distributed expression for the shape gradient is more accurate than the boundary counterpart, when finite elements are employed to discretize the arising PDEs.

We further explore these observations in two directions: first, we work in a parabolic setting and second, we explicitly address the fact that finite element solutions live on polygons/polyhedra, but they approximate functions defined on smooth domains. We therefore prove, and numerically verify, semidiscrete estimates in a spatially semidiscrete setting, and fully discrete estimates when the implicit Euler or Crank-Nicolson methods are adopted for the time discretization.

Our analysis is based on a model shape optimization problem for the heat equation, where the goal is to determine the shape of a zero temperature inclusion given the temperature and heat flux at an external boundary. For such problem, the shape gradient is derived, a star-shaped ansatz is applied, and numerical results are presented and discussed.

Contents

1. Introduction

To simulate PDE-constrained shape optimization problems, a discretization of several "continuous" quantities has to be performed. In particular, suitable numerical methods for the involved partial differential equations must be adopted, and then, an optimization routine has to be implemented, so as to obtain a hopefully reasonable estimate of the sought analytical solution.

The accuracy of the optimization procedure is influenced by many factors. In particular, when using gradient based optimization, one would like the discretized shape gradient to be best possible approximation to the continuous counterpart. There is a major design choice playing a role here, which is whether a boundary or distributed/volumetric approach is taken: when sufficient smoothness is available, the boundary and distributed expressions of the shape gradient are equivalent, on the continous level, and this is the content of the so-called "structure theorem" (see theorem 1.4 of [59]). This equivalence, however, often breaks down on the discrete level, and one has to decide the form with which to work. There are of course advantages and disadvantages to both views (see e.g. [59]), but there seems to be numerical evidence for a superior accuracy of the latter over the former, at least when the finite element method is adopted to approximate partial differential equations. Theoretical analysis backing up this observation was presented in the work [40]. They analyzed a model elliptic problem, and showed that the discretized shape gradient can be expected to be a second order approximation to the continuous one in the volumetric case, only a first order one with the boundary approach. The use of the FEM method is motivated there by its popularity, generality and flexibility, for engineering applications.

Such conclusions are however only drawn in an elliptic setting, but parabolic shape optimization has important applications too (see e.g. [12], [38] to mention a few), and deserves further analysis. With this in mind, we try to extend the observations of [40] in two ways:

- on one hand, we consider a time-dependent setting
- on the other one we try to account for the fact that continuous shape gradients are based on a smooth domain, whereas the discretized quantities naturally live on simplicial meshings of the latter

To this end, we borrow a model parabolic shape optimization problem from [38] and center our arguments around it. In [38], boundary expressions for the shape gradients are derived, and PDEs are approximated using the boundary element method. While this choice provides computational efficiency, it sacrifices generality (more complicated PDEs need not to be easily convertible to boundary integral equations). We take, in contrast, a distributed/volumetric approach and employ finite elements for the partial differential equations. As a byproduct, we obtain a very easy implementation that is amenable to pre-existing, high-performance software packages, such as FEniCS ([49]) and dolfin-adjoint ([32], [23], [52]).

This thesis is then structured as follows:

- in chapter 2, we introduce the model parabolic shape optimization problem, and proceed to compute the continuous shape gradient. We also discuss the star-shaped parametrization of domains that we adopted, for simplicity, in the implementation
- chapter 3 is then about the finite element discretization of the PDEs and of the geometry. Estimates for the errors between discrete and continuous shape gradients are given, under the assumptions that the discrete domain interpolates the continuous domain at the boundary nodes. The analysis is satisfactory when the implicit Euler method is adopted in time, where we show that optimization and discretization commute, by employing a suitable scheme for the adjoints. We conjecture that such commutation is achievable also when adopting the Crank-Nicolson method and motivate this belief with theoretical and numerical arguments. In any case, as a replacement, similar estimates for the Crank-Nicolson method are derived in an optimize-then-discretize setting
- in chapter 4 we discuss our implementation and conduct two sets of experiments: on one hand we illustrate results for the shape optimization of the model problem, and on the other hand we provide numerical evidence for the error estimates of chapter 3
- chapter 5 contains a brief summary of the thesis and lists some possible future research directions

For exposition purposes, we delegated many technicalities to appendices:

- some useful results from functional analysis are collected in appendix A
- many details about the parabolic equations that appear in the thesis can be found in appendix B
- several facts about domains deformations are found in appendix C
- in appendix D, the adopted finite element framework, in the context of smooth geometries, is explained

2. Infinite dimensional setting

This chapter is devoted to the analysis of the non-discretized shape optimization problem:

- in section 2.1 we introduce the shape identification problem we are interested in
- in section 2.2 we reformulate it as a shape optimization problem, and compute the shape gradient of the cost functional to be minimized
- in section 2.3, we discuss the ansatz that the sought domains are star-shaped, to give some justification to our computer implementation
- in section 2.4 we further justify our implementation, that is fully discussed in section 4.1, with respect to the scalar product in which optimization is performed

2.1. Shape identification problem

Let $D \subseteq \mathbb{R}^n$ be a sufficiently smooth domain, and $\Omega \subset\subset D$. We then call $\Gamma_f = \partial D$, $\Gamma_m = \partial \Omega$. We let $T > 0$ and $I = (0, T)$, $\Sigma_f = I \times \Gamma_f$, $\Sigma_m = I \times \Gamma_m$.
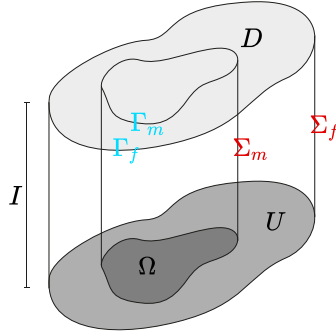

Figure 2.1.: Space-time cylinder with labels

Let us interpret D as a uniform and isotropic body, inside which an inclusion of zero temperature Ω is present (think of an ice cube submerged in water). The temperature u inside $D \setminus \Omega = U$ evolves over time according to the heat equation, at least approximately. We are interested in obtaining the shape of the inclusion, which we suppose to be not accessible, i.e. we cannot directly measure it. We are however allowed to access the outer boundary ∂D and measure surface temperature and normal heat flux: we ask ourselves how to recover such shape from the knowledge of this boundary data only. This is a non-linear and ill-posed inverse problem (according to e.g. [38]).

Summing up, our task is, given the outer temperature and heat flux, to reconstruct the shape of Ω that induced, through heat diffusion, those boundary quantities.

In more mathematical terms, let us consider a heat equation on the unknown cylinder $U \times I$, with zero initial condition and no volumetric forcing term, where on Σ_f are prescribed smooth enough Dirichlet and Neumann data simultaneously (call them f and g, they correspond to the outer temperature and heat flux), while on Σ_m, homogeneous Dirichlet conditions.

> **Problem 2.1.1** (Overdetermined heat equation)
> Call $U := D \setminus \Omega$. We look for $u : U \times I \to \mathbb{R}$ solving:
> $$\begin{cases} u_t - \Delta u = 0 & \text{on } U \times I \\ u(0) = 0 \\ u = f, \partial_\nu u = g & \text{on } \Sigma_f \\ u = 0 & \text{on } \Sigma_m \end{cases}$$
>
> We introduce the splitting:
>
> $$\begin{cases} v_t - \Delta v = 0 & \text{on } U \times I \\ v(0) = 0 \\ v = f & \text{on } \Sigma_f \\ v = 0 & \text{on } \Sigma_m \end{cases} \quad , \quad \begin{cases} w_t - \Delta w = 0 & \text{on } U \times I \\ w(0) = 0 \\ \partial_\nu w = g & \text{on } \Sigma_f \\ w = 0 & \text{on } \Sigma_m \end{cases}$$

It can be in fact shown that, for arbitrary f, g, there exists at most one Ω such that problem 2.1.1 is solvable (see [18], [17])

We can leverage this property to find a numerical approximation for such domain. In particular, the equations for v, w are always uniquely solvable, and $u = v, u = w$, in case u exists, i.e. when the shape identification problem admits a solution. One way to proceed is therefore, given data f, g and a guess $\hat{\Omega}$ of the sought domain, to simulate v, w on $\hat{\Omega}$, measure their discrepancy $\|v - w\|$ and use this knowledge to improve the iterate $\hat{\Omega}$ and get closer to the actual inclusion Ω, by trying to minimize $\|v - w\|$.

Summing up, the thesis is devoted to the analysis of the following problem.

> **Problem 2.1.2** (Shape identification problem)
> We aim at finding Ω such that u, defined in problem 2.1.1, exists, i.e. such that $v = w$.

This same problem was addressed in [38] using a slightly different approach than us, involving boundary integral equations, boundary element methods and non-standard time stepping schemes. On the other hand our focus has a rather "volumetric" flavour, as we will make clear in the following chapters, and we make use of the well known implicit Euler or Crank-Nicolson algorithms.

As already mentioned, some uniqueness results for problem 2.1.2 are already available. We are not concerned with the problem of existence of Ω, likewise this aspect is not addressed in the aforementioned work [38]. Some advances in this direction were made in the case where Ω is allowed to evolve with time, this is addressed in [14].

In the following we will formalize assumptions, setting and notation, and we will tackle problem 2.1.2 by shape optimization techniques.

2.2. Treatment by shape optimization

> **Assumption 2.2.1** (Geometry assumptions for the shape optimization problem)
> Let $D \subseteq \mathbb{R}^n$ be a bounded Lipschitz domain, and $\Omega_r \subset\subset D$ also bounded Lipschitz. Call $U_r := D \setminus \Omega_r$, another bounded Lipschitz domain, the so-called "reference domain".

> **Definition 2.2.2** (Admissible transformations)
> Given D, we consider the set $\mathcal{T}$ of bi-Lipschitz homeomorphshisms of $\mathbb{R}^n$ that fix D^c, endowed with the "perturbation space" Θ of Lipschitz deformation fields that vanish on D^c. See also definition C.1.3.
> We will consider transformations of U_r that belong to $\mathcal{T}_a := \mathcal{T} \cap \{\tau \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n), \|\tau - \mathrm{Id}\|_{W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)} < C(U_r)\}$, where the presence of the bound by $C(U_r)$ is to ensure that $\tau(U_r) \subset\subset D$ is also bounded Lipschitz, and the existence of such constant is guaranteed by theorem C.1.6.

We remark that there exists a unique Lipschitz continuous representative T of $\tau \in \mathcal{T}_a$ (see proposition A.1.2), and that we denote it also by τ, for simplicity: by $\tau(U_r)$ we precisely mean $T(U_r)$.

We now recast problem 2.1.2 into a new form, suitable for shape optimization, as done in [38]. We mention that the equations for v, w of problem 2.1.1 are well posed, this is discussed in detail in the appendix, for the sake of presentation. We remark that, given any extension $\bar{u}$ to f onto $U \times I$, then v decomposes as $v = v_0 + \bar{u}$, where v_0 solves another heat equation with zero Dirichlet conditions. We therefore write $v^\tau = v_0^\tau + \bar{u}, w^\tau$ to emphasize the dependence on τ, and refer the reader to problem B.2.2, eq. (B.2.7) and problem C.4.3 for additional details.

> **Problem 2.2.3** (Shape optimization problem)
> Suppose that assumption 2.2.1, assumption B.2.1 (applied to problem 2.1.1) hold. We want to solve:
> $$\inf_{\tau \in \mathcal{T}_a} \frac{1}{2} \|v^\tau - w^\tau\|^2_{L^2(I, H_\tau)} =: J(\tau)$$
> The notation for the spaces also comes from problem C.4.3: $\cdot_\tau$ means that the space is based on the moving domain $\tau(U_r)$, and $H = L^2, \mathtt{V} = H_0^1, \mathtt{W} = H_{0,m}^1 = \{v \in H^1, v(\Gamma_m) = 0\}$ (see also appendix B.2 for the last space).

Therefore, we are now concerned with finding a function τ, instead of a generic set Ω: this way we can make use of functional analytic techniques and results from optimal control.

> *Observation* 2.2.4 (Tracking type cost functional).
> We have chosen the $L^2(I, L^2)$ norm to measure the discrepancy $v \simeq w$. Apart from having favourable functional analytic properties (Fréchet differentiability, to mention one), such cost functional will also allow us to obtain "better behaved" adjoint states. In fact, contrary to [38], the heat equations for the adjoint states (see proposition 2.2.10) will have more compatibility between initial condition and boundary conditions. This potentially simplifies the numerical analysis of such equations.

Now, let $U := \tau(U_r)$, for $\tau \in \mathcal{T}_a$ and let $\delta\theta \in \Theta$. To find a better (in the sense of the energy J) candidate τ for the solution of problem 2.2.3, we can use gradient information, i.e. perturb our current guess τ in the direction of steepest descent for J, i.e. the shape gradient dJ of J. We are hence interested in finding $J'(\tau) \in \Theta^*$ such that, for all null sequences $\delta\theta_k \to 0$ in Θ, we have:

$$\lim_k \frac{|J(\tau + \delta\theta_k) - J(\tau) - J'(\tau)[\delta\theta_k]|}{\|\delta\theta_k\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}} = 0$$

Note, thanks to proposition C.1.5, a small $\delta\theta \in \Theta$ perturbation of $\tau \in \mathcal{T}_a$, small with respect to the $W^{1,\infty}(D;\mathbb{R}^n)$ topology: it follows that, for k large enough, $\tau + \delta\theta_k \in \mathcal{T}_a$.

> *Observation* 2.2.5.
> To carry out all the reasonings with such a general form of tranformation τ, an assumption of "smallness" (such as the one involving $C(U_r)$) is necessary, to keep $\tau(U_r)$ Lipschitz. A more transparent way of obtaining $\tau(U_r) \subset\subset D$ to be Lipschitz can be found in section 2.3.
> Also note, that τ has a Lipschitz inverse yields $\tau(U_r) \subset\subset D$: for $x \in D$, we have in fact $0 < \delta = \inf_{d \in \partial D} |x - d| \leq \left\|\tau^{-1}\right\|_{W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n)} \inf_{d \in \partial D} |\tau(x) - d|$.

Now, $\tau + \delta\theta_k = (\mathrm{Id} + \delta\theta_k \circ \tau^{-1}) \circ \tau$, and $\mathrm{Id} + \delta\theta_k \circ \tau^{-1}$ is in $\mathcal{T}_a$ (it is in $\mathcal{T}$ by proposition C.1.5 and the reasoning above shows it is also in $\mathcal{T}_a$). We are then equivalently interested in:

$$\lim_k \frac{|J((\mathrm{Id} + \delta\theta_k \circ \tau^{-1}) \circ \tau) - J(\tau) - J'(\tau)[\delta\theta_k]|}{\|\delta\theta_k\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}}$$

We now introduce a Lagrangian functional, so as to derive the expression of the shape gradient dJ of J. There are several ways about this task in the literature (see [59], [16] or [46]). We will adopt that contained in [59]. It requires the PDEs corresponding to $\tau + \delta\theta_k$ to be all reformulated on the base domain $\tau(U_r)$. To transform the PDEs to a different domain we need to consider the variational formulations of $v^{\tau + \delta\theta_k}$ and $w^{\tau + \delta\theta_k}$ and then apply a change of variables to the appearing integrals. This is precisely addressed theorem C.4.2 (whose applicability is ensured by assumption C.4.1, which holds by assumption 2.2.1).

Remembering that k large, i.e. $k \geq K(\tau)$, we have $\tau_k := \mathrm{Id} + \delta\theta_k \circ \tau^{-1} \in \mathcal{T}_a$, as seen above, and having theorem C.4.2 in mind we can set:

$$L_\tau(k, w, v_0, q, p) :=$$

$$\frac{1}{2} \int_I \int_{\tau(U_r)} |v_0 + \bar{u} \circ \tau_k - w|^2 |\det(D\tau_k)| +$$

$$\int_I (w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla w, \nabla q)_{H_\tau} - \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)} +$$

$$\int_I (v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla v_0, \nabla p)_{H_\tau} + \int_I ((\bar{u} \circ \tau_k)', p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla(\bar{u} \circ \tau_k), \nabla p)_{H_\tau}$$

Here $w \in Q_0(I, \mathtt{W}_\tau), v_0 \in Q_0(I, \mathtt{V}_\tau), q \in Q^0(I, \mathtt{W}_\tau), p \in Q^0(I, \mathtt{V}_\tau)$, where the space Q is thoroughly described after its introduction in definition B.3.2, which we recall: $Q(I, V) = H^{1,1} = L^2(I, V) \cap H^1(I, H)$, and Q^0 means the imposition of a zero terminal condition (Q_0 stands for zero initial condition). We have set $A_\tau := (D\tau)^{-1}(D\tau)^{-t}|\det(D\tau)|$.

L_τ is composed of three parts: the cost functional and the two variational formulation of v_0^τ and w^τ, transported to the domain $\tau(U_r)$, which will remain fixed, for the sake of computing the shape gradient.

Note that to be precise, $\bar{u}$ is an extension (any extension in fact, satisfying the conditions of eq. (B.2.7)) of the Dirichlet datum f, on the moving domain $\tau_k(\tau(U_r))$. Because of this, let's fix $\bar{u}_\tau$, an extension of f on $\tau(U_r)$ and choose $\bar{u} := \bar{u}_\tau \circ \tau_k^{-1}$ (note that $\bar{u}$ is a legitimate extension of f, and in particular it satisfies alle the required conditions stated before eq. (B.2.7)).

Therefore, we can state the following definition.

> **Definition 2.2.6** (Lagrangian)
> For a fixed $\tau \in \mathcal{T}_a$ and $k \geq K(\tau)$, for $\tau_k := \mathrm{Id} + \delta\theta_k \circ \tau^{-1} \in \mathcal{T}_a$, we define:
>
> $$L_\tau(k, w, v_0, q, p) =$$
>
> $$\frac{1}{2} \int_I \int_{\tau(U_r)} |v_0 + \bar{u}_\tau - w|^2 |\det(D\tau_k)| +$$
>
> $$\int_I (w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla w, \nabla q)_{H_\tau} - \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)} +$$
>
> $$\int_I (v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla v_0, \nabla p)_{H_\tau} + \int_I (\bar{u}_\tau', p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla \bar{u}_\tau, \nabla p)_{H_\tau}$$
>
> L_τ is defined as a map $\{k \geq K(\tau)\} \times Q_0(I, \mathtt{W}_\tau) \times Q_0(I, \mathtt{V}_\tau) \times Q^0(I, \mathtt{W}_\tau) \times Q^0(I, \mathtt{V}_\tau) \to \mathbb{R}$.
> We call $u = (w, v_0)$, $\pi = (q, p)$ (states and adjoints), $G(k, u, \pi) = L_\tau(k, w, v_0, q, p)$ to ease the notation.
> We also call $b(k, u) = \frac{1}{2} \int_I \int_{\tau(U_r)} |v_0 + \bar{u}_\tau - w|^2 |\det(D\tau_k)|$ and $a(k, u, \pi) = G(k, u, \pi) - b(k, u)$, $E = Q_0(I, \mathtt{W}_\tau) \times Q_0(I, \mathtt{V}_\tau)$, $F = Q^0(I, \mathtt{W}_\tau) \times Q^0(I, \mathtt{V}_\tau)$, the state and adjoint space.

The rest of this section is devoted to applying the averaged adjoint method [59] to our problem, so as to identify the shape gradient expression. To this end we will have to state some properties of the Lagrangian L_τ.

Proposition 2.2.7 (Properties of the Lagrangian)

L_τ satisfies the following properties:

1. $\psi \mapsto a(k, \phi, \psi)$ is linear, no matter what ϕ, k

2. G is Fréchet differentiable with respect to ψ at $(k, \phi, 0)$ for all k, ϕ

3. $d_\psi G(k, \phi, 0)[\delta\psi] = 0$ for all $\delta\psi \in F$, admits a unique solution $\phi = u^k$

4. $[0,1] \ni s \mapsto G(k, su^k + (1-s)u^0, \psi)$ is $AC[0,1]$, no matter what k, ψ

5. G is Fréchet differentiable with respect to ϕ at (k, ψ, ϕ) for all k, ψ, ϕ

6. $[0,1] \ni s \mapsto d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]$ is $L^1(0,1)$, no matter what $k, \psi, \delta\phi$

7. there exists a unique solution $\psi = \pi^k$ to $\int_0^1 d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]ds = 0$ for all $\delta\psi$

In particular $\pi^k = (Q^k \circ \tau^k, P^k \circ \tau^k)$, where we introduced the averaged adjoint problems on the moving domain:

Problem 2.2.8 (Averaged adjoint equations)

$$\begin{cases} -Q^k_t - \Delta Q^k = \frac{v^k_0 - w^k + v^0_0 - w^0}{2} \circ \tau^{-1}_k + \bar{u}_\tau \circ \tau^{-1}_k \\ Q^k(T) = 0 \\ \partial_\nu Q^k = 0 \text{ on } \Sigma_f \\ Q^k = 0 \text{ on } \Sigma_m \end{cases}, \qquad \begin{cases} -P^k_t - \Delta P^k = -\frac{v^k_0 - w^k + v^0_0 - w^0}{2} \circ \tau^{-1}_k - \bar{u}_\tau \circ \tau^{-1}_k \\ P^k(T) = 0 \\ P^k = 0 \text{ on } \Sigma_f \\ P^k = 0 \text{ on } \Sigma_m \end{cases}$$

Proof.

We give some comments for the non trivial points.

Proof of 3

Testing $d_\psi G(k, \phi, 0)[\delta\psi] = $ separately with $\delta\psi = (\delta q, 0)$ and $\delta\psi = (0, \delta p)$ we get back the state equations, so that a unique solution exists by theorem C.4.2 and theorem B.2.6.

Proof of 7

It is readily seen that:

$$\int_0^1 d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]ds =$$

$$\int_I (((v^k_0 + \bar{u}_\tau - w^k) + (v^0_0 + \bar{u}_\tau - w^0))/2|\det(D\tau_k)|, \delta v_0 - \delta w)_{H_\tau} +$$

$$\int_I (\delta w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla\delta w, \nabla q)_{H_\tau} + \int_I (\delta v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla\delta v_0, \nabla p)_{H_\tau} = ...$$

As in proposition C.3.1, for example, $\delta w_t = (\delta w \circ \tau^{-1}_k)_t \circ \tau_k$, where $\delta w \circ \tau^{-1}_k \in Q_0(I, \mathbb{W}_{\tau_k \circ \tau})$ by proposition C.3.1 (that can be applied thanks to the smallness of τ_k). Applying a change of variables we are left with:

$$... = \int_I \left(\frac{v^k_0 - w^k}{2} \circ \tau^{-1}_k + \frac{v^0_0 - w^0}{2} \circ \tau^{-1}_k + \bar{u}_\tau \circ \tau^{-1}_k, \delta v_0 \circ \tau^{-1}_k - \delta w \circ \tau^{-1}_k\right)_{H_{\tau_k \circ \tau}} +$$

$$\int_I ((\delta w \circ \tau^{-1}_k)_t, q \circ \tau^{-1}_k)_{H_{\tau_k \circ \tau}} + (\nabla(\delta w \circ \tau^{-1}_k), \nabla(q \circ \tau^{-1}_k))_{H_{\tau_k \circ \tau}} + \int_I ((\delta v_0 \circ \tau^{-1}_k)_t, p \circ \tau^{-1}_k)_{H_{\tau_k \circ \tau}} + (\nabla\delta(v_0 \circ \tau^{-1}_k), \nabla(p \circ \tau^{-1}_k))_{H_{\tau_k \circ \tau}}$$

Here, as we saw in proposition C.3.1, we have $\delta w \circ \tau^{-1}_k, w \circ \tau^{-1}_k \in Q_0(I, \mathbb{W}_{\tau_k \circ \tau}), \delta v_0 \circ \tau^{-1}_k, v_0 \circ \tau^{-1}_k \in Q_0(I, \mathbb{V}_{\tau_k \circ \tau}), q \circ \tau^{-1}_k \in Q^0(I, \mathbb{W}_{\tau_k \circ \tau})$ and $p \circ \tau^{-1}_k \in Q^0(I, \mathbb{V}_{\tau_k \circ \tau})$.

Because $\circ \tau^{-1}_k$ is a bijection of $Q_0(I, \mathbb{V}_{\tau_k \circ \tau})$ and $Q_0(I, \mathbb{V}_{\tau_k})$ as we saw in proposition C.3.1 (and analogously for $\mathbb{W}$), we have that $\int_0^1 d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]ds = 0$ for all $\delta\phi \in E$ if and only if:

$$\int_I \left(\frac{v^k_0 + w^k}{2} \circ \tau^{-1}_k - \frac{v^0_0 + w^0}{2} \circ \tau^{-1}_k + \bar{u}_\tau \circ \tau^{-1}_k, \delta V_0 - \delta W\right)_{H_{\tau_k \circ \tau}} +$$

$$\int_I (\delta W_t, q \circ \tau^{-1}_k)_{H_{\tau_k \circ \tau}} + (\nabla\delta W, \nabla(q \circ \tau^{-1}_k))_{H_{\tau_k \circ \tau}} +$$

$$\int_I (\delta V_{0t}, p \circ \tau^{-1}_k)_{H_{\tau_k \circ \tau}} + (\nabla\delta V_0, \nabla(p \circ \tau^{-1}_k))_{H_{\tau_k \circ \tau}} = 0$$

for all $\delta W \in Q_0(I, \mathbb{W}_{\tau_k \circ \tau})$, $\delta V_0 \in Q_0(I, \mathbb{V}_{\tau_k \circ \tau})$.

We wish to find a (unique) solution $(q^k, p^k) \in Q^0(I, \mathbb{W}_\tau) \times Q^0(I, \mathbb{V}_\tau)$ of this problem. We can equivalently (by proposition C.3.1) find $(Q^k, P^k) \in Q^0(I, \mathbb{W}_{\tau_k \circ \tau}) \times Q^0(I, \mathbb{V}_{\tau_k \circ \tau})$ satisfying:

$$\int_I \left(\frac{v_0^k - w^k}{2} \circ \tau_k^{-1} + \frac{v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1}, \delta V_0 - \delta W \right)_{H_{\tau_k \circ \tau}} +$$

$$\int_I (\delta W_t, Q^k)_{H_{\tau_k \circ \tau}} + (\nabla \delta W, \nabla Q^k)_{H_{\tau_k \circ \tau}} +$$

$$\int_I (\delta V_{0t}, P^k)_{H_{\tau_k \circ \tau}} + (\nabla \delta V_0, \nabla P^k)_{H_{\tau_k \circ \tau}} = 0$$

for all $\delta W, \in Q_0(I, \mathbb{W}_{\tau_k \circ \tau})$, $\delta V_0 \in Q_0(I, \mathbb{V}_{\tau_k \circ \tau})$.

Upon testing first with $\delta W = 0$ and then with $\delta V_0 = 0$, an application of integration by parts in time (see proposition B.3.3) yields the problems which are the weak formulations (cfr. theorem C.4.2, problem B.2.2 and problem B.2.2) of the PDEs:

$$\begin{cases} -Q_t^k - \Delta Q^k = \frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1} \\ Q^k(T) = 0 \\ \partial_\nu Q^k = 0 \text{ on } \Sigma_f \\ Q^k = 0 \text{ on } \Sigma_m \end{cases}, \quad \begin{cases} -P_t^k - \Delta P^k = -\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} - \bar{u}_\tau \circ \tau_k^{-1} \\ P^k(T) = 0 \\ P^k = 0 \text{ on } \Sigma_f \\ P^k = 0 \text{ on } \Sigma_m \end{cases}$$

Applying the time reversal $t \mapsto T - t$ (where $I = (0,T)$), these are a couple of standard heat equations for which we have available existence, uniqueness and stability results (see appendix B, and theorem B.2.6).

By calling then $\pi^k = (Q^k \circ \tau^k, P^k \circ \tau^k)$ we conclude the proof. $\square$

We now turn to the verification of Gateaux differentiability of J, applying the techniques proposed in [59].

> **Proposition 2.2.9** (Averaged adjoint method for Gateaux derivatives)
> If $J'(\tau) \in \Theta^*$ satisfies:
> $$\lim_k \frac{G(k, u^0, \pi^k) - G(0, u^0, \pi^k)}{t_k} = J'(\tau)[\delta\theta]$$
> where $\delta\theta_k = t_k \delta\theta$ for $t_k \to 0$, then $J'(\tau)$ is the Gateaux derivative of J at τ.

Proof.
See theorem 3.1, [59]. $\square$

> **Proposition 2.2.10** (Gateaux differentiability of J)
> Given $\tau \in \mathcal{T}_a$, J is Gateaux differentiable at τ with respect to the $W^{1,\infty}$ topology. The Gateaux differential is:
> $$J'(\tau)[\delta\theta] =$$
> $$\int_I (w_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), q^\tau)_{L^2(\tau(U_r))} + \int_I (A'(\delta\theta \circ \tau^{-1})\nabla v^\tau, \nabla p^\tau)_{L^2(\tau(U_r))} +$$
> $$\int_I (v_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), p^\tau)_{L^2(\tau(U_r))} + \int_I (A'(\delta\theta \circ \tau^{-1})\nabla w^\tau, \nabla q^\tau)_{L^2(\tau(U_r))} +$$
> $$\frac{1}{2} \int_I \int_{\tau(U_r)} |v^\tau - w^\tau|^2 \operatorname{div}(\delta\theta \circ \tau^{-1})$$
> where p^τ, q^τ solve:
> $$\begin{cases} -q_t^\tau - \Delta q^\tau = v^\tau - w^\tau \\ q^\tau(T) = 0 \\ \partial_\nu q^\tau = 0 \text{ on } \Sigma_f \\ q^\tau = 0 \text{ on } \Sigma_m \end{cases}, \quad \begin{cases} -p_t^\tau - \Delta p^\tau = -v^\tau + w^\tau \\ p^\tau(T) = 0 \\ p^\tau = 0 \text{ on } \Sigma_f \\ p^\tau = 0 \text{ on } \Sigma_m \end{cases}$$
> and where $A'(\delta\theta) = -D\delta\theta - (D\delta\theta)^t + \operatorname{div}(\delta\theta)I$.

Proof.
The shape derivative is linear and bounded
Linearity is immediate. For the boundedness, with C independent of $\delta\theta$, τ:

$$|J'(\tau)[\delta\theta]| \leq C\left(\left\|\operatorname{div}(\delta\theta \circ \tau^{-1})\right\|_{L^\infty(\tau(U_r))} + \left(\sum_{ij}\left\|(A'(\delta\theta \circ \tau^{-1})_{ij}\right\|_{L^\infty(\tau(U_r))}\right)\right) \leq C\left\|\delta\theta\right\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$$

where in the last step we applied proposition C.1.7.

Conclusion

Assume at first that $p^k \rightharpoonup p^0$ in $Q(I, \mathbb{V}_\tau)$ and $q^k \rightharpoonup q^0$ in $Q(I, \mathbb{W}_\tau)$, something which will be later verified. Using that $u^0 = (w^\tau, v_0^\tau)$, and cancelling the boundary integrals:

$$G(k, u^0, \pi^k) - G(0, u^0, \pi^k) =$$

$$\frac{1}{2}\int_I\int_{\tau(U_r)}|v^\tau - w^\tau|^2(|\det(D\tau_k)| - 1)+$$

$$\int_I(w_t^\tau(|\det(D\tau_k)| - 1), q^k)_{H_\tau} + ((A_{\tau_k} - I)\nabla w^\tau, \nabla q^k)_{H_\tau} + \int_I(v_t^\tau(|\det(D\tau_k)| - 1), p^k)_{H_\tau} + ((A_{\tau_k} - I)\nabla v^\tau, \nabla p^k)_{H_\tau}$$

Now, the application $\delta\theta \mapsto \mathrm{Id} + \delta\theta \circ \tau^{-1}$ is Fréchet differentiable at $\delta\theta = 0$, as a map of Θ into $\mathcal{V}^1$, with Fréchet derivative $\delta\theta \circ \tau^{-1}$, which is linear and bounded in $\delta\theta$ by proposition C.1.7.

Also, the maps $\delta\eta \mapsto |\det(D\eta)|$ and $\eta \mapsto (D\eta)^{-1}(D\eta)^{-t}|\det D\eta|$ are Fréchet differentiable at Id, from $\mathcal{V}^1$ into $L^\infty(\mathbb{R}^n;\mathbb{R})$ and $L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})$, as stated in lemma 4.16, page 80 of [46]. Their Fréchet derivatives are $\operatorname{div}(\beta)$ and $I - D\beta - (D\beta)^t$, respectively.

Therefore, composition with $\delta\theta \mapsto \mathrm{Id} + \delta\theta \circ \tau^{-1}$ yields two Fréchet differentiable maps, $\delta\theta_k \mapsto |\det(D\tau_k)|$ and $\delta\theta_k \mapsto A_{\tau_k}$, whose derivatives at 0, in direction $\delta\theta \in \Theta$, are exactly $\operatorname{div}(\delta\theta \circ \tau^{-1})$ and $A'(\delta\theta \circ \tau^{-1})$, so that:

- $|\det(D\tau_k)| - 1 = |\det(D\tau_k)| - 1 - t_k\operatorname{div}(\delta\theta \circ \tau^{-1}) + t_k\operatorname{div}(\delta\theta \circ \tau^{-1}) = o_k^1 + t_k\operatorname{div}(\delta\theta \circ \tau^{-1})$
- $A_{\tau_k} - I = A_{\tau_k} - I - t_kA'(\delta\theta \circ \tau^{-1}) + t_kA'(\delta\theta \circ \tau^{-1}) = o_k^2 + t_kA'(\delta\theta \circ \tau^{-1})$

where $o_1^k \in L^\infty(\mathbb{R}^n;\mathbb{R})$ and $o_2^k \in L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})$ are higher order terms, in L^∞ and with respect to t_k. We can then write $(G(k, u^0, \pi^k) - G(0, u^0, \pi^k))/t_k = a_k + o_k$.

Here:

$$a_k := \frac{1}{2}\int_I\int_{\tau(U_r)}|v^\tau - w^\tau|^2\operatorname{div}(\delta\theta \circ \tau^{-1})+$$

$$\int_I(w_t^\tau\operatorname{div}(\delta\theta \circ \tau^{-1}), q^k)_{H_\tau} + (A'(\delta\theta \circ \tau^{-1})\nabla w^\tau, \nabla q^k)_{H_\tau} + \int_I(v_t^\tau\operatorname{div}(\delta\theta \circ \tau^{-1}), p^k)_{H_\tau} + (A'(\delta\theta \circ \tau^{-1})\nabla v^\tau, \nabla p^k)_{H_\tau}$$

Thanks to the assumed weak convergence, $a_k \to J'(\tau)[\delta\theta]$. So, we still have to show that:

$$o_k := \frac{1}{2}\int_I\int_{\tau(U_r)}|v^\tau - w^\tau|^2 o_k^1 t_k^{-1} + \int_I(w_t^\tau o_k^1 t_k^{-1}, q^k)_{H_\tau} + (t_k^{-1}o_k^2\nabla w^\tau, \nabla q^k)_{H_\tau} + \int_I(v_t^\tau o_k^1 t_k^{-1}, p^k)_{H_\tau} + (t_k^{-1}o_k^2\nabla v^\tau, \nabla p^k)_{H_\tau}$$

goes to zero. This is true thanks to the boundedness of the averaged adjoint states, which stems from their weak convergence, and the properties of o_k^1, o_k^2.

Weak convergence of states

We assumed $p^k \rightharpoonup p^0$ in $Q(I, \mathbb{V}_\tau)$ and $q^k \rightharpoonup q^0$ in $Q(I, \mathbb{W}_\tau)$. We now prove these claims. We show at first $v_0^k \rightharpoonup v_0^0$ in $Q(I, \mathbb{V}_\tau)$ and $w^k \rightharpoonup w^0$ in $Q(I, \mathbb{W}_\tau)$. We do this by uniformly estimating these quantities on k. To do this, we use the equations of $V_0^k := v_0^k \circ \tau_k^{-1}$ and $W^k := w^k \circ \tau_k^{-1}$ (see theorem C.4.2) and theorem B.2.6, to obtain the stability estimates:

$$\left\|V^k\right\|_{C([0;T],H_{\tau_k\circ\tau})}^2 + \left\|V^k\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 + \left\|\nabla V^k\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 + \left\|(V^k)_t\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 \leq C\left\|U^k\right\|_{H^1(I,\mathbb{W}_{\tau_k\circ\tau})}^2$$

$$\left\|W^k\right\|_{C([0;T],H_{\tau_k\circ\tau})}^2 + \left\|W^k\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 + \left\|\nabla W^k\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 + \left\|W_t^k\right\|_{L^2(I,H_{\tau_k\circ\tau})}^2 \leq C\left\|g\right\|_{H^1(I,L^2(\Gamma_f))}^2$$

where C is independent of k.

Now, consider theorem C.2.1. It says that for almost every time:

$$\left\|U^k\right\|_{\mathbb{W}_{\tau_k\circ\tau}} \leq \left(1 + \left\|\det D\tau_k\right\|_{L^\infty(\mathbb{R}^n)}\right)^{1/2}\left\|(D\tau_k)^{-1}\right\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})}\left\|\bar{u}\right\|_{H^1(\tau(U_r));\mathbb{R}^n)}$$

and a similar estimate we have for the first derivative. This bound is uniform on k by proposition C.1.7.

We conclude that $\left\|U^k\right\|_{H^1(I,\mathbb{W}_{\tau_k\circ\tau})}^2$ is bounded and we thus have that $W^k \in Q_0(I, \mathbb{W}_{\tau_k\circ\tau}), V_0^k \in Q_0(I, \mathbb{V}_{\tau_k\circ\tau})$ are bounded.

Now, for almost all times, using theorem C.2.1, we obtain that, for instance:

$$\left\|v_0^k\right\|_{\mathbb{W}_\tau} \leq \left(1 + \left\|\det(D\tau_k)^{-1}\right\|_{L^\infty(\mathbb{R}^n)}\right)^{1/2}\left\|D\tau_k\right\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})}\left\|V_0^k\right\|_{H^1(\tau_K(\tau(U_r)))}$$

where we remember that H_0^1 was chosen to be normed with the full H^1 norm.

The same goes for w^k and the first derivatives in time, yielding that $w^k \in Q_0(I, \mathtt{W}_\tau), v_0^k \in Q_0(I, \mathtt{V}_\tau)$ are bounded.

We thus have $w^k \rightharpoonup w^? \in Q_0(I, \mathtt{W}_\tau)$, $v_0^k \rightharpoonup v_0^? \in Q_0(I, \mathtt{V}_\tau)$, in the weak topologies of, respectively, $Q(I, \mathtt{W}_\tau), Q(I, W_\tau)$, and modulo subsequences. The initial values are preserved because Q_0 is closed and convex in the Hilbert space Q (see also proposition B.3.3).

We now prove that $w^? = w^0$, $v^? = v^0$, and this will yield the weak convergence of the whole sequence. To prove e.g. that $v^? = v^0$, let us look at the weak formulations of v_0^k:

$$\int_I (v_{0t}^k, p | \det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla v_0^k, \nabla p)_{H_\tau} + (\bar{u}', p | \det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla \bar{u}, \nabla p)_{H_\tau} = 0$$

for all $p \in Q_0(I, \mathtt{V}_\tau)$. Let's analyze the first term, which is $\int_I (v_{0t}^k, p | \det(D\tau_k)|)_{H_\tau} = (v_{0t}^k, p | \det(D\tau_k)|)_{L^2(I, H_\tau)}$. We can write:

$$(v_{0t}^k, p | \det(D\tau_k)|)_{L^2(I, H_\tau)} = (v_{0t}^k, p)_{L^2(I, H_\tau)} + (v_{0t}^k, p(| \det(D\tau_k)| - 1))_{L^2(I, H_\tau)}$$

Because $p \in Q(I, \mathtt{V}_\tau)$, the first term converges to $(v_{0t}^?, p)_{L^2(I, H_\tau)}$. The other term can be estimated as follows:

$$|(v_{0t}^k, p(| \det(D\tau_k)| - 1))_{L^2(I, H_\tau)}| \le \left\| v_{0t}^k \right\|_{L^2(I, H_\tau)} \|p\|_{L^2(I, H_\tau)} \|| \det(D\tau_k)| - 1\|_{L^\infty}$$

where the first term in the product is bounded by the weak convergence property, and the last one goes to 0 by continuity, see again proposition C.1.7. In a similar fashion for the other pieces, and by passing to the limit:

$$\int_I (v_{0t}^?, p)_{H_\tau} + (\nabla v_0^?, \nabla p)_{H_\tau} + (\bar{u}', p)_{H_\tau} + (\nabla \bar{u}, \nabla p)_{H_\tau} = 0$$

so that $v^? = v^0$.

Weak convergence of averages adjoint states

So, $v_0^k \rightharpoonup v_0^0, w^k \rightharpoonup w^0$ in $Q(I, \mathtt{V}_\tau)$ and $Q(I, \mathtt{W}_\tau)$. We now claim that $p^k \rightharpoonup p^0, q^k \rightharpoonup q^0$, and prove this similarly to before. We bound $P^k := p^k \circ \tau_k^{-1}$ and $Q^k := q^k \circ \tau_k^{-1}$. By proposition B.1.8, we will obtain a bound in Q as soon as we have a bound on $\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1}$ in the $L^2(I, H)$ norm, and of $U^k := \bar{u}_\tau \circ \tau_k^{-1}$. The latter was proven above.

So, by theorem C.2.1 and proposition C.1.7, it suffices to have an $L^2(I, H)$ bound on $\frac{v_0^k + w^k + v_0^0 + w^0}{2} \circ \tau_k^{-1} \circ \tau_k = \frac{v_0^k + w^k + v_0^0 + w^0}{2}$ which we have, since we just proved that v_0^k, w^k are weakly convergent in e.g. $L^2(I, H)$. We conclude that Q^k, P^k are bounded in the $Q(I, \mathtt{W}_{\tau_k \circ \tau})$ and $Q(I, \mathtt{V}_{\tau_k \circ \tau})$ sense, so that, just as above, a bound on q^k, p^k in the $Q(I, \mathtt{W}_\tau)$ and $Q(I, \mathtt{V}_\tau)$ can be obtained.

We conclude that there exist $q^?, p^?$ in $Q^0(I, \mathtt{W}_\tau), Q^0(I, \mathtt{V}_\tau)$, that are, modulo subsequences, the weak limits of q^k, p^k. To show e.g. $q^? = q^0$ and conclude the convergence of the full sequence, we analyze the weak formulation of q^k, which reads, after going to the moving domain and applying integration by parts in time (see proposition B.3.3):

$$-\int_I \left(\frac{((v_0^k + \bar{u}_\tau - w^k) + (v_0^0 + \bar{u}_\tau - w^0)}{2} \right) | \det(D\tau_k)|, \delta w)_{H_\tau} = -\int_I (q_t^k, \delta w | \det(D\tau_k)|)_{H_\tau} + (A_{\tau_k} \nabla \delta w, \nabla q^k)_{H_\tau}$$

for all $\delta w \in Q_0(I, \mathtt{W}_\tau)$.

We show the convergence of e.g. the member: $\int_I (v_0^k | \det(D\tau_k)|, \delta w)_{H_\tau}$. By splitting the scalar product as we saw above, we are left with checking that $\int_I (v_0^k, \delta w)_{H_\tau} \to \int_I (v_0^0, \delta w)_{H_\tau}$, which is true, since we proved that $v_0^k \rightharpoonup v_0^0$ in $Q(I, \mathtt{V}_\tau)$. We conclude, upon passing to the limit, that:

$$-\int_I \left(\frac{((v_0^0 + \bar{u}_\tau - w^0) + (v_0^0 + \bar{u}_\tau - w^0)}{2}), \delta w \right)_{H_\tau} = -\int_I (q_t^?, \delta w)_{H_\tau} + (\nabla \delta w, \nabla q^?)_{H_\tau}$$

which is satisfied also by q^0, therefore $q^? = q^0$ and we have weak convergence of the entire sequence. $\qquad\square$

2.3. Star-shaped reparametrization

Here we reparametrize the shape optimization problem assuming the domains $D, \Omega = \tau(\Omega_r)$ to be star-shaped with respect to the origin. We do this to justify our computer implementation. In particular, we define and analyze certain maps that convert functions defined on spheres to "radial" deformation fields on $D \setminus \Omega$ (see below for details), and based on those, detail the expression of the shape gradient of proposition 2.2.10. This will be the result of proposition 2.3.6. Essentially, this section is concerned with connecting the analysis done previously with general tranformations τ, to more special radial transformations, employing and adapting the framework of [22]. We start by recalling the definition of star-shaped domain.

Proposition 2.3.1 (Star shaped boundary)
Let $f \in C(\mathbb{S}^{n-1})$, $f > 0$. Define $\Omega_f := \{x, |x| < f(\hat{x})\} \cup \{0\}$, where $\hat{x} = x/|x|$. Then:

- Ω_f is open

- Ω_f has boundary $\{x, |x| = f(\hat{x})\}$

- Ω_f is a bounded Lipschitz domain

Proof.

For $x \in \partial \Omega_f$ (so, $x \neq 0$) we find $x_n, y_n \to x$ with $|x_n| < f(\widehat{x_n})$ and $|y_n| \geq f(\widehat{y_n})$. For large n and by continuity, $|x| = f(\hat{x})$ and we have shown one inclusion.

For the reverse, and $x, |x| = f(\hat{x})$ (so, $x \neq 0$), we define $x_n = \frac{n}{n+1}x$ which satisfies $|x_n| < |x| = f(\hat{x}) = f(\widehat{x_n})$, that is, $x_n \in \Omega_f$, and also $x_n \to x$. This shows that $x \in \partial \Omega_f$.

It is a bounded Lipschitz domain by lemma 2 at page 96 of [15], and lemma 5 at page 151 also of [15]. Note that the definition of Lipschitz domain of [15] is completely equivalent to that of [3] (and at least implies that of [50], [36], [45], [1], a fact which is needed in the sequel), by an application of the Lebesgue number lemma, whose statement can be found at e.g. page 179 of [53]. $\square$

We now define maps relating a radial function to its correspondent a star-shaped domain. We choose $0 < \epsilon < f_D \in W^{1,\infty}(\mathbb{S}^{n-1})$, to parametrize the non moving part of the optimization domain. The reference domain U_r is taken to be $U_r := \Omega_{f_D} \setminus \overline{B}_\epsilon$, and we call $D := \Omega_{f_D}$

Proposition 2.3.2 (H_f, A_f)
Let $\epsilon < f_D \in W^{1,\infty}(\mathbb{S}^{n-1})$ and $0 < f \in W^{1,\infty}(\mathbb{S}^{n-1})$, $f < f_D$, and define:

- $H_f(x) := \begin{cases} \frac{x}{\epsilon}f(\hat{x}) & x \neq 0 \\ 0 & x = 0 \end{cases}$, as a function $\mathbb{R}^n \to \mathbb{R}^n$

- $A_f(x) := \left(f(\hat{x}) + \frac{f_D(\hat{x})-f(\hat{x})}{f_D(\hat{x})-\epsilon}(|x|-\epsilon) \right) \hat{x}$, as a function $\mathbb{R}^n \setminus \{0\} \to \mathbb{R}^n$

They enjoy the following properties:

1. $H_f(B_\epsilon) = \Omega_f$, $H_f(\epsilon \mathbb{S}^{n-1}) = \partial \Omega_f$

2. $A_f(D \setminus \overline{B}_\epsilon) = D \setminus \overline{\Omega_f}$, $A_f(\partial D) = \text{Id}$, $A_f(\epsilon \mathbb{S}^{n-1}) = \partial \Omega_f$

3. $A_f = H_f$ on $\epsilon \mathbb{S}^{n-1}$

4. $H_f^{-1}(y) := \begin{cases} \epsilon \frac{y}{f(\hat{y})} & y \neq 0 \\ 0 & y = 0 \end{cases}$, as a function $\mathbb{R}^n \to \mathbb{R}^n$

5. $A_f^{-1}(y) := \left(\epsilon + \frac{f_D(\hat{y})-\epsilon}{f_D(\hat{y})-f(\hat{y})}(|y| - f(\hat{y})) \right) \hat{y}$, as a function $\overline{D} \setminus \Omega_f \to \overline{D} \setminus B_\epsilon$

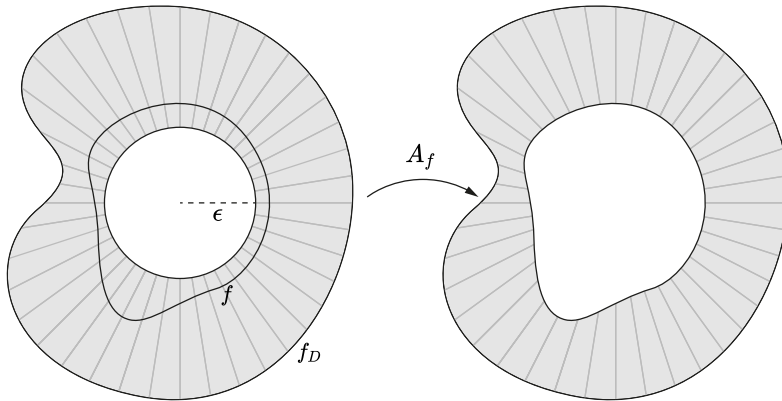Figure 2.2.: Illustration of the action of A_f

Proof.

All the properties are straightforward from the definitions. It helps to recognize that A_f is just the linear map from the radial segment $[\epsilon, f_D(\hat{x})]$ to $[f(\hat{x}), f_D(\hat{x})]$ and that $\overline{\Omega_{f_D}} \setminus \Omega_f = \{f(\hat{x}) \leq |x| \leq f_D(\hat{x})\}$ $\square$

They also satisfy a bi-Lipschitz condition.

Proposition 2.3.3 (Bi-Lipschitz condition)
We have that $A_f : \overline{D} \setminus B_\epsilon \to \overline{D} \setminus \Omega_f$ is Lipschitz with Lipschitz inverse (bi-Lipschitz), and so is $H_f : \mathbb{R}^n \to \mathbb{R}^n$.

Proof.

The second part of the proposition is contained in [22] in a weaker form, we therefore proceed to prove all the statements.

$\underline{H_f}$

We can assume both $x, y \neq 0$. Then $|f(\hat{x})x - f(\hat{y})y| \leq |x||f(\hat{x}) - f(\hat{y})| + f(\hat{y})|x - y|$. Employing direct and reverse triangle inequalities we get $|\hat{x} - \hat{y}| \leq \frac{2}{|x|}|x - y|$. As f is Lipschitz (see [22]) we obtain: $|f(\hat{x})x - f(\hat{y})y| \leq |x|C(f)\frac{2}{|x|}|x - y| + C(f)|x - y|$.

Now, $1/f$ is also Lipschitz and bounded, because $f > 0$ and is continuous on a compact set. Thus the same proof shows the Lipschitz property also for H_f^{-1}.

$\underline{A_f}$

Call $A_f(x) = \left(f(\hat{x}) + \frac{f_D(\hat{x}) - f(\hat{x})}{f_D(\hat{x}) - \epsilon}(|x| - \epsilon) \right) \hat{x} =: Q(x)\hat{x}$. Because $|x| \geq \epsilon$, as before, we obtain $|A_f(x) - A_f(y)| \leq 2/\epsilon Q(x)|x - y| + |Q(x) - Q(y)|$, so that we need to show that Q is bounded Lipschitz.

By continuity and compactness, $f_D(\hat{x}) - \epsilon \geq \delta > 0$ and boundedness follows. The Lipschitz property follows because Q is a sum of products of bounded Lipschitz functions. For instance, $f_D(\hat{x})$ is bounded and Lipschitz because $|x| \geq \epsilon$, as before, and so is $f_D(\hat{x}) - \epsilon$. It is a bounded Lipschitz function that is uniformly greater than δ, so that its reciprocal is also a bounded Lipschitz function.

Analogous reasonings let us prove also the Lipschitz property of A_f^{-1}. $\qquad\square$

We now try to glue H_f, A_f together to still obtain a bi-Lipschitz function. Even the Lipschitz property doesn't hold in general, see page 7 of [63] for a counterexample. We therefore proceed to the proof of this fact.

Proposition 2.3.4 (Gluing H_f^{-1}, A_f^{-1})
H_f^{-1}, A_f^{-1}, or also A_f, H_f can be glued into a Lipschitz function $\overline{D} \to \overline{D}$.

Proof.

Call τ_f^{-1} the gluing. It is Lipschitz $\overline{D} \to \overline{D}$ if and only if $\tau_f^{-1} \circ H_f$ is Lipschitz $H_f^{-1}(\overline{D}) \to \mathbb{R}^n$, because we proved that H_f is bi-Lipschitz $\mathbb{R}^n \to \mathbb{R}^n$. We are therefore left to prove that gluing Lipschitz functions along $\mathbb{S}^{n-1}$ produces a Lipschitz function, which would also yield the claim for τ_f, that is the gluing of A_f, H_f. Note that by the preceding proposition, all the functions to be glued are Lipschitz and agree on their overlaps.

Gluing lemma for Lipschitz functions on $\mathbb{S}^{n-1}$

Let $A \supseteq \overline{B_\epsilon}$ be a set. Suppose that $g : A \to \mathbb{R}^n$ and $h : \overline{B_\epsilon} \to \mathbb{R}^n$ are Lipschitz and that they agree on $\epsilon \mathbb{S}^{n-1}$. Call f their gluing.

For the proof we can assume that $x \in B_\epsilon$, $y \in A \setminus \overline{B_\epsilon}$. Then, $|f(x) - f(y)| \leq |h(x) - h(\epsilon \hat{y})| + |g(\epsilon \hat{y}) - g(y)|$.

We claim at first that $|y - \epsilon \hat{y}| \leq |x - y|$. To see this, choose $n := \hat{y}$. Then $|y - x|^2 \geq |(y - x) \cdot nn|^2$ by Pythagoras' theorem, so that $|y - x| \geq |(y - x) \cdot n| = |(y - \epsilon \hat{y}) \cdot n + (\epsilon \hat{y} - x) \cdot n|$. But $(y - \epsilon \hat{y}) \cdot n = |y| - \epsilon \geq 0$, and $(\epsilon \hat{y} - x) \cdot n = \epsilon - x \cdot n \geq 0$ as $x \cdot n \leq |x| \leq \epsilon$. Thus $|y - x| \geq |(y - \epsilon \hat{y}) \cdot n| + |(\epsilon \hat{y} - x) \cdot n| \geq |(y - \epsilon \hat{y}) \cdot n| = |y - \epsilon \hat{y}|$.

We also claim that $|x - \epsilon \hat{y}| \leq |x - y|$. To do so, pick $n := \frac{\epsilon \hat{y} - x}{|\epsilon \hat{y} - x|}$. By Pythagoras' theorem we obtain $|y - x| \geq |(y - x) \cdot n| = |(y - \epsilon \hat{y}) \cdot n + (\epsilon \hat{y} - x) \cdot n|$. The second summand is non-negative and for the first one, it is directly proportional to $(y - \epsilon \hat{y}) \cdot (\epsilon \hat{y} - x) = (|y| - \epsilon)(\epsilon - \hat{y} \cdot x) \geq 0$. So, $|x - y| \geq |(\epsilon \hat{y} - x) \cdot n| = |\epsilon \hat{y} - x|$.

Thus $|f(x) - f(y)| \leq C|x - y|$ as desired. $\qquad\square$

Corollary 2.3.5 (Radial to volumetric transformation)
Let again $\epsilon < f_D \in W^{1,\infty}(\mathbb{S}^{n-1})$ and $0 < f \in W^{1,\infty}(\mathbb{S}^{n-1}), f < f_D$. Define:

- $\tau_f(x) := \begin{cases} x & |x| \geq f_D(\hat{x}) \\ \left(f(\hat{x}) + \frac{f_D(\hat{x}) - f(\hat{x})}{f_D(\hat{x}) - \epsilon}(|x| - \epsilon) \right) \hat{x} & \epsilon \leq |x| \leq f_D(\hat{x}) \\ \frac{x}{\epsilon} f(\hat{x}) & 0 < |x| \leq \epsilon \\ 0 & |x| = 0 \end{cases}$

- $\tau_f^{-1}(y) := \begin{cases} x & |y| \geq f_D(\hat{y}) \\ \left(\epsilon + \frac{f_D(\hat{y}) - \epsilon}{f_D(\hat{y}) - f(\hat{y})}(|y| - f(\hat{y})) \right) \hat{y} & f(\hat{y}) \leq |y| \leq f_D(\hat{y}) \\ \epsilon \frac{y}{f(\hat{y})} & 0 < |y| \leq f(\hat{y}) \\ 0 & |y| = 0 \end{cases}$

Then $\tau_f \in \mathcal{T}$, i.e. it is a bi-Lipschitz homeomorphism.

Proof.

The final gluing on the border of D yields a Lipschitz function: we can see this by taking $\mathrm{Id} - \tau_f^{\pm 1}$, which is Lipschitz and vanishing on ∂D, so that we are considering the zero extension outside D of a Lipschitz function, null on ∂D. Such extension is readily shown to be Lipschitz. $\qquad\square$

Note that, as long as $f < f_D$, $\tau_f(B_\epsilon)$ will always be a bounded Lipschitz domain.

We finally have a look at shape derivatives in this radial framework. The reparametrized cost functional is $j(q) := J(\tau_{\epsilon+q})$, where $0 < q + \epsilon < f_D$. We are interested, for $h \in W^{1,\infty}(\mathbb{S}^{n-1})$, in the limit

$$\lim_{t \to 0} \frac{j(q + th) - j(q)}{t} = \lim_{t \to 0} \frac{J(\tau_{\epsilon+q+th}) - J(\tau_{q+\epsilon})}{t}$$

Now, we derive the expression of a displacement field V_h, to connect this difference quotient to the already computed shape derivative, see also [22]. The ansatz $\tau_{q+th} = (\mathrm{Id} + tV_h \circ \tau_q^{-1}) \circ \tau_q$ brings us to $V_h = \frac{\tau_{q+th} - \tau_q}{t}$, and by some computations, we obtain:

$$V_h(x) := \begin{cases} 0 & |x| \geq f_D(\hat{x}) \\ h(\hat{x}) \frac{f_D(\hat{x}) - |x|}{f_D(\hat{x}) - \epsilon} \hat{x} & \epsilon \leq |x| \leq f_D(\hat{x}) \\ \frac{x}{\epsilon} h(\hat{x}) & 0 < |x| \leq \epsilon \\ 0 & |x| = 0 \end{cases}$$

This expression only depends on h and is the gluing of Lipschitz functions, that are either 0 at the gluing points, or such that the gluing points lie in $\epsilon \mathbb{S}^{n-1}$. Note, this vector field is just moving $\epsilon \mathbb{S}^{n-1}$ radially by h and radially damping this movement to 0 close to ∂D. Therefore:

> **Proposition 2.3.6** (Shape derivative, star shaped case)
> We have the following facts, for $h \in W^{1,\infty}(\mathbb{S}^{n-1})$, $0 < q < f_D$, $q \in W^{1,\infty}(\mathbb{S}^{n-1})$:
>
> - $\tau_{q+th} = (\mathrm{Id} + tV_h \circ \tau_q^{-1}) \circ \tau_q$
>
> - $V_h \in \Theta$
>
> - j is Gateaux differentiable at every $0 < q < f_D$, $q \in W^{1,\infty}(\mathbb{S}^{n-1})$, with $j'(q)[h] = J'(\tau_{\epsilon+q})[V_h]$

Proof.

We only need to show that $h \mapsto V_h$ is linear bounded between $W^{1,\infty}(\mathbb{S}^{n-1}) \to \Theta$. Linearity is immediate and for the boundedness: $\sup_x |V_h(x)| = \|h\|_\infty$, and we only therefore need to bound the Lipschitz constant of V_h.

We only need to restrict ourselves to $\overline{D}$, as extending to zero a Lipschitz function doesn't increase its Lipschitz constant.

The gluing lemma from the proof of proposition 2.3.4 shows that it is sufficient to bound the Lipschitz constants of the two branches of V_h, separately. These bounds are, respectively: $C(\|h\|_\infty + 2\|D_T h\|_\infty)$ and $[2\epsilon^{-1}(\|D_T h\|_\infty + \|h\|_\infty)]C + C\|h\|_\infty$, where $C = (\epsilon, f_D) > 0$, which concludes the proof. $\square$

2.3.1. Smooth star-shaped domains

To ensure that U has the smoothness required to perform numerical analysis, we want to increase the regularity of f and see an increase in the regularity of $\partial \Omega_f$.

> **Proposition 2.3.1.1** (Smooth radial function yields smooth star shaped domain)
> Let $f > 0$ which is either $C^{1,1}(\mathbb{S}^{n-1})$ (that is, C^1 with all the components of $D_T f$ Lipschitz) or $C^2(\mathbb{S}^{n-1})$.
> Then, Ω_f has boundary of class $C^{1,1}$ or C^2.

Proof.

In what follows we generically write C^o, $o = 1, 1$ or $o = 2$.

A punctured diffeomorphism of class C^o

We consider H_f, setting $\epsilon = 1$ for simplicity. It has gradient (see [22]) $DH_f(x) = f(\hat{x})I + \hat{x} \otimes D_T f(\hat{x})$, and $DH_f^{-1}(y) = 1/f(\hat{y})I - 1/f(\hat{y})^2 \hat{y} \otimes D_T f(\hat{y})$. These quantities are C^o away from the origin. In particular H_f is C^o outside of $B_\delta(0)$, $\delta < 1$. $H_f(B_\delta)$ contains a ball around the origin, and the complement $H_f(B_\delta)^c$ contains Ω_f.

We conclude that $H_f : \overline{B_\delta(0)}^c \to \overline{H_f(B_\delta(0))}^c$ is a C^o diffeomorphism, where the set on the right is open by H_f being a homeomorphism of $\mathbb{R}^n$. The Lipschitz regularity of the gradients follows from the Lipschitz property and boundedness of every factor, and the fact that we are working away from the origin. In particular, $D_T f$ is Lipschitz, therefore continuous, on the sphere, and so bounded too.

We have therefore obtained a homeomorphism $\mathbb{R}^n \to \mathbb{R}^n$, which is C^o as $\overline{B_\delta(0)}^c \to \overline{H_f(B_\delta(0))}^c$, so, in a neighbourhood of $\partial \Omega_f$. For simplicity let's refer to such maps as C^o punctured diffeomorphisms for Ω_f.

Punctured diffeomorphism and C^o domains

Let Ω be of class C^o (always locally) and bounded. Assume we have F, a punctured diffeomorphism for Ω, so, $F : \mathbb{R}^n \to \mathbb{R}^n$ is a homeomorphism, and $F : U \to F(U)$ is C^o, $\partial \Omega \subset\subset U$. Then, by analyzing the composition of F with (small enough) charts of Ω we see that $F(\Omega)$ is another C^o domain.

From diffeomorphisms to graphs

Let Ω be any C^o domain, $x \in \partial \Omega$. We obtain $A \ni x, B$ open, and $\phi : A \to B$ a C^o diffeomorphism, with $\phi^{-1}(B \cap \mathbb{R}^n_+) = A \cap \Omega$, and $\phi(x) = 0$.

Applying the implicit function theorem in a suitable way (e.g. through minor reworkings of the proofs at page 310, 311 of [34]), we obtain:

- a "square" and an interval V', I with $V' \times I \ni x$
- $\eta : V' \to I$, Lipschitz, of class C^o
- $\phi(V') \subset\subset J \subset\subset I$
- $z \in V' \times I, z_n < \eta_n(z) \iff z \in (V' \times I) \cap \Omega$
- (and consequently, $z \in V' \times I, z_n = \eta_n(z) \iff z \in (V' \times I) \cap \partial\Omega$)

<u>Conclusion</u>

Let a radial function $f > 0$ be of class C^o. H_f is punctured diffeomorphism of class C^o, so that we have that $\partial\Omega_f$ is the image of $\epsilon\mathbb{S}^{n-1}$, a domain of class C^o as well, locally. So Ω_f is of class C^o locally, in the sense of diffeomorphisms, and by what we showed, also in the sense of graphs.

So, for $x \in \partial\Omega_f$ we can find a change of coordinates and a parallelepiped $V = V' \times I$ with $\phi : V' \to I$, ϕ of class C^o and also Lipschitz, and $V \cap \Omega_f = V \cap \{x_n < \phi(x')\}$. We have moreover that $\phi \in J \subset\subset I$ for some open interval J. By a compactness argument, finitely many $V_j = V'_j \times (a^j_n, b^j_n)$ are necessary to cover $\partial\Omega_f$.

So, we have $V_j \cap \Omega_f = V_j \cap \{x_n < \phi_j(x')\} = V \cap \{a^j_n < x_n < \phi_j(x'), x' \in V'_j\}$. Choose $d > 0$ to be the minimum gap between ϕ_j and I_j. $d > 0$ by the existence of $J_j \subset\subset I_j$. We call L the maximum Lipschitz constant of ϕ_j. We have therefore a Lipschitz and C^o domain in the style of [15], which yields, modulo an application of the Lebesgue number lemma, a C^o and Lipschitz domain in the style of [36], whose definition we are working with. $\qquad\square$

2.4. Hilbertian regularization

To approximate a solution of problem 2.2.3 one must apply a discretization strategy and solve an optimization problem in finite dimensions instead. We will adopt derivative based algorithms, where we compute search directions from the knowledge of the discretized shape derivative. In general, the shape derivative on the continuous level is just a functional: one can try to extract a descent direction from its knowledge using the Riesz representation theorem. The choice of the inner product in which to find the representative is usually dictated by the control space, in optimal control.

In shape optimization, however, one works with spaces which are not Hilbert, e.g. $W^{1,\infty}$. A way to tackle this is illustrated in [22], where descent directions are directly searched in $W^{1,\infty}$ without relying on the Riesz theorem. The Hilbert space approach is nonetheless of easier implementation, and we decided to stick with it, in this work. We therefore face two problems. On one hand, this approach is not completely rigorous, as we discuss below, and on the other hand it is not immediate which inner product to use in the finite dimensional optimization. Unfortunately, choosing the "wrong" scalar product can yield descent directions that are too "squiggly" (see section 4.2 for an example, in particulare fig. 4.7), or mesh-dependence effects, where finer and finer meshes require more and more optimization iterations to converge (see [56]).

In our implementation in particular, see chapter 4 and specifically section 4.1, we perform optimization with respect to the H^1 scalar product. On a continuous level, and in the star-shaped setting we put ourselves into, this means finding descent directions $h \in H^1(\mathbb{S}^{n-1})$ from:

$$(r(q), h)_{H^1(\mathbb{S}^{n-1})} = j'(q)[h]$$

where $r(q)$ represents, via the Riesz representation theorem, the functional $j'(q)$. The reason for this is again to be able to find good enough (in the sense of smoothness) descent directions and to avoid mesh-dependence, as opposed to when the L^2 product is used instead. Despite not being a fully rigorous procedure, it is standard trick in shape optimization, and it worked well for us (see chapter 4). It is not rigorous because we pretend to simultaneously have q smooth ($q \in H^2(\mathbb{S}^{n-1})$, for instance) while $r(q) \in H^1(\mathbb{S}^{n-1})$: $q - \alpha r(q)$ need not to be smooth too! For further details regarding this so-called "Hilbertian regularization" procedure, we refer to [2]. We just sketch a proof of the fact that $j'(q)$ can act on the larger space $H^1(\mathbb{S}^{n-1})$ and that it is continuous in the H^1 topology, thus making the operation $r(q)$ well defined.

At first we remark that $h \mapsto V_h$ maps $H^1(\mathbb{S}^{n-1})$ functions into $H^1(\mathbb{R}^n; \mathbb{R}^n)$ functions. To see this, note that h can be approximated by smooth functions h_k, in the H^1 norm (see definition 2.3 of [4]). For the generic term of the approximating sequence we can employ integration in spherical coordinates and use the fact that h_k is Cauchy, to get that V_{h_k} is Cauchy in $H^1(\mathbb{R}^n; \mathbb{R}^n)$, and that it converges to V_h.

Now, consider the expression of the shape derivative, given in proposition 2.2.10. We identify three different terms. We write u for a state v or w, and a for the corresponding adjoint, leaving out the dependence on τ for simplicity:

$$\int_I (u_t, \operatorname{div}(\delta\theta \circ \tau_q^{-1})a)_{L^2(U)}, \quad \int_I (A'(\delta\theta \circ \tau_q^{-1})\nabla u, \nabla a)_{L^2(U)}, \quad \frac{1}{2}\int_I \int_U |v - w|^2 \operatorname{div}(\delta\theta \circ \tau_q^{-1})$$

Here, $U = \tau_q(U_r)$, $\delta\theta = V_h$.

By theorem C.2.1, we observe that $\operatorname{div}(\delta\theta \circ \tau_q^{-1})$, $A'(\delta\theta \circ \tau_q^{-1})$ are square integrable. Moreover, as we will discuss very soon, we can make hypothesis on the data and a suitable modification to the cost function so that $u, a \in H^1(I, H^2(U))$, see assumption 3.1.2, where we need the regularity of q, to have ∂U smooth enough to guarantee H^2 regularity (we have discussed this in proposition 2.3.1.1). Now, the Sobolev embedding $H^1 \hookrightarrow L^4$ (for spatial dimensions $n = 2, 3$, see e.g. [1]) and the Hölder's inequality, allow us to deduce that $j(q)$ can be indeed continuously extended to $H^1(\mathbb{S}^{n-1})$.

For the sake of generality, the same conclusions follow (more easily) when the star-shaped parametrization is not employed.

3. Discretization

In this chapter we focus on giving justification to the numerical observations contained in chapter 4. Linear finite elements are used to discretize the partial differential equations in space, whereas the implicit Euler or the Crank-Nicolson methods are used for advancing in time.

We take into account the fact non-discretized domains are smooth, while the computational ones is polygonal/polyhedral.

We are not focusing here on optimization algorithms to solve the shape identification problem, nor on the specific boundary parametrization. This will be done in chapter 4.

As a summary of the discretization approach:

- the PDEs are numerically solved on a polygonal/polyhedral approximation of the smooth domain U
- such approximation involves only knowing a finite number of points of ∂U, and not its entire parametrization
- only such nodal values of the boundary data are required (compatible, for instance, with the case where only finite number of measurements are available)
- implicit Euler or Crank-Nicolson time steppings are adopted

We chose such time steppings because of their simplicity, overall low regularity requirements (compared to more sofisticated e.g. Runge-Kutta methods), and the fact that they are unconditionally stable, i.e. no restriction on the time step size must be made, relative to the spatial discretization, to obtain convergence. We can reach the required smoothness in time for the state equations, by requiring smooth data, and certain compatibility relations between them (see e.g. chapter 2 of [47] and assumption B.2.3). Smoothness of the data alone is not enough: a regular solution would be obtained, but only away from the starting time, where a singularity can develop (see e.g. the discussion in [38]). We have full control over the compatibility relations for the states, but the adjoint equations are, in a certain sense, fixed by the particular cost functional we chose, and the state equations themselves: unfortunately, for the adjoints, compatibility relations do not hold, in general.

In [38], the authors work in fact with adjoint equations that have incompatible boundary data, and devise a non-standard time stepping scheme to deal with this. On the other hand, our choice of cost functional makes it possible to obtain compatibility of "order zero" in the adjoints. This would be enough for a low order space-time method without time quadrature (see e.g. [51]), but not for the chosen fully discrete schemes. To obtain more compatibility we need to modify the data that enters the adjoint equations, and since we cannot modify the structure of the PDEs solved by the states w, v, we can only tweak the cost functional. This is what we will do, with the introduction of a suitable temporal weight in the cost functional of problem 2.2.3. Such operation will yield compatibility of arbitrary order, at the price of partially modifying the nature of the shape optimization problem. See section 3.1 for a more thorough discussion.

An in-depth presentation and analysis of the discretization algorithms for states and adjoints is discussed in appendix D. In what follows we will build on the results therein.

As a last note, let us mention the two canonical ways, in the literature on optimal control, of discretizing a problem posed on an infinite-dimensional level:

- optimize-then-discretize: the gradient of the cost functional is derived on the continuous level (see e.g. proposition 2.2.10 in our case), some adjoint states appear and first order conditions can be formulated. Then, one proceeds with discretizing states and adjoints and the continuous optimality system, and obtains one on the discrete level
- discretize-then-optimize: the states and cost function, i.e. the continuous problem (problem 2.1.1 and problem 2.2.3) are discretized, to obtain an optimization problem posed on the discrete level. Finite dimensional optimality conditions can now be derived

In any case, one starts from an infinite-dimensional problem and obtains discrete optimality conditions, that can be employed for a numerical implementation. When the obtained discrete optimality system is the same, we say that the two strategies, optimize-then-discretize and discretize-them-optimize commute. With a diagram:
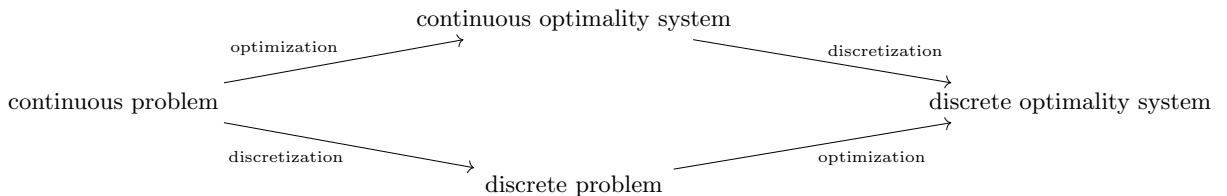
Although in general not a trivial task, there are several benefits implied by realizing a commutative scheme, we refer to the introduction of [48] for a comparison between the two strategies, and a discussion of advantages and disadvantages of each. See also [30], in the context of parabolic optimal control.

We can show that optimization and discretization commute, when using the implicit Euler case for states, and a suitable variant for adjoints. We strongly suspect that commutatoion holds also when Crank-Nicolson is used, see the work of [30].

Now:

- in section 3.1, the continuous states and adjoints are discretized and the error in doing so, is quantified: we make heavy use here

of the results from appendix D. In particular, optimal order estimates for the FEM solutions are recalled (optimal with respect to the approximation properties of the finite element spaces and time stepping schemes)

- in section 3.2, results about the convergence of the discrete shape gradient, to the continuous one, are presented in different settings: a spatially semidiscrete one, and two fully discrete ones, i.e. one with implicit Euler applied to the states and an overall discretize-then-optimize (and commutative) approach, the other with the Crank-Nicolson method applied to states and adjoints, in an optimize-then-discretize fashion

In what follows, $\lesssim$ stands for $\leq C$, with $C > 0$ independent on time and space discretization parameters.

3.1. Approximation of PDEs

Consider the state and adjoint equations as seen in problem 2.1.1 and proposition 2.2.10. Let us have for simplicity a unified notation (just like in problem B.2.2).

> **Problem 3.1.1** (Unified notation for state and adjoint equations)
> State equations:
>
> $$\begin{cases} u_t - \Delta u = 0 & \text{in } U \times (0,T) \\ u = u_D & \text{on } \Gamma_D \times (0,T) =: \Sigma_D \\ \partial_\nu u = u_N & \text{on } \Gamma_N \times (0,T) =: \Sigma_N \\ u(0) = 0 \end{cases}, \quad \begin{cases} -a_t - \Delta a = (-1)^{[a=v]} \eta(v-w) & \text{in } U \times (0,T) \\ a = 0 & \text{on } \Gamma_D \times (0,T) \\ \partial_\nu a = 0 & \text{on } \Gamma_N \times (0,T) \\ a(T) = 0 \end{cases}$$
>
> We mean that u stands either for v, in which case a is p, or u is w and then a is q.

We have dropped, for simplicity, all the references to the domain transformation τ. Let us discuss the presence of the temporal weight η. This is a function $\eta : [0,T] \to \mathbb{R}$. Its presence in the right hand side of the adjoint equation can be justified by modifying the energy function in problem 2.2.3 to be:

$$J_\eta(\tau) = \frac{1}{2} \int_I \eta \, \|v_\tau - w_\tau\|_{H_\tau}^2$$

This modification's main purpose is to facilitate the analysis of the numerical discretization. In particular, we choose η to be a smooth cut-off function that is positive in $(0,T)$ and 0 in $[T, +\infty)$. Note that in case a solution to the "classical" problem exists, then it is also a solution to this new perturbed problem, and viceversa. In fact, $J_\eta(\tau) = 0 \implies \eta \|v_\tau - w_\tau\|_{H_\tau}^2 = 0 \implies v_\tau = w_\tau$. This equality holds on all $I = [0,T]$ by the time continuity of the states.

Modifying the final-time behaviour of the energy might of course have detrimental effects if the boundary data exhibits strong variations close to final time. However, for boundary conditions that e.g. stabilyze over time, then a heat equation will also produce a solution tending to a steady state, so that the presence of η shouldn't play a significant role. In any case, the shape of η can be adjusted according to the user's needs.

We now proceed to discretize states and adjoints using the scheme presented in problem D.3.2 (the adjoint equation can be cast into a standard heat equation by time reversal). In short, finite elements are used in space, a finite difference time stepping, in time. Note that the adjoints discretization we are about to discuss is an optimize-then-discretize one. We will see alternative approaches in the case of implicit Euler.

Now, the spatial discretization is done on a polygonal approximation U_h of U, a smooth domain. We explicitly account for this discrepancy, see the introductory discussion in appendix D. Note, the next assumption is formulated as if U, U_h were given, i.e. as if they were not deformations of initial reference domains. This will be remarked later on, too.

Throughout, set $\theta = 1$ to obtain the implicit Euler method, $\theta = 1/2$ for the Crank-Nicolson method.

> **Assumption 3.1.2** (Hypothesis for the numerical discretization of problem 3.1.1)
>
> 1. $\partial U \in C^2$ (for instance, the star shaped functions must be of class C^2, see proposition 2.3.1.1), U_h is polygonal/polyhedral and ∂U_h interpolates ∂U. The mesh family of U_h must be (shape) regular and quasi-uniform (for such definitions, see [13])
>
> 2. $u_D \in H^{1/\theta+1}(I, H^{3/2}(\Gamma_D)) \cap H^1(I, H^2(\Gamma_D))$, $u_N \in H^{1/\theta+1}(I, H^{3/2}(\Gamma_N)) \cap L^2(I, H^2(\Gamma_N))$
>
> 3. $g_D(0) = 0$ and $g_N^{(k)}(0), g_D^{(k+1)}(0) = 0$ for $k = 0, ..., 1/\theta - 1$
>
> 4. $\eta^{(k)}(T) = 0$ for $k = 0, ..., 1/\theta - 1$, $\eta \geq 0$ and $\eta \in C^\infty([0,T]; \mathbb{R})$

We have written $u_N, u_D, \Gamma_D, \Gamma_N$ to mantain a flexible notation. With reference to problem 2.1.1 this translates to:

- state v: $u_D = f$ on Γ_f, $= 0$ on Γ_m, $\Gamma_D = \partial U = \tau(U_r)$, $\Gamma_N = \emptyset$
- state w: $u_N = g$ on Γ_f, $u_D = 0$ on Γ_m, $\Gamma_D = \Gamma_m$ and $\Gamma_f = \Gamma_N$

Call now h the maximum element size of U_h, and δt the size of one of the K uniform length intervals $[t^k, t^{k+1}]$, $k = 0, ..., K - 1$, into which we subdivide I.

Problem 3.1.3 (Numerical discretization of problem 3.1.1 in an optimize-then-discretize fashion)
Consider $g_{N,h}^k, g_{D,h}^k$ to be the Lagrange interpolant of $g_N(t^k), g_{D,h}^k$. For the state u, we look for $u_h^k \in S_h^1$, $k = 0, ..., K$, with:

$$\left(\frac{u_h^{k+1} - u_h^k}{\delta t}, v_h \right)_{L^2(U_h)} + (\nabla(\theta u_h^{k+1} + (1-\theta)u_h^k), \nabla v_h)_{L^2(U_h)} = (\theta g_{N,h}^{k+1} + (1-\theta)g_{N,h}^k, v_h)_{L^2(\Gamma_{N_h})}, \quad 1 \le k \le K$$

$$u_h^{k+1}|_{\Gamma_{D_h}} = g_{D,h}^{k+1}, \quad 1 \le k \le K$$

$$u_h^0 = 0$$

and $v_h \in S_{h,0,D_h}^1$. Here $\Gamma_{D_h}, \Gamma_{N_h}$ are the discrete counterparts of Γ_D, Γ_N, and $S_{h,0,D_h}^1$ is the linear finite element space on U_h, with the constraint of vanishing on Γ_{D_h}.
The same scheme is applied to the adjoint equations. Further details can be found in the appendix after problem D.3.2, of which problem 3.1.3 is an instance.

We now state the error estimates for problem 3.1.1. Before doing so, we remark again that the continuous solution is defined on a smooth domain U, whereas the discretized solution on a polygonal/polyhedral approximation U_h. To compare e.g. u and u_h we must have a way of "lifting" u_h to u or viceversa. This procedure is possible and we denote its action by $(\cdot)^l$: we thus compare $u : U \times I \to \mathbb{R}$ and $u_h^l : U \times \{0, ..., K\} \to \mathbb{R}$. For details regarding the lifting action we refer to proposition D.1.3.
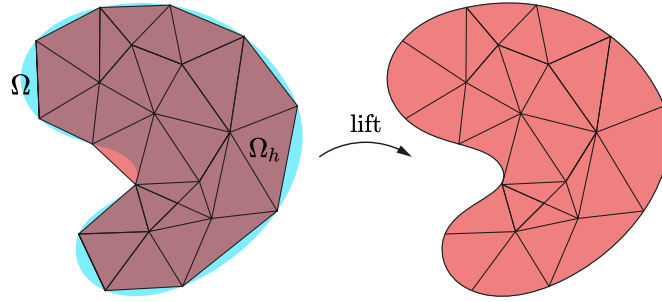

Figure 3.1.: Lifting action

Proposition 3.1.4 (Optimize-then-discretize approximation of state and adjoint equations)
Let assumption 3.1.2 be fulfilled. Then, for $0 \le k \le K$:

$$\left\| u(t^k) - (u_h^k)^l \right\|_{L^2(U)} \lesssim h^2 + (\delta t)^{1/\theta}$$

$$\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h^{k+1})^l) + (1-\theta)(u(t^k) - u_h^k)^l) \right\|_{H^1(U)}^2} \lesssim h + (\delta t)^{1/\theta}$$

$$\left| \int_I (\partial_t u, w_K)_{L^2(U)} - \delta t \sum_{k=0}^{K-1} \left(\frac{(u_h^{k+1})^l - (u_h^k)^l}{\delta t}, w_{K,k} \right)_{L^2(U)} \right| \lesssim \left(h^2 + (\delta t)^{1/\theta} \right) \left\| w_K \right\|_{L^2(I, H_{0,D}^1(U))}$$

and

$$\left\| a(t^k) - (a_h^k)^l \right\|_{L^2(U)} \lesssim h^2 + (\delta t)^{1/\theta}$$

$$\sqrt{\delta t \sum_{k=1}^{K} \left\| (1-\theta)(a(t^k) - a_h^k)^l) + \theta(a(t^{k-1}) - a_h^{k-1})^l) \right\|_{H^1(U)}^2} \lesssim h + (\delta t)^{1/\theta}$$

$$\left| - \int_I (\partial_t a, w_K)_{L^2(U)} - \delta t \sum_{k=1}^{K} \left(\frac{(a_h^{k-1})^l - (a_h^k)^l}{\delta t}, w_{K,k} \right)_{L^2(U)} \right| \lesssim \left(h^2 + (\delta t)^{1/\theta} \right) \left\| w_K \right\|_{L^2(I, H_{0,D}^1(U))}$$

where w_K is piecewise constant on the time discretization, and with values $w_{K,k}$, on $[t^k, t^{k+1}]$, that belong to $H_{0,D}^1(U)$ (i.e. it is 0 on the Dirichlet boundary), and $\lesssim$ means $\le C$, with $C > 0$ independent of h and δt.
For the states, we will also need the following estimate:

$$\left\| u(t^k) - (u_h^k)^l \right\|_{L^2(\Omega)} \lesssim \left\| u(t^k) - u_h^l(t^k) \right\|_{L^2(\Omega)} + \left\| u_h(t^k) - u_h^k \right\|_{L^2(\Omega)} \lesssim \delta t^{1/\theta} + h$$

Note, the Dirichlet boundary varies between v, w. So, for v, $H^1_{0,D} = H^1_0$, whereas for w we have $H^1_{0,D} = H^1_{0,m} = \{u \in H^1, u(\Gamma_m) = 0\}$.

Proof.

We show the satisfaction of all the hypothesis necessary to obtain theorem D.3.10 (where we track from there all the necessary assumptions), and then bound the constants therein, uniformly with respect to the space/time discretization. We do this for u at first, then for a. We do not track the dependency on the domain U as already remarked.

We note at first that in the star-shaped setting, $\partial U \in C^2$ can be ensured by proposition 2.3.1.1.

Smoothness of u: assumption D.2.4 and assumption B.2.1: we need to guarantee that $u \in H^1(I, H^2(U))$. To do so we turn to theorem B.2.6, which we apply with $k = 1$. Hypothesis 1 to 3 suffice for this.

Assumptions for spatial semidiscretization of u: assumption D.2.6: they are also satisfied by $1 - 3$.

Assumptions for full discretization of u: assumption D.3.1: the smoothness of the problem data is ensured by point 2. We turn to the compatibility conditions of order $1, ..., 1/\theta$. The compatibility "residuals" $\delta^k_h(0)$ are all 0 (see assumption D.3.1 for the notation) by hypothesis 3, so that the compatibility relations are satisfied.

Bounding the constants A, B, C, D of u: theorem D.3.10: to bound A, B uniformly with respect to h we only need to note that the equation for u has no source term. To bound C, this last fact, together with $\delta^k_h(0) = 0$, $k = 0, ..., 1/\theta$, suffices. $D = 0$, in turn.

We now turn verify the same facts for the adjoint states a.

Smoothness of a: we need to ensure that $a \in H^1(I, H^2(U))$. To apply theorem B.2.6 with $k = 1$ we see that $\eta(T)(v(T) - w(T))$ should be zero on the Dirichlet boundary, which it is, given the fact that $\eta(T) = 0$. We also need v, w (so, generically, u), to be $H^1(I, L^2(U))$, which we have already checked (we even have $u \in H^1(I, H^2(U))$); assumption B.2.1 is also easily verified.

Assumptions for spatial semidiscretization of a: to fulfill assumption D.2.6 we see by the triangle inequality that $\left\| \eta(u - u^l_h) \right\|_{L^2(U)} \lesssim C_u h^2$ would suffice, for a suitable C_u (see assumption D.2.6 for the definition of C_u). Actually, given the properties of η, only $\left\| u - u^l_h \right\|_{L^2(U)} \lesssim C_u h^2$ has to be asked. But the hypothesis we have verified for u were sufficient for the conclusions of theorem D.2.10 to hold. We can therefore take $C_u = A = A(u)$, which is a constant in space and time, independent of δt and h, as we saw before.

Assumptions for full discretization of a: the compatibility conditions listed in assumption D.3.1 are satisfied as long as $\eta(T) = 0$ in the case $\theta = 1$, and additionally $\eta'(T) = 0$ in the case $\theta = 1/2$. We also have $u_h \in H^{1/\theta}(I, S^1_h)$ by 2.

Bounding the constants $A(a), B(a), C(a), D(a)$ of a: this would be the last step to ensure the thesis of theorem D.3.10, for a. Starting from $D(a)^2$, we see, thanks to the boundedness of η, that $D(a)^2 \lesssim \delta t \sum_{k=0}^{K-1} \left\| \theta(u_h(t^{k+1}) - u^{k+1}_h) + (1 - \theta)(u_h(t^k) - u^k_h) \right\|^2_{L^2(U_h)}$. This is $O(\delta t^{2/\theta})$ by proposition D.3.3 and the above reasonings ($D = D(u) = 0$, $C = C(u)$ is bounded uniformly).

Moving on to $C(a)$. By the triangle inequality, the already checked compatibility relations and the boundedness of η, we see that there only remains to bound the term $\int_I \left\| u^{1/\theta}_h \right\|^2_{-1,h} \lesssim \int_I \left\| u^{1/\theta}_h \right\|^2_{L^2(U_h)}$. This can be done as above eq. (D.3.7).

To bound $A(a)$ (equivalently $B(a)$), we need to check the boundedness of $\int_I C^2_{\eta(v-w)} + \int_I \|\eta(v_h - w_h)\|^2_{H^1(U_h)}$ (the definition of $C_{\eta(v-w)}$ comes directly from assumption D.2.6). In fact, we have chosen $\eta(v_h - w_h) \in S^1_h$ as a right hand side for the semidiscrete equation of a_h. A triangle inequality and basic stability estimates yield a bound for the second term. $C_{\eta(v-w)}$, thanks to theorem D.2.10, is dominated by $A(v) + A(w)$, which we have in turn already estimated.

The last estimate Is the content of proposition D.3.11, where the constant E can be bounded by the data as above, and the source terms f^k_h are all zero. $\qquad \square$

Only for $\theta = 1$, we now define a discretized shape optimization problem, where we employ continuous and piecewise linear transformations τ_h, that thus preserve the finite element spaces and the polygonal/polyhedral nature of the discrete reference domain $U_{r,h}$. This is necessary to fully justify that optimization and discretization commute, for $\theta = 1$.

At this level, and for the rest of the chapter, for simplicity but also for the sake of generality, we work again with with general transformations, in place of radial fields.

Problem 3.1.5 (Discrete shape optimization problem)

Given a polygonal/polyhedral reference domain $U_{r,h}$ and transformations τ_h, vector valued finite element fields that are the identity on $\Gamma_{m,h}$, we solve:

$$\inf_{\tau_h} \frac{\delta t}{2} \sum_{k=1}^{K} \left\| v^k_h - w^k_h \right\|^2_{L^2(\tau_h(U_{r,h}))} =: J_{h,\delta t}(\tau_h)$$

where v^k_h, w^k_h are defined in problem 3.1.3, and their dependence on τ_h is not highlited in the notation. We also ask τ_h to have small enough $W^{1,\infty}$ norm, so as to keep $U_{r,h}$ bounded Lipschitz and preserve the mesh quality.

Proposition 3.1.6 (Discrete shape gradient)

The discrete shape gradient of problem 3.1.5 is:

$$J'_{h,\delta t}(\tau_h)[\delta\theta_h] =$$

$$\delta t \sum_{k=1}^{K}\left(\frac{w_h^k - w_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h \circ \tau_h^{-1})q_h^{k-1}\right)_{L^2(\tau_h(U_{r,h}))} + \delta t \sum_{k=1}^{K}(A'(\delta\theta_h \circ \tau_h^{-1})\nabla w_h^k, \nabla q_h^{k-1})_{L^2(\tau_h(U_{r,h}))} +$$

$$\delta t \sum_{k=1}^{K}\left(\frac{v_h^k - v_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h \circ \tau_h^{-1})p_h^{k-1}\right)_{L^2(\tau_h(U_{r,h}))} + \delta t \sum_{k=1}^{K}(A'(\delta\theta_h \circ \tau_h^{-1})\nabla v_h^k, \nabla p_h^{k-1})_{L^2(\tau_h(U_{r,h}))} +$$

$$\frac{\delta t}{2}\sum_{k=1}^{K}\int_{\tau_h(U_{r,h})}\eta(t^k)|v_h^k - w_h^k|^2 \operatorname{div}(\delta\theta_h \circ \tau_h^{-1})$$

Again, we dropped the dependence of v, w on τ_h, for simplicity. Here, the discretized adjoint states satisfy:

Problem 3.1.7

$$\left(\frac{p_h^{k-1} - p_h^k}{\delta t}, v_h\right)_{L^2(\tau_h(U_{r,h}))} + (\nabla p_h^{k-1}, \nabla v_h)_{L^2(\tau_h(U_{r,h}))} + \eta(t^k)(v_h^k - w_h^k, v_h)_{L^2(\tau_h(U_{r,h}))} = 0, \quad 1 \le k \le K$$

$$p_h^k = 0 \text{ on } \tau_h(\partial U_{h,r}), \quad 1 \le k \le K$$

$$p_h^K = 0$$

and

$$\left(\frac{q_h^{k-1} - q_h^k}{\delta t}, v_h\right)_{L^2(\tau_h(U_{r,h}))} + (\nabla q_h^{k-1}, \nabla v_h)_{L^2(\tau_h(U_{r,h}))} - \eta(t^k)(v_h^k - w_h^k, v_h)_{L^2(\tau_h(U_{r,h}))} = 0, \quad 1 \le k \le K$$

$$q_h^k = 0 \text{ on } \tau_h(\Gamma_{D_h,r}), \quad 1 \le k \le K$$

$$q_h^K = 0$$

The test functions are zero on the entire discrete boundary for the equation of p_h^k, and only on the moving boundary for q_h^k.

Proof.
One can adopt the same techniques employed in the continuous case, or, use of the method proposed in and [12], section 4 (or more generally, [46]).

Also note, it is important that τ_h is piecewise linear on the discretization, and continous, so that finite element functions remain finite element functions after an application of τ_h, and the geometry remains of polygonal/polyhedral nature. See again [12] for further details on this matter. □

Observation 3.1.8 (τ and τ_h).
Throughout the rest of the chapter, we won't try to take into account the fact that the reference domains U_r and $U_{r,h}$ are changing under the actions of τ and τ_h. It means that the estimates are τ, τ_h dependent, but the dependence is not tracked. Therefore we will fix $U = \tau(U_r)$ and $U_h = \tau_h(U_{r,h})$ once and for all. Remember that assumption 3.1.2 must hold, which implies a specific form of τ_h, i.e. that it must interpolate τ. Given therefore a reference discretization $U_{r,h}$ interpolating U_r, then τ_h is completely determined by τ.

Choosing such $U_{r,h}$ is not restrictive, but confining τ_h to be the interpolant of τ, is: we refrain from generalizing the estimate to more arbitrary τ_h, and we note that our result may be a first step of a more general argument (just like in finite element error estimates, the error between exact and discretized solution is decomposed into two parts by the introduction of a suitable interpolant).

This is in any case a novelty with respect to e.g. [40], which contains similar estimates to the ones we are up to derive, but in which H^2 regularity is demanded on non-convex polygonal domains.

We now give a quantitative estimate on the approximation power of the discrete adjoints we just obtained, for $\theta = 1$. This is needed, because the scheme they satisfy is not exactly the implicit Euler treated in proposition 3.1.4.

Proposition 3.1.9 (Error estimates for adjoint states in a discretize-then-optimize fashion)
The discretize-then-optimize adjoints with implicit Euler satisfy the same asymptotic, optimal order error estimates of proposition 3.1.4, under the same assumptions.

Proof.
The proof is exactly that of proposition 3.1.4. The only difference comes from the fact that the right hand sides of the adjoints are not "correct", i.e. they are shifted by δt. But this is not an issue, as we shall now show.

We see that we only need to show a bound of $\delta t \sum_{k=1}^{K} \left\| \eta(t^{k-1})u_h(t^{k-1}) - \eta(t^k)u_h^k \right\|_{L^2(U_h)}^2$, where u denotes the generic state corresponding state to the generic adjoint a (this is the same notation as in the proof of proposition 3.1.4), and where $U_h = \tau_h(U_{r,h})$.

Applying the triangle inequality and using again the proof of proposition 3.1.4, we see that we actually only need to bound the term:

$$\delta t \sum_{k=1}^{K} \left\| \eta(t^{k-1})u_h(t^{k-1}) - \eta(t^k)u_h^k \right\|_{L^2(U_h)}^2 \lesssim$$

$$\underbrace{\delta t \sum_{k=1}^{K} \left\| \eta(t^{k-1})(u_h(t^{k-1}) - u_h(t^k)) \right\|_{L^2(U_h)}^2}_{\text{①}} + \underbrace{\delta t \sum_{k=1}^{K} \left\| (\eta(t^{k-1}) - \eta(t^k))u_h(t^k) \right\|_{L^2(U_h)}^2}_{\text{②}} + \underbrace{\delta t \sum_{k=1}^{K} \left\| \eta(t^k)(u_h^k - u_h(t^k)) \right\|_{L^2(U_h)}^2}_{\text{③}}$$

There holds $\text{②} \leq \left\| \eta' \right\|_\infty^2 \delta t^3 \sum_{k=1}^{K} \left\| u_h(t^k) \right\|_{L^2(U_h)}^2$. Call $\pi u_h := u_h(t^k)$ for $t \in (t^k, t^{k+1})$. By lemma A.2.7 we see that, for δt small enough, one has $\left\| \pi u_h \right\|_{L^2(I,L^2(U_h))} \lesssim \delta t \left\| u_h' \right\|_{L^2(I,L^2(U_h))}$. This yields:

$$\text{②} \leq \left\| \eta' \right\|_\infty^2 \delta t^3 \sum_{k=1}^{K} \left\| u_h(t^k) \right\|_{L^2(U_h)}^2 = \left\| \eta' \right\|_\infty^2 \delta t^2 \int_I \left\| \pi_h u_h \right\|_{L^2(U_h)}^2 \lesssim \delta t^2 \left\| u_h' \right\|_{L^2(I,L^2(U_h))}^2 \left\| \eta' \right\|_\infty^2$$

On the other hand, $\text{①} \leq \left\| \eta \right\|_\infty^2 \delta t \sum_{k=1}^{K} \left\| u_h(t^{k-1}) - u_h(t^k) \right\|_{L^2(U_h)}^2$, and with a similar reasoning as in the proof of lemma A.2.7, we conclude $\text{①} \leq \left\| \eta \right\|_\infty^2 \delta t \sum_{k=1}^{K} \delta t \int_{I_k} \left\| u_h' \right\|_{L^2(I_k,L^2(U_h))}^2$.

In both cases, $\left\| u_h' \right\|_{L^2(I,L^2(U_h))}^2$ can be bounded, uniformly with respect to h (and δt), by stability estimates (see e.g. corollary D.2.17). It is clear from this estimate that a very steep η may yield higher discretization errors.

Finally, by proposition D.3.3 (which we can apply by assumption 3.1.2), we obtain $\text{③} \lesssim (h^2 + \delta t) \left\| \eta \right\|_\infty^2$. $\qquad\square$

Observation 3.1.10 (Optimization and discretization commute).
So, optimization and discretization commute, for $\theta = 1$, the perturbed implicit Euler method of proposition 3.1.6, applied to the adjoints, being a "legitimate" scheme, as we have just shown in proposition 3.1.9). With a diagram:
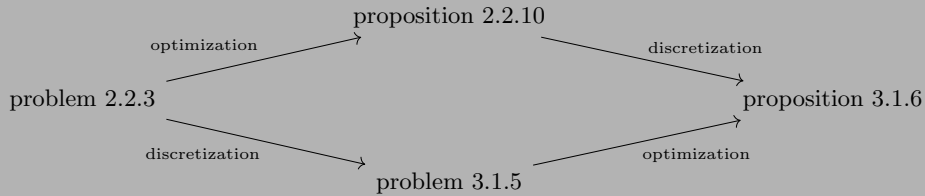
Let us also briefly introduce the spatially semidiscretized shape optimization problem, and its shape gradient. This is an interesting quantity on its own, but it also plays a role in obtaining fully discrete estimates.

Proposition 3.1.11 (Semidiscrete shape optimization problem)
We introduce the spatially semidiscrete state equation, with unified notation u_h, similarly to problem 3.1.3. Calling $g_{N,h}$ and $g_{D,h}$ the Lagrange interpolants (defined a.e. in time) of g_N, g_D, we consider $u_h : I \to S_h^1$ as:

$$\left(u_h', v_h \right)_{L^2(U_h)} + (\nabla u_h, \nabla v_h)_{L^2(U_h)} = (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}, \quad \text{for a.e. } t \in I$$

$$u_h|_{\Sigma_{D_h}} = g_{D,h}$$

$$u_h(0) = 0$$

and $v_h \in S_{h,0,D_h}^1$. This is an instance of problem D.2.5, to which we refer for further details. The shape optimization problem is to find τ_h, a vector valued finite element field that is the identity on $\Gamma_{m,h}$ (and with small enough $W^{1,\infty}$ norm, so as to keep $U_{r,h}$ bounded Lipschitz and preserve the mesh quality), minimizing:

$$J_h(\tau_h) = \int_I \int_{\tau_h(U_{r,h})} \eta |v_h - w_h|^2$$

The adjoint state $a_h : I \to S_h^1$ to u_h solves:

$$- \left(a_h', v_h\right)_{L^2(U_h)} + (\nabla a_h, \nabla v_h)_{L^2(U_h)} = (-1)^{[u_h = v_h]} \eta(v_h - w_h), \quad \text{for a.e. } t \in I$$

$$a_h|_{\Sigma_{D_h}} = 0$$

$$a_h(T) = 0$$

and the semidiscrete shape gradient in direction $\delta\theta_h$ (a vector valued finite element field that is zero on $\Gamma_{m,h}$) reads:

$$dJ_h(\tau_h)[\delta\theta_h] =$$

$$\int_I (w_h' \text{div}(\delta\theta_h \circ \tau_h^{-1}), q_h)_{L^2(\tau_h(U_{r,h}))} + \int_I (A'(\delta\theta_h \circ \tau_h^{-1})\nabla v_h, \nabla p_h)_{L^2(\tau_h(U_{r,h}))} +$$

$$\int_I (v_h' \text{div}(\delta\theta_h \circ \tau_h^{-1}), p_h)_{L^2(\tau_h(U_{r,h}))} + \int_I (A'(\delta\theta_h \circ \tau_h^{-1})\nabla w_h, \nabla q_h)_{L^2(\tau_h(U_{r,h}))} +$$

$$\frac{1}{2} \int_I \int_{\tau(U_{r,h})} |v_h - w_h|^2 \text{div}(\delta\theta_h \circ \tau_h^{-1})$$

Proof.

It can be done similarly to proposition 2.2.10 or proposition 3.1.6. □

3.2. Approximation of shape gradient

In our numerical experiments (see chapter 4) we adopt a discretize-then-optimize approach. When employing the implicit Euler method in time, we can see that optimization and discretization commute, as explained below. We are moreover able to quantify the error generated when substituting the continuous shape gradient with the fully discretized one.

A future line of research could be to extend such conclusions to the case of the Crank-Nicolson method, in a discretize-then-optimize setting, so as to fully justify the adopted algorithms in some of the numerical experiments we conducted. A promising direction would be to find a way to adapt the arguments of [30], at least to show commutativity of optimization and discretization. We will prove, as a partial replacement, optimize-then-discretize error estimates for the shape gradient.

In particular, similar estimates to those in [40] will be derived, although in a slightly different context: in a time-dependent setting, and with a more precise handling of the geometry mismatch. In [40], order 2 estimates (in space) are obtained: this is because the deformation field $\delta\theta$ in which the shape gradient is tested, is assumed to have two orders of differentiability, so that certain duality techniques may be employed. Such a result doesn't fully explain why superconvergence happens in the context of just $W^{1,\infty}$ displacements, a fact which is indeed observable in our experiments.

For smooth displacement fields $\delta\theta$ that vanish in a neighbourhood of the fixed boundary, a similar superconvergence result for the shape gradient is available also in our context. Such "compact support" assumption is not very strong: admissible displacements must already be zero at the fixed boundary, so as to preserve Γ_f.

This result, is shown initially for the spatial semidiscretization, a fact that alone suggests that such a result may be available also in the fully discrete case. This is also confirmed by the experiments in section 4.2. In a commutative setting, we are able to give full theoretical justification for the implicit Euler scheme. In the Crank-Nicolson case, we could only arrive at optimize-then-discretize estimates.

In case displacement fields are not smooth enough, $O(h^2)$ orders, as noted in [40], don't seem to be so easily obtainable: we are also are able to only prove $O(h)$ estimates.

Theorem 3.2.1 (Semidiscrete error estimates for shape gradient)
Let U be fixed and U_h as in assumption 3.1.2. Let assumption 3.1.2 itself hold, $\delta\theta \in W^{2,\infty}(U; \mathbb{R}^n)$, with $D\delta\theta = 0$ on the fixed boundary Γ_f. There exists a constant γ that depends on U, the shape regularity and quasi-uniformity of the meshes, but independent of h, such that, for h small enough, we have:

$$\left| dJ(U)[\delta\theta] - dJ_h(U_h)[\delta\theta^{-l}] \right| \leq \gamma h^2 \|\delta\theta\|_{W^{2,\infty}(U;\mathbb{R}^n)}$$

If otherwise $\delta\theta \in W^{1,\infty}(U; \mathbb{R}^n)$, we obtain:

$$\left| dJ(U)[\delta\theta] - dJ_h(U_h)[\delta\theta^{-l}] \right| \leq \gamma h \|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)}$$

The notation $dJ(U)[\delta\theta] := dJ(\tau)[\delta\theta \circ \tau]$, if $U = \tau(U_r)$, is to emphasize that the dependence on τ is not tracked. Analogously $dJ_h(U_h)[\delta\theta] := dJ_{h,\delta t}(\tau_h)[\delta\theta_h \circ \tau]$, with $U_h = \tau_h(U_{r,h})$ and a suitable τ_h that (linearly) interpolates τ on the spatial discretization nodes.

Proof.

We compare "time derivative" terms, "gradient" terms and "cost function" terms, and use proposition D.1.5, apart from the semidiscretization error estimates for the partial differential equations, to obtain an overall $O(h^2)$ term, or $O(h)$ term. For the expression of

the semidiscretized shape gradient we make use of proposition 3.1.11. We also call $\delta\theta_h := \delta\theta^{-l}$.

<u>Derivatives</u>

We recover the notation $u \to$ generic state (v or w), $a \to$ adjoint state of u. We have:

$$\int_I (u', a\mathrm{div}(\delta\theta))_{L^2(U)} - \int_I (u'_h, a_h \mathrm{div}(\delta\theta_h))_{L^2(U_h)} =$$

$$\underbrace{\int_I ((u - u_h^l)', a\mathrm{div}(\delta\theta))_{L^2(U)}}_{\text{①}} + \underbrace{\int_I ((u'_h)^l, (a - a_h^l)\mathrm{div}(\delta\theta))_{L^2(U)}}_{\text{②}} + \underbrace{\int_I ((u'_h)^l, a_h^l \mathrm{div}(\delta\theta_h^l))_{L^2(U)} - \int_I (u'_h, a_h \mathrm{div}(\delta\theta_h))_{L^2(U_h)}}_{\text{③}} +$$

$$\underbrace{\int_I ((u'_h)^l, a_h^l (\mathrm{div}(\delta\theta) - \mathrm{div}(\delta\theta_h^l)))_{L^2(U)}}_{\text{③'}}$$

We apply corollary D.2.17 to ①, which we can do by assumption 3.1.2 and by the reasonings of proposition 3.1.4, to obtain $\left|\text{①}\right| \lesssim h^2 \|\mathrm{div}\delta\theta\|_{W^{1,\infty}(U)}$. It is crucial here that $\delta\theta$ has two weak derivatives, so that $a\delta\theta$ is as smooth as required by corollary D.2.18. Otherwise, we can only assume $\delta\theta \in W^{1,\infty}$ and apply corollary D.2.17, which yields $\left|\text{①}\right| \lesssim h \|\mathrm{div}\delta\theta\|_{L^\infty(U)}$.

On the other hand, employing theorem D.2.10, proposition D.1.3 and suitable stability estimates to u'_h (which are avaliable by assumption D.3.1), we come as well to $\left|\text{②}\right| \lesssim h^2 \|\mathrm{div}\delta\theta\|_{L^\infty(U)}$.

Employing proposition D.1.5, and proposition D.1.3, we find:

$$\left|\text{③}\right| \lesssim h^2 \|u'_h\|_{L^2(I,H^1(U_h))} \|a_h\|_{L^2(I,H^1(U_h))} \|\delta\theta\|_{W^{1,\infty}(U)} \lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$$

Lastly, $\text{③'} \lesssim \left\|\delta\theta - \delta\theta_h^l\right\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$, where we applied proposition D.1.3 and suitable stability estimates to bound u'_h and a_h in the $L^2(I, L^2)$ norm.

<u>Gradients</u>

We perform the splitting:

$$\int_I (A'(\delta\theta)\nabla u, \nabla a)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u_h, \nabla a_h)_{L^2(U_h)} =$$

$$\underbrace{\int_I (A'(\delta\theta) - A'(\delta\theta_h^l)\nabla u, \nabla a)_{L^2(U)}}_{\text{④'}} + \underbrace{\int_I (A'(\delta\theta_h^l)\nabla u, \nabla a)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u^{-l}, \nabla a^{-l})_{L^2(U_h)}}_{\text{④}} +$$

$$\underbrace{\int_I (A'(\delta\theta_h^l)\nabla(u_h^l - u), \nabla a_h^l)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla(u_h - u^{-l}), \nabla a_h)_{L^2(U_h)}}_{\text{⑤}} +$$

$$\underbrace{\int_I (A'(\delta\theta_h^l)\nabla u, \nabla(a_h^l - a))_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u^{-l}, \nabla(a_h - a^{-l}))_{L^2(U_h)}}_{\text{⑥}} +$$

$$-\underbrace{\int_I (A'(\delta\theta_h^l)\nabla(u_h^l - u), \nabla(a_h^l - a))_{L^2(U)}}_{\text{⑦}} - \underbrace{\int_I (A'(\delta\theta_h^l)\nabla u, \nabla(a_h^l - a))_{L^2(U)}}_{\text{⑧}} - \underbrace{\int_I (A'(\delta\theta_h^l)\nabla(u_h^l - u), \nabla a)_{L^2(U)}}_{\text{⑨}}$$

We refer directly to proposition D.1.5 to show that $\left|\text{④}\right| \lesssim h^2 \left\|\delta\theta_h^l\right\|_{W^{1,\infty}(U)}$. We also obtain, by additionally invoking proposition D.1.3 and suitable stability estimates:

$$\left|\text{⑤}\right|, \left|\text{⑥}\right| \lesssim h \left\|\delta\theta_h^l\right\|_{W^{1,\infty}(U)} \left\|u_h^l - u\right\|_{L^2(I,H^1(U))}, h \left\|\delta\theta_h^l\right\|_{W^{1,\infty}(U)} \left\|a_h^l - a\right\|_{L^2(I,H^1(U))} \lesssim h^2 \left\|\delta\theta_h^l\right\|_{W^{1,\infty}(U)}$$

having used theorem D.2.10 in the last step. The same theorem D.2.10 is sufficient to conclude the bound $\left|\text{⑦}\right| \lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$. The remaining terms are treated in the same way, we thus focus on ⑨. Using integration by parts theorem A.1.1, the assumption on $D\delta\theta_h^l$ and the fact that $u, u_h^l = 0$ on the moving boundary Γ_m, we obtain:

$$\left|\textcircled{9}\right| = \left|\int_I (\mathrm{div}(A'(\delta\theta)\nabla a), u_h^l - u)_{L^2(U)}\right| \lesssim h^2 \|\delta\theta\|_{W^{2,\infty}(U)}$$

where we used again theorem D.2.10. Alternatively, if $\delta\theta_h^l$ is not twice differentiable, theorem D.2.10 yields $\left|\textcircled{9}\right| \lesssim h \|\delta\theta\|_{W^{1,\infty}(U)}$.

Cost function

There holds:

$$\int_I \int_U \eta |v - w|^2 \mathrm{div}(\delta\theta) - \int_I \int_{U_h} \eta |v_h - w_h|^2 \mathrm{div}(\delta\theta_h) =$$

$$\underbrace{\int_I \int_U \eta((v - v_h^l) - (w - w_h^l))((v + v_h^l) - (w + w_h^l))\mathrm{div}(\delta\theta)}_{\textcircled{10}} + \underbrace{\int_I \int_U \eta(v_h^l - w_h^l)^2 \mathrm{div}(\delta\theta_h^l) - \int_I \int_{U_h} \eta(v_h - w_h)^2 \mathrm{div}(\delta\theta_h)}_{\textcircled{11}} +$$

$$\underbrace{\int_I \int_U \eta(v_h^l - w_h^l)^2 (\mathrm{div}(\delta\theta) - \mathrm{div}(\delta\theta_h^l))}_{\textcircled{11'}}$$

There holds $\textcircled{10} \lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$ thanks to the Cauchy-Schwarz inequality and theorem D.2.10, the same holds for $\textcircled{11}$ but because of proposition D.1.5. Lastly, by suitable stability estimates, $\textcircled{11'} \lesssim \left\|\delta\theta - \delta\theta_h^l\right\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$. $\qquad\square$

Corollary 3.2.2 (Fully discrete error estimates for discretize-then-optimize shape gradient, implicit Euler case)
With the same assumptions and notation of theorem 3.2.1 and in the discretize-then-optimize framework of section 3.2, we can conclude, in the smooth case:

$$\left|dJ(U)[\delta\theta] - dJ_{h,\delta t}(U_h)[\delta\theta^{-l}]\right| \leq \gamma(h^2 + \delta t)\|\delta\theta\|_{W^{2,\infty}(U)}$$

and, in the rough case:

$$\left|dJ(U)[\delta\theta] - dJ_{h,\delta t}(U_h)[\delta\theta^{-l}]\right| \leq \gamma(h + \delta t)\|\delta\theta\|_{W^{1,\infty}(U)}$$

Proof.

The overall argument amounts to "inserting dJ_h between dJ and $dJ_{h,\delta t}$". Two pieces must then be estimated, and the first is exactly addressed in theorem 3.2.1. The second one is $dJ_h(U)[\delta\theta^{-l}] - dJ_{h,\delta t}(U_h)[\delta\theta^{-l}]$. Of this member, we give an appropriate splitting, where every piece is $O(\delta t)$. This splitting is:

$$\int_I \int_{U_h} u_h' a_h \mathrm{div}(\delta\theta^{-l}) - \delta t \sum_{k=1}^K \int_{U_h} \frac{u_h^k - u_h^{k-1}}{\delta t} a_h^k \mathrm{div}(\delta\theta^{-l}) =$$

$$\underbrace{\int_I \int_{U_h} u_h'(a_h - \pi a_h)\mathrm{div}(\delta\theta^{-l})}_{\textcircled{12}} + \underbrace{\delta t \sum_{k=1}^K \int_{U_h} \frac{u_h(t^k) - u_h(t^{k-1})}{\delta t}(a_h(t^k) - a_h^k)\mathrm{div}(\delta\theta^{-l})}_{\textcircled{13}} +$$

$$\underbrace{\delta t \sum_{k=1}^K \int_{U_h} \left(\frac{u_h(t^k) - u_h(t^{k-1})}{\delta t} - \frac{u_h^k - u_h^{k-1}}{\delta t}\right) a_h^k \mathrm{div}(\delta\theta^{-l})}_{\textcircled{14}}$$

and:

$$\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla u_h)\nabla a_h - \delta t \sum_{k=1}^K \int_{U_h} (A'(\delta\theta^{-l})\nabla u_h^k)\nabla a_h^{k-1} =$$

$$\underbrace{\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla(u_h - \tilde\pi u_h)\nabla a_h}_{\text{(15)}} + \underbrace{\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla\tilde\pi u_h)\nabla(a_h - \pi a_h)}_{\text{(16)}} +$$

$$\underbrace{\delta t \sum_{k=1}^K \int_{U_h} (A'(\delta\theta^{-l})\nabla u_h(t^k))\nabla(a_h(t^{k-1}) - a_h^{k-1})}_{\text{(17)}} + \underbrace{\delta t \sum_{k=1}^K \int_{U_h} (A'(\delta\theta^{-l})\nabla(u_h(t^k) - u_h^k)\nabla a_h^{k-1}}_{\text{(18)}}$$

Finally:

$$\frac{1}{2}\int_I \int_{U_h} \eta|v_h - w_h|^2 \text{div}(\delta\theta^{-l}) - \frac{\delta t}{2}\sum_{k=1}^K \int_{U_h} \eta(t^k)(v_h^k - w_h^k)^2 \text{div}(\delta\theta^{-l}) =$$

$$\underbrace{\frac{1}{2}\int_I \int_{U_h} (\eta - \tilde\pi\eta)|v_h - w_h|^2 \text{div}(\delta\theta^{-l})}_{\text{(19)}} + \underbrace{\frac{1}{2}\int_I \int_{U_h} \tilde\pi\eta(|v_h - w_h|^2 - |\tilde\pi v_h - \tilde\pi w_h|^2)\text{div}(\delta\theta^{-l})}_{\text{(20)}} +$$

$$\underbrace{\frac{1}{2}\sum_{k=1}^K \int_{U_h} \eta(t^k)((v_h(t^k) - w_h(t^k))^2 - (v_h^k - w_h^k)^2)\text{div}(\delta\theta^{-l})}_{\text{(21)}}$$

We can treat (12), (15), (16), (19), (20) with lemma A.2.7 and suitable stability estimates: we obtain terms that are $O(\delta t)\,\|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)}$. The terms (13), (17) necessitate proposition 3.1.9 and stability estimates: they also are $O(\delta t)\,\|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)}$.

For the remaining pieces (14), (18), (21) the same conclusions apply, but this time we make use of proposition D.3.11 and proposition 3.1.4 (only their semidiscrete counterpart is necessary, such estimate can be readily extracted from the proof of those propositions). $\qquad\square$

As previously mentioned, we couldn't prove convergence for the adjoint states obtained after discretization, with $\theta = 1/2$. As a partial replacement for this, we derive a fully discrete estimate similar to the above ones, but in an optimize-them-discretize setting.

Corollary 3.2.3 (Fully discrete error estimates for optimize-then-discretize shape gradient, Crank-Nicolson case)
With the same assumptions and notation of theorem 3.2.1, and defining the optimize-then-discretize shape gradient as:

$$\tilde{d}J_{h,\delta t}(U_h)[\delta\theta^{-l}] :=$$

$$\delta t \sum_{k=0}^{K-1} \int_{U_h} \frac{w_h^{k+1} - w_h^k}{\delta t}\frac{q_h^k + q_h^{k+1}}{2}\text{div}(\delta\theta^{-l}) + \delta t \sum_{k=1}^K \int_{U_h} \left(A'(\delta\theta^{-l})\nabla\frac{w_h^k + w_h^{k+1}}{2}\right)\nabla\frac{q_h^k + q_h^{k+1}}{2}$$

$$\delta t \sum_{k=0}^{K-1} \int_{U_h} \frac{v_h^{k+1} - v_h^k}{\delta t}\frac{p_h^k + p_h^{k+1}}{2}\text{div}(\delta\theta^{-l}) + \delta t \sum_{k=1}^K \int_{U_h} \left(A'(\delta\theta^{-l})\nabla\frac{v_h^k + v_h^{k+1}}{2}\right)\nabla\frac{p_h^k + p_h^{k+1}}{2}$$

$$\frac{\delta t}{2}\sum_{k=0}^{K-1} \int_{U_h} \frac{\eta(t^k)(v_h^k - w_h^k)^2 + \eta(t^{k+1})(v_h^{k+1} - w_h^{k+1})^2}{2}\text{div}(\delta\theta^{-l})$$

we have, in the smooth case:

$$\left|dJ(U)[\delta\theta] - \tilde{d}J_{h,\delta t}(U_h)[\delta\theta^{-l}]\right| \le \gamma(h^2 + \delta t^2)\,\|\delta\theta\|_{W^{2,\infty}(U)}$$

and, in the rough case:

$$\left|dJ(U)[\delta\theta] - \tilde{d}J_{h,\delta t}(U_h)[\delta\theta^{-l}]\right| \le \gamma(h + \delta t^2)\,\|\delta\theta\|_{W^{1,\infty}(U)}$$

Proof.
Also here we only need to compare the semidiscrete and the fully discrete shape gradients, and to proceed to a suitable splitting of such discrepancy. We begin by the time derivatives terms:

$$\int_I \int_{U_h} u_h' a_h \mathrm{div}(\delta\theta^{-l}) - \delta t \sum_{k=0}^{K-1} \int_{U_h} \frac{u_h^{k+1} - u_h^k}{\delta t} \frac{a_h^k + a_h^{k+1}}{2} \mathrm{div}(\delta\theta^{-l}) =$$

$$\underbrace{\int_I \int_{U_h} (u_h - \pi_1 u_h)' a_h \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{12}}} + \underbrace{\int_I \int_{U_h} \frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} (a_h - \pi_1 a_h) \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{13}}} +$$

$$\underbrace{\delta t \sum_{k=0}^{K-1} \int_{U_h} \left(\frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} - \frac{u_h^{k+1} - u_h^k}{\delta t} \right) T_k a_h \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{14}}} + \underbrace{\delta t \sum_{k=0}^{K-1} \int_{U_h} \frac{u_h^{k+1} - u_h^k}{\delta t} \left(T_k a_h - \frac{a_h^k + a_h^{k+1}}{2} \right) \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{15}}}$$

For the gradients:

$$\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla u_h)\nabla a_h - \delta t \sum_{k=1}^{K} \int_{U_h} \left(A'(\delta\theta^{-l})\nabla\frac{u_h^k + u_h^{k+1}}{2} \right) \nabla \frac{a_h^k + a_h^{k+1}}{2} =$$

$$\underbrace{\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla(u_h - \pi_1 u_h))\nabla a_h + (A'(\delta\theta^{-l})\nabla\pi_1 u_h)\nabla(a_h - \pi_1 a_h)}_{\text{\textcircled{16}}} + \underbrace{\int_I \int_{U_h} (A'(\delta\theta^{-l})\nabla\pi_1 u_h)\nabla\pi_1 a_h - \delta t \sum_{k=0}^{K-1}(A'(\delta\theta^{-l})T_k\nabla u_h)\nabla T_k a_h}_{\text{\textcircled{17}}}$$

$$\underbrace{+ \delta t \sum_{k=0}^{K-1} \left(A'(\delta\theta^{-l}) \left(T_k\nabla u_h - \nabla\frac{u_h(t^k) + u_h(t^{k+1})}{2} \right) \right) \nabla T_k a_h}_{\text{\textcircled{18}}} + \underbrace{\delta t \sum_{k=0}^{K-1} \left(A'(\delta\theta^{-l})\nabla\frac{u_h(t^k) + u_h(t^{k+1})}{2} \right) \nabla \left(T_k a_h - \frac{a_h(t^k) + a_h(t^{k+1})}{2} \right)}_{\text{\textcircled{19}}}$$

For the cost functions:

$$\frac{1}{2} \int_I \int_{U_h} \eta|v_h - w_h|^2 \mathrm{div}(\delta\theta^{-l}) - \frac{\delta t}{2} \sum_{k=0}^{K-1} \int_{U_h} \frac{\eta(t^k)(v_h^k - w_h^k)^2 + \eta(t^{k+1})(v_h^{k+1} - w_h^{k+1})^2}{2} \mathrm{div}(\delta\theta^{-l}) =$$

$$\underbrace{\int_I \int_{U_h} \eta(v_h - w_h)^2 \mathrm{div}(\delta\theta^{-l}) - \delta t \sum_{k=0}^{K-1} \int_{U_h} T_k \left[\eta(v_h - w_h)^2 \right] \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{20}}} +$$

$$\underbrace{\frac{\delta t}{2} \sum_{k=0}^{K-1} \int_{U_h} \frac{\eta(t^k)((v_h(t^k) - w_h(t^k))^2 - (v_h^k - w_h^k)^2) + \eta(t^{k+1})((v_h(t^{k+1}) - w_h(t^{k+1}))^2 - (v_h^{k+1} - w_h^{k+1})^2)}{2} \mathrm{div}(\delta\theta^{-l})}_{\text{\textcircled{21}}}$$

Now, \textcircled{12}, \textcircled{13}, \textcircled{16} can be treated with with lemma A.2.7, remembering that $\|u_h''\|_{L^2(I,L^2)}$ is bounded as in the proof of proposition D.3.11 for \textcircled{12}, and that the difference quotient of \textcircled{13} can be handled as in the proof of proposition D.3.11. We obtain bounds by $\|\delta\theta_h\|_{W^{1,\infty}(U_h;\mathbb{R}^n)} \delta t^2$.

For \textcircled{14}, \textcircled{15}, \textcircled{18}, \textcircled{19}, \textcircled{21} we must use the finite element estimates 3.1.4, or proposition D.3.11, in the case of \textcircled{14}: we obtain bounds by $\|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)} \delta t^2$.

Consider now the function $I \ni t \mapsto i(t) := \eta(t) \int_{U_h} (v_h(t) - w_h(t))^2 \mathrm{div}(\delta\theta^{-l})$, where $T_k f = (f(t^k) + f(t^{k+1}))/2$. Using basic properties of Sobolev and Bochner spaces (see at the end of the proof), it can be shown that $i \in W^{2,1}(I;\mathbb{R})$, and the same arguments as in [21] ensure that $\text{\textcircled{20}} \leq \delta t^2 \int_I |i''|$. The latter term can be bounded as $\lesssim \|\delta\theta_h\|_{W^{1,\infty}(U_h;\mathbb{R}^n)} \delta t^2$, where we have to use the boundedness of v_h'', w_h'' in $L^2(I, L^2)$ as we saw it in the proof of proposition D.3.11.

Let us now come to \textcircled{17}. In this case some algebraic computations show that:

$$\text{\textcircled{17}} = \frac{\delta t^2}{12} \delta t \sum_{k=0}^{K-1} \left(A'(\delta\theta^{-l}) \nabla \frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t}, \nabla \frac{a_h(t^{k+1}) - a_h(t^k)}{\delta t} \right)_{L^2(U_h)}$$

Let us call $\overline{u'}_h$ the function that on each I_k is $\delta t^{-1} \int_{I_k} u'_h = \dfrac{u_h(t^{k+1}) - u_h(t^k)}{\delta t}$. We immediately get:

$$\left| \underset{}{\textcircled{17}} \right| \lesssim \delta t^2 \, \|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \overline{u'}_h|_{I_k} \right\|_{H^1(U_h)}^2} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \overline{a'}_h|_{I_k} \right\|_{H^1(U_h)}^2}$$

A minor reworking of lemma 3.2 of [41] gives $\left| \textcircled{17} \right| \lesssim \delta t^2 \, \|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)} \|u'_h\|_{L^2(I,H^1(U_h))} \|a'_h\|_{L^2(I,H^1(U_h))}$. Now we only need to apply stability estimates to conclude $\left| \textcircled{17} \right| \lesssim \delta t^2 \, \|\delta\theta\|_{W^{1,\infty}(U;\mathbb{R}^n)}$.

A technicality

Here is why i'' is $W^{2,1}(I;\mathbb{R})$. η is smooth in time, so that we want $j(t) := \int_{U_h} (v_h(t) - w_h(t))^2 \mathrm{div}(\delta\theta^{-l})$ to be $W^{2,1}(I;\mathbb{R})$. But by corollary A.2.2 it suffices $t \mapsto (v_h(t) - w_h(t))^2 \mathrm{div}(\delta\theta^{-l})$ to be in $W^{2,1}(I;L^1)$. First of all, the constant factor $\mathrm{div}(\delta\theta^{-l})$ doesn't play a role in time smoothness, so that we now only need to check that $(v_h - w_h)^2 \in W^{2,1}(I;L^1)$. This will follow from repeated application of the following lemma: $uv \in W^{1,1}(I,L^1)$ if $u,v \in H^1(I,L^2)$, with $(uv)' = uv' + u'v$.

The latter claim follows by density of smooth functions $C^\infty(\overline{I}, L^2)$ in $H^k(I, L^2)$, see [44], corollary 3.12.

$\square$

4. Implementation

We now discuss our implementation and verify some of the results that were previously shown:

- section 4.1 is devoted to the illustration of the computer implementation of the shape optimization problem, problem 2.2.3
- in section 4.2 some numerical experiments are reported and commented: we focus on shape optimization results and on the error estimates for shape gradients of section 3.2

4.1. Algorithmic set-up

We anticipate that all the experiments and the code are hosted at the following GitHub page:

`https://github.com/leom97/Master-s-thesis.git`.

We wrote our code in Python, making substantial use of the FEniCS package ([49]). This is the main tool to simulate the partial differential equations. One of the reasons for choosing FEniCS is the compatibility with dolfin-adjoint, an automatic differentiation toolbox that "derives the discrete adjoint and tangent linear models from a forward model written in the Python interface to FEniCS" (see [32], [23] and [52]). That is, we only needed to code the "forward model" (cost functional and partial differential equations), whereas the shape gradients, that are exact on the discrete level, would be automatically derived for us by dolfin-adjoint. The correctness of the gradients was also checked through comparisons based on proposition 3.1.6 and through Taylor tests. In addition, for the shape optimization part, we made use of Moola, "a set of optimisation algorithms specifically designed for PDE-constrained optimisation problems" (see here). GMSH ([33]) was used for the meshing.

The shape identification problem, problem 2.1.2, lends itself very well to debugging and numerical experimentation, as one can build "exact" solutions (on the discrete level) and then analyze whether that is recovered by the optimization process. One can for instance artificially create the "optimal" inclusion Ω_e, invent Neumann measurements g, simulate the heat equation for w (see problem 2.1.1) and then obtain the correct Dirichlet data f. Starting then from an initial guess for the inclusion and making use of g, f, optimization can be started: Ω_e should be recovered.

Before delving into more details, here is an overview of the different components of the shape optimization code:

1. meshing the reference domain
2. transforming the reference domain to the "optimal domain" Ω_e
3. simulating the heat equation on Ω_e with artificial Neumann data g, to obtain the synthetic Dirichlet data f
4. running the optimization routines with f, g as data form a guess of Ω_e

Let us now discuss more thoroughly some of the above components.

Meshing

We want to remark that in the meshing procedure, we started from a smooth shape modeled in GMSH, and then triangulated it into a mesh, whose boundary nodes lie on the boundary of the smooth shape, as is required in e.g. assumption 3.1.2 and appendix D. Instead of choosing a base mesh and then performing (uniform) refinements on it, we loaded a sequence of meshes with increasingly finer mesh widths. In fact, after a uniform refinement, not all discrete boundary nodes need to be again on the smooth boundary. One would need to correct for this effect, and to do so, have knowledge of a parametrization of the entire boundary: as we tried to use the least possible knowledge of the smooth boundary, we opted for generating a mesh sequence, instead of performing refinements.
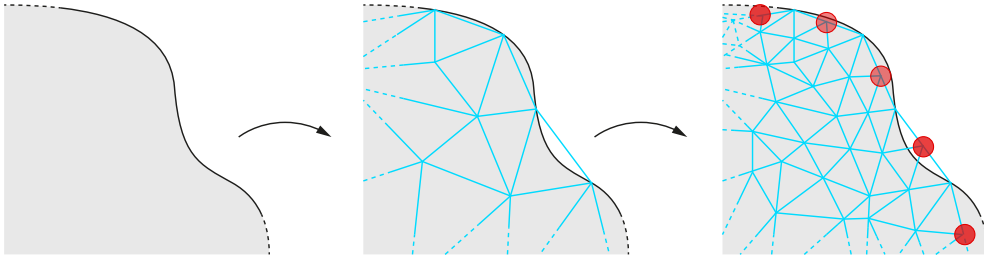

Figure 4.1.: Problems with uniform refinements

Star-shaped parametrization

For simplicity, we assume that the computational domain can only undergo radial displacements of the form given in corollary 2.3.5. This is realized as follows. The reference domain is fixed to be a triangular meshing of $D \setminus \overline{B_\epsilon(0)} =: U_r$, meshing which induces the space of linear finite elements S_h^1, as we have denoted it in e.g. appendix D. Consider another meshing of the unit sphere $\mathbb{S}^{n-1}$,

potentially independent of the previous one to allow some flexibility, inducing the space of (surface) linear finite elements $B^1_{\tilde{h}}$. Our control, i.e. our optimization variable, will be a function $q_{\tilde{h}} \in B^1_{\tilde{h}}$, and we should be solving:

$$\min_{q_{\tilde{h}} \in B^1_{\tilde{h}}} J_{h,\delta t}(\tau_{\epsilon + q_{\tilde{h}}}) = J_{h,\delta t}(\mathrm{Id} + V_{q_{\tilde{h}}})$$

with $V_{q_{\tilde{h}}}$ being the replacement vector field described in corollary 2.3.5. The issue with this formulation is that $V_{q_{\tilde{h}}}$ doesn't preserve the polygonal/polyhedral nature of the volume meshes. Therefore, we actually implement:

$$\min_{q_{\tilde{h}} \in B^1_{\tilde{h}}} J_{h,\delta t}(\mathrm{Id} + I_h V_{q_{\tilde{h}}})$$

where I_h means Lagrange interpolation onto piecewise linears. The transformation $q_{\tilde{h}} \mapsto I_h V_{q_{\tilde{h}}}$ is implemented in a user defined dolfin-adjoint module.

Synthetic data

As previously mentioned, to obtain the needed boundary data to perform shape optimization, we simulate the heat equation for w on the exact computational domain $\Omega_{e,h}$. Because we are in a "volumetric" setting, we give the Neumann data and obtain the Dirichlet nodal values, unlike in [38], where the opposite is done. In fact, in our setting, the discrete Neumann trace need not to have a boundary representation.

Using the same discretization parameters to generate the synthetic data, and then perform shape optimization, will result in committing an "inverse crime" (see [65]). To avoid this, there are at least two possibilities: either some noise is added to the synthetic data, or different computational models must be employed in synthesis and inversion/optimization. We experiment with both options, and in particular, for the second, we synthethize the data with a finer discretization than during the optimization process. We mention that in [38], synthesis and inversion are performed by solving integral equations of different kinds, but on the same discretization. The authors also add noise to the synthetic data.

Finite elements

We are adopting, as already mentioned, linear (instead of e.g. quadratic) finite elements, for simplicity, but also computational efficiency. This is in constrast with [38], where the authors employ order 2 isoparametric elements (in the context of the boundary element method). The framework of appendix D can be moreover potentially accommodate higher order isoparametric elements, see the works of e.g. [25], [27], [26]. Isoparametric elements elements are necessary, when adopting higher order basis functions, in order to preserve optimal accuracy (see section 4.4 of [58] for a discussion on this). The version of FEniCS we are using (2019.1) doesn't provide support for curved geometries, and the latest release FEniCSx is not yet interfaced with dolfin-adjoint. Alternatively, Firedrake could be employed, which has compatibility with dolfin-adjoint, although we encountered several difficulties in the transfering of functions between non conforming meshes, something we needed at several places throughout our code.

Also, we recall that the motivation for using the FEM method is that the analysis of [40], which we partially repeated in our setting, suggests that the volume form of the shape gradient is more accurate a boundary form, when PDEs are discretized with the finite element method. Finite elements are also appreciated and widespread in the engineering community. The main drawback of adopting a distributed setting is the added computational cost: the entire domain must be meshed, and the solution computed on interior nodes too.

Optimization

As previously mentioned, we make use of the package Moola. This is because of its capabilities to natively handle optimization with respect to custom scalar products, and we found this to be especially important in our case, see section 2.4 for a theoretical justification and section 4.2 for a further discussion.

We mostly experimented with an L-BFGS algorithm, but also with a modified Newton's method. We implemented the latter following the observations contained in [28], a work centered around a very similar shape optimization problem to ours, in an attempt to alleviate some spurious oscillations we observed, most likely coming from the ill-posedness of the shape identification problem. We will soon discuss these aspects in section 4.2.

With regards to the temporal weight (see section 3.1 for details), we chose $\eta(t) = \exp\{-a/(t-T)^2\}$, with a suitable $a > 0$ ($a = 0.005$ in our runs). η roughly looks like this:
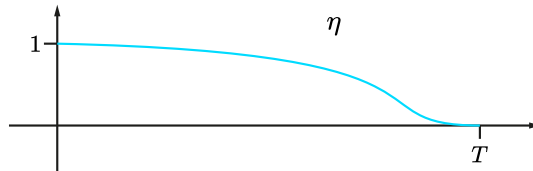

Figure 4.2.: The temporal weight η

4.2. Experiments

All the experiments were run on a laptop with an Intel® i7-6700HQ CPU at 2.60GHz, and 16 GB of RAM.

For simplicity we work in two dimensions and with $D := B_2(0)$, $\Omega_r := B_1(0)$, so that U_r is an annulus centered at the origin.

4.2.1. Shape optimization results

We set $T = 2$ throughout. Note that in the following plots, the "exact" control (yielding the exact domain $\Omega_{e,h}$ is always interpolated into the finite element space of the control $\tilde{q}_h$, to emphasize what is the best possible result that can be attained by the optimization routine.

Some exploratory runs

Let us illustrate a few runs, performed with different Neumann data g and with an hourglass-shaped inclusion. The challenge of this example is to correctly resolve the "corners" in the middle of the hourglass, which have a strong derivative (in the sense of radial functions), are far away from the external boundary (so that the influence on the boundary data of the heat equations may be weak), and where the mesh becomes very distorted, which worsens the quality of the mesh and thus, possibly, of the finite element solution.

To avoid the inverse crime, the Dirichlet data is generated on a mesh that is twice as fine as the to-be-optimized one, and with 120 steps of the Crank-Nicolson method, whereas 60 are used in the simulation. The parameter $\tilde{h}$ is set to 0.03 during synthesis, and to 0.15 during inversion. Such configuration will be referred to as "standard configuration".

We show the results of six runs performed with six different Neumann sources, having a common behaviour in time: $g_1 = t^2$, $g_2 = x_1 g_1$, $g_3 = x_2 g_2$, $g_4 = t^2 \sin(4t)$, $g_5 = t$, $g_6 = 1$. The examples took $25, 20, 20, 25, 25, 25$ L-BFGS iterations to converge, amounting to around 4 minutes for each run.

g_2, g_3, g_4 represent various complications of the base example g_1, and we experiment with them to point out that there doesn't seem to exist a recurring "error shape" when varying the boundary data.
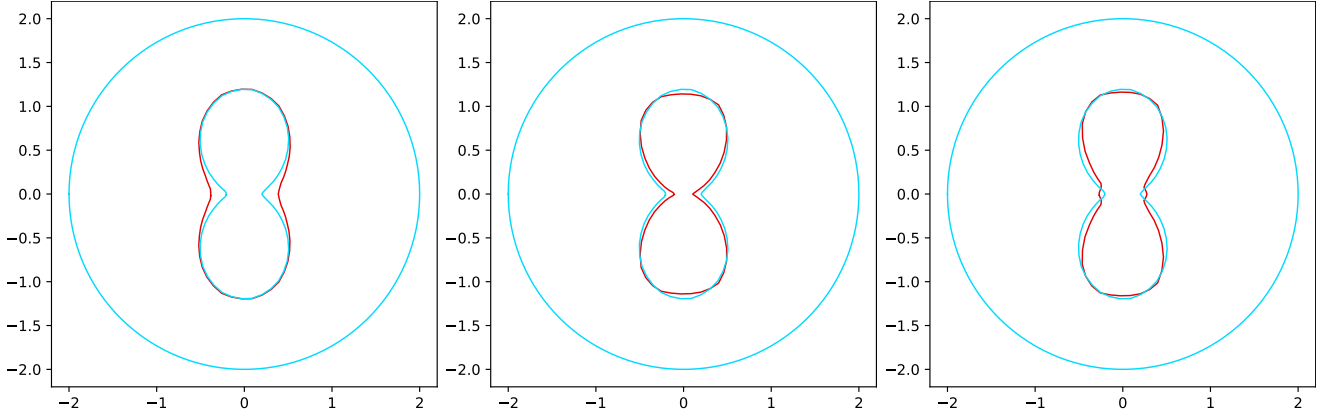

Figure 4.3.: Exact and simulated inclusion (in red) for the runs with g_2, g_3 adn g_4, in order from left to right

On the other hand, the heat equations with g_5, g_6 lack, respectively, one and two orders of compatibility, that are required in assumption 3.1.2. We can see a better result in g_1, then in g_5 and lastly in g_6:
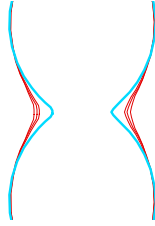

Figure 4.4.: From the outside to the inside: run with g_6, g_5, g_1 and exact solution in blue

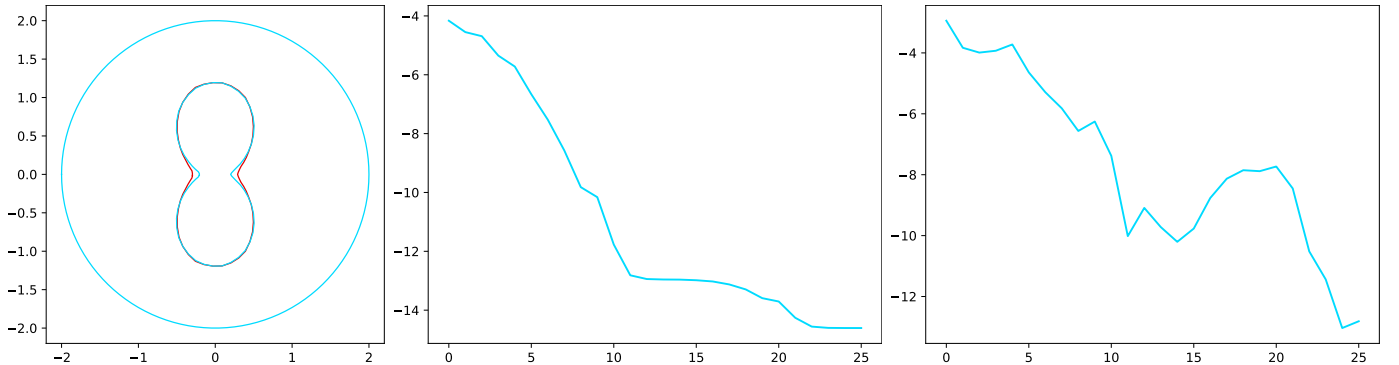For completeness, with g_1, we also report the history of the cost function and the gradient l^∞ norm:

Figure 4.5.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 25 iterations

We now show a visual comparison of the same example g_1, run with three different values a for $\eta(t) = \exp\{-a/(t-T)^2\}$, which are $a = 0.005, a = 0.05$ and $a = 0$.

Figure 4.6.: From outside to inside: run with g_1 and $a = 0$, $a = 0.05$, $a = 0.005$ and exact solution in blue

Some very small differences can be noticed: it seems that small values of a yield an improvement over a 0 value of a. Our hypothesis for this is in accordance with the behaviour of fig. 4.4: $a = 0$ means losing some compatibility. A too large value of a, on the other hand, perturbs the problem too much (so that the plot corresponding to $a = 0.005$ is yields the best result here). From here, we conjecture that a should be chosen small enough, but positive.

Inner product

We found it beneficial to work with smooth descent directions by making use of the H^1 inner product during optimization, instead of the L^2 one. This is natively handled by Moola. In doing so we obtained less squiggly boundaries, and more admissible ones: note in fact that we are working in an unconstrained setting for simplicity, whereas the optimization variable $\tilde{q}_h$ should be positive and small enough for the computational domain to be contained in $B_2(0)$. With the L^2 scalar product we found that iterates were sometimes assuming negative values.
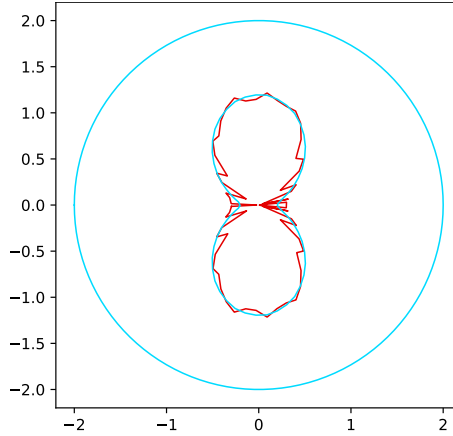

Figure 4.7.: Reconstruction for the run g_1 and the L^2 inner product

Ill-posedness

Degeneration of the boundary

It has already been noted in [38] that problem 2.1.2 is "severely ill-posed". The ill-posedness of the inverse problem is mirrored in the ill-posedness of the shape optimization problem, problem 2.2.3, where the responsible for such ill-posedness is the compactness of the continuous shape Hessian at the optimal domain: this phenomenon has been exhaustively analyzed in [28] in an "elliptic" version of problem 2.1.2, but we expect their conclusions to apply also to our case.

We computed the shape Hessian at the optimal domain with the help of dolfin-adjoint and observed indeed large condition numbers, as expected (with values $\simeq 10^5$).

This means that small changes in the problem data might yield large changes in the reconstruction, and instabilities in the reconstruction process. In fact, as is commonplace in solving ill-posed inverse problems, proceeding further with the iterations of the solution algorithm will only at first improve the reconstruction, but later result in a degradation of the result (see e.g. [42], section 2.1). As a remedy, one should impose prior knowledge on the reconstruction through regularization, and/or adopt some form of early stopping.

We did experience these phenomena: up to a certain number of L-BFGS iterations, we obtained acceptable results, the ones we showed above. Proceeding further led to a degradation of the inner boundary. The run with g_1 and stopping at 75 iterations instead 25, produced:
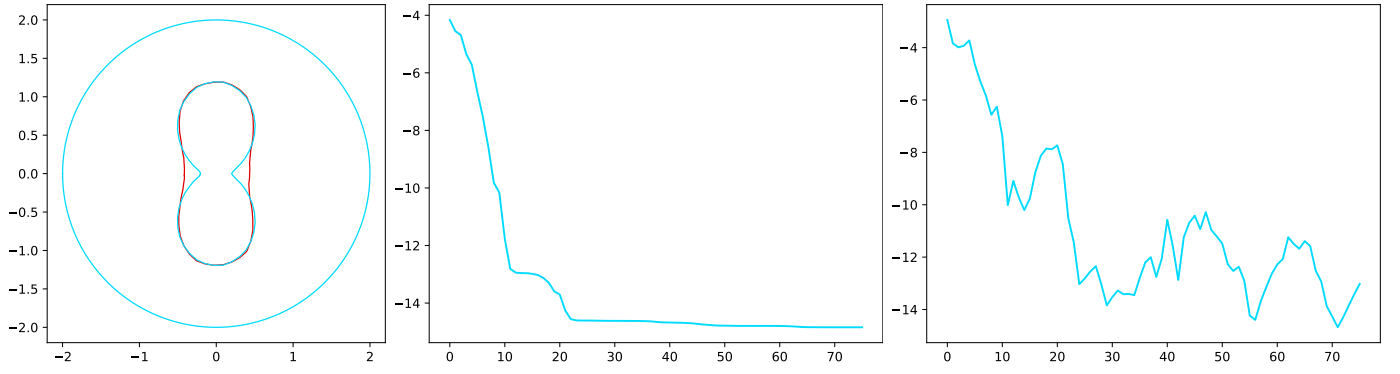
Figure 4.8.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 75 iterations

The solution obtained at around 25 iterations remains unchanged and stable until about iteration 35, then the cost function is further reduced, along some spurious descent direction.

This degeneration is even more evident and quicker, in case the implicit Euler method is used during optimization, in place of the Crank-Nicolson one, all the other parameters being unchanged (so that the exact data is still generated with the Crank-Nicolson method). This is because the implicit Euler's method converges more slowly in time, so that the discrepancy in the computed PDEs and the synthetic PDEs, is $O(\delta t)$ and not $O(\delta t^2)$. This is one of the reasons for adopting the Crank-Nicolson method: the implicit Euler method yields a faster, worse degeneration of the boundary, and a less accurate one, when early stopping is applied. We have nonetheless analyzed the implicit Euler case in chapter 3 because this method has already been successfully employed in less ill-posed parabolic shape optimization (see [12]). We show reconstruction, cost function and gradient history for a run with implicit Euler.
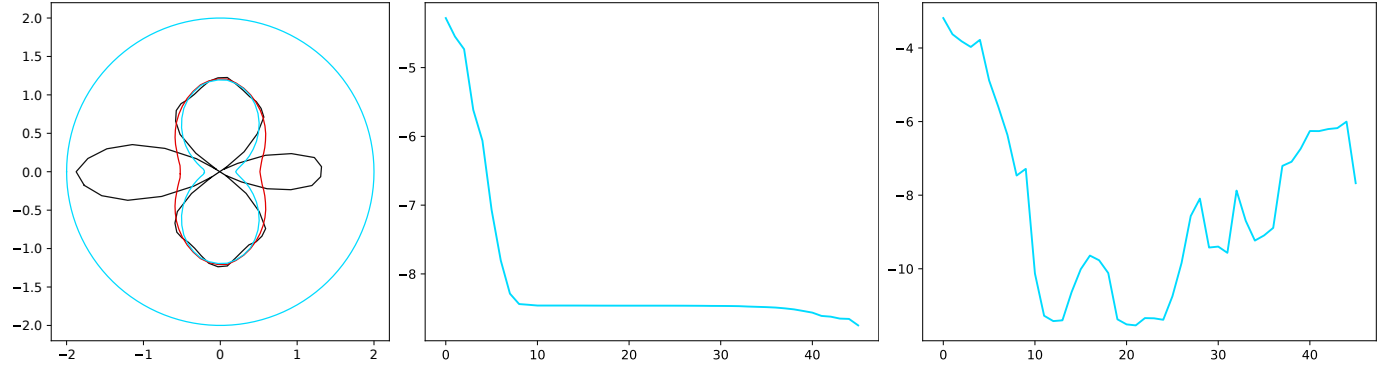

Figure 4.9.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run. The black boundary corresponds to 45 iterations, the blue one to 25. The presence of the lateral lobes in the black reconstruction indicates a negative radial function.

About the inverse crime

Let us avoid the inverse crime in a different way, through application of noise to the problem data f, g. We therefore set the discretization parameters for the synthetization, equal to those used for the inversion. The noise level is 1%, with respect to the $L^\infty(I, L^\infty)$ norm of the data, and the perturbation is random uniform.

We noticed that the optimization process is much more stable with the number of iterations, than when different discretizations are adopted, for inversion and synthesis. The reconstructed boundary is very similar to those of the above runs, and it starts to present spurious oscillations very late (only after iteration 80, in the case of the g_1 run). In the present case, the discrepancy between exact data, and data available during optimization, is randomly distributed and of zero mean, whereas we noted that it presents a "trend" given by the chosen PDEs discretization algorithm, when different discretizations are employed. This seems to be a key ingredient to the degeneration behaviour that we observed.

We did most of the experiments with different discretizations between inversion and synthesis, because this approach better highlited the ill-posedness of the problem. Moreover, in a real-world situation, the data can be interpreted to be sampled from a solution with discretization parameters tending to zero, this is another reason to proceed as we did.

Second order information

As previously mentioned, there is evidence for saying that the shape optimization problem is ill-posed: this is reflected in an ill-conditioned Hessian, at the optimal domain. This can cause undesired oscillations when employing only first order optimization methods, a possible way out being the usage of additional second order information, like the shape Hessian.

We thus experimented with a regularized Newton method, following the observations of [28] (to which we refer the reader for further details about the method), and found out that, indeed, spurious oscillations don't seem to happen: using g_1 as Neumann data, we find that it takes about 20 iterations for the shape to stabilize. However, the runtime increases to about 2.75 minutes per iteration, the shape Hessian being automatically computed by dolfin-adjoint. On top of this, the reconstruction seems to be less precise than when employing the L-BFGS method, with early stopping. This convinced us to stick with the L-BFGS method.
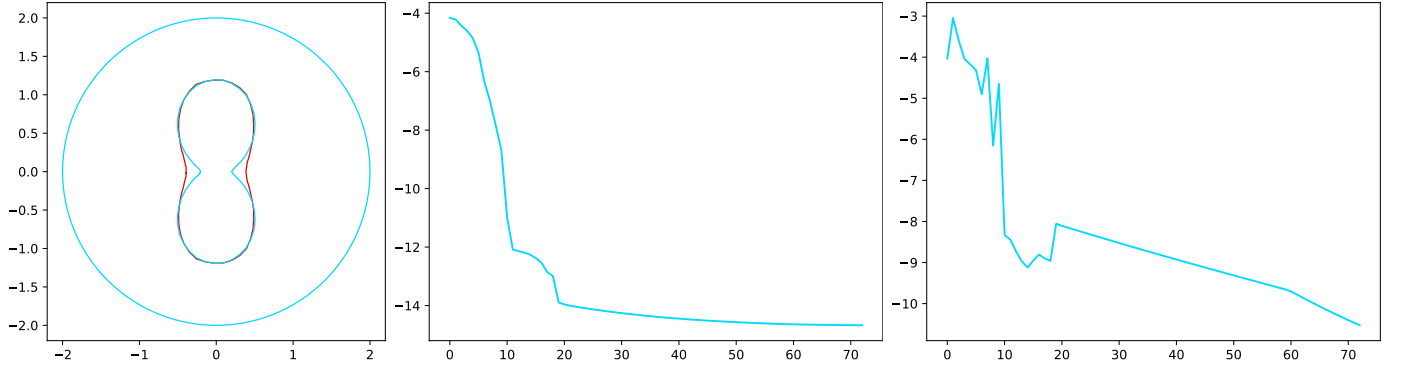
Figure 4.10.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run, and the regularized Newton method from [28]. The reconstructions after 20 and 70 shape are visually indistinguishable.

Sea urchin

Lastly, we show the reconstruction of a 2D version of the more complicated "sea urchin" inclusion of [38]. The discretization configuration is the standard one. The reconstruction ran for 30 iterations. This time, for completeness, we applied also 1% noise to the data, apart from employing different discretizations in inversion and synthesis.
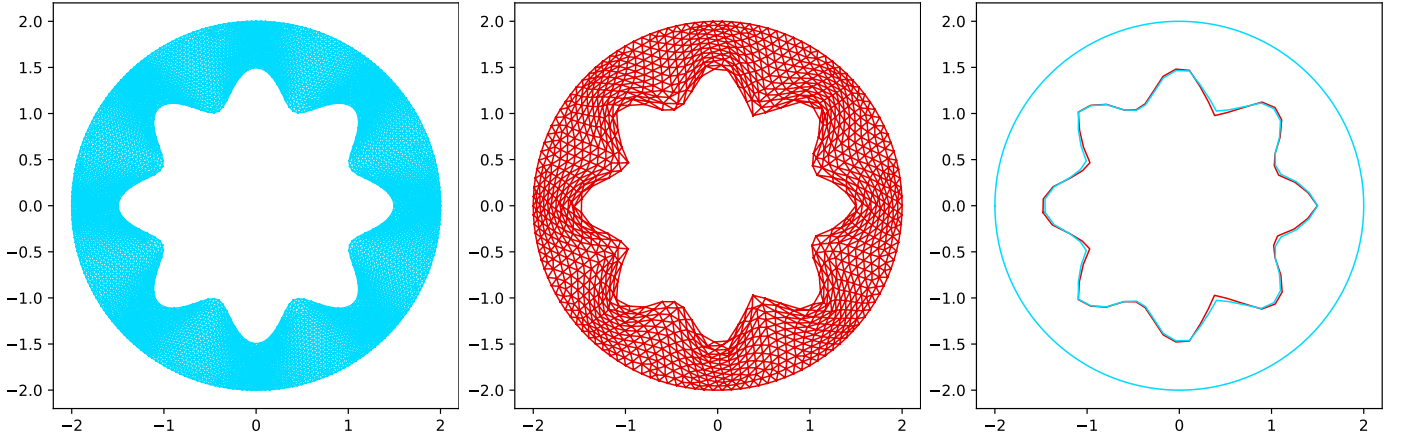

Figure 4.11.: "Exact" domain, reconstruction, and comparison between reconstruction and the exact domain, interpolated to the optimization finite element space.

4.2.2. Estimates for the shape gradients

We now present some numerical evidence of the estimates shown in section 3.2. Throughout, U_h will be approximating $U = B_2(0) \setminus \overline{B_1(0)}$.

For $\theta = 1$ (implicit Euler) or $\theta = 1/2$ (Crank-Nicolson), we set $\delta t = Ch^{2\theta}$, $C > 0$. We choose a number of spikes s from 0 to 9, an amplitude among 0.1 and 0.2 and we consider the resulting sinusoidal radial function $q(t) = A\cos(st)$, interpolated on a spherical mesh of size $\tilde{h} = 0.5$. This mesh parameter stays fixed across all the runs, when h varies. Note, this yields a very coarse spherical mesh: the rationale is to have the resulting displacement fields (finite element vector fields on the mesh of size h) approximating a vector field that is in $W^{1,\infty}$ but not $W^{2,\infty}$, as h is refined. We thus obtain 20 different displacement fields $\delta\theta^i_{h,\tilde{h}}$, $i = 1,...,20$, with which we test the shape gradients.

Not being able to represent non-discretized shape gradients, we content ourselves with analyzing the asymptotic behaviour of the quantity:

$$Q_h := \max_{i=1,...,20} \frac{|dJ_{h_f,\delta t_f}(U_{h_f})[\delta\theta^i_{h_f,\tilde{h}}] - dJ_{h,\delta t}(U_h)[\delta\theta^i_{h,\tilde{h}}]|}{\left\|\delta\theta^i_{h,\tilde{h}}\right\|_{W^{1,\infty}(U_{h_f})}}$$

where $h_f \ll h$, $\delta t_f \ll \delta t$.

In particular, we set $h_f = 0.03125$, and $h = 2^l h_f$, for l integer, where we refer to 2^l as "multiplier". We report the orders of convergence $\frac{\log Q_h - \log Q_{2h}}{\log h - \log 2h}$ in four cases, corresponding to $\theta = 1, 1/2$ and $a = 0.05, 0$, where $\eta = \exp\{-a/(t-T)^2\}$. We set $C = 1$ (for $\delta t = Ch^{2\theta}$) for Crank-Nicolson, and $C = 5$ for implicit Euler, to have a number of timesteps that is always greater than 1. For reasons of computational resources, we made one less refinement in the implicit Euler case.

Of course we register an infinite order of convergence when the refinement brings us from $2h_f$ to h_f. Moreover, the order of convergence value in the refinement before this is larger than expected, most probably because of a "saturation" effect. We nonetheless think that, at least in the case $a > 0$, these results confirm the theoretical considerations in section 3.2. In particular, we note the following facts:

Run with Crank-Nicolson, $a = 0.05$ and $C = 1$						
Multiplier	32	16	8	4	2	1
Q_h	0.0557	0.0139	0.0047	0.0013	0.0003	0.0
OOC	2.356	1.8261	2.0785	2.4573	∞	−
Run with Crank-Nicolson, $a = 0$ and $C = 1$						
Multiplier	32	16	8	4	2	1
Q_h	0.0697	0.0078	0.0021	0.0006	0.0001	0.0
OOC	3.7204	2.1859	2.1446	2.3489	∞	−

Table 4.1.: Order of convergence study with Crank-Nicolson

Run with implicit Euler, $a = 0.05$ and $C = 5$					
Multiplier	16	8	4	2	1
Q_h	0.0549	0.0154	0.0047	0.001	0.0
OOC	2.1202	1.9637	2.3004	∞	−
Run with implicit Euler, $a = 0$ and $C = 5$					
Multiplier	16	8	4	2	1
Q_h	0.0594	0.0126	0.005	0.0011	0.0
OOC	2.5864	1.5225	2.2349	∞	−

Table 4.2.: Order of convergence study with implicit Euler

- the above tables suggest a superconvergence effect, for the implicit Euler's method, even with "rough" displacement vector fields, cfr. corollary 3.2.2

- although we haven't given a proof of the convergence behaviour in the case of the Crank-Nicolson method and a discretize-then-optimize approach, the above results suggest that the quantity Q_h is $O(h^2 + \delta t^2)$, as we suspected. Note, also here it suffices to test with $W^{1,\infty}$ displacements, to obtain the spatial superconvergence effect

- the value of 1.5225 in table 4.1 might be due to a lack of regularity of the adjoint states, since $a = 0$. This does not contradict our predictions, which were done in conditions of $a > 0$

5. Conclusion

We considered a model parabolic shape optimization problem and treated it in a volumetric fashion: the expression of the distributed shape gradient was derived, also in connection to a star-shaped parametrization of the domains.

The finite element method was employed to perform the spatial discretization of the arising PDEs, whereas a Crank-Nicolson or implicit Euler scheme was adopted for the temporal one. In the latter case, optimization and discretization are seen to commute.

We derived a semidiscrete (in space) error estimate relating the continuous shape gradient at a smooth enough domain U, and the discrete shape gradient at a polygonal/polyhedral interpolation U_h of U. In the case of the implicit Euler method, we were able to derive fully discrete estimates in a discretize-then-optimize commutative setting, for the Crank-Nicolson one only in an optimize-then-discretize framework.

Numerical experiments support such conclusions, and even suggest that what was only proved for the implicit Euler method, might be obtainable with the Crank-Nicolson method. We also show the results from the shape optimization process itself.

There are some interesting directions in which our work can be expanded:

- one could at first prove that discretization and optimization commute also for Crank-Nicolson, as [30] suggests
- from here, fully discrete estimates analogous to those for implicit Euler, should be derivable
- the error estimates for the shape gradients were derived assuming a specific form of U_h: it could be worth to try to eliminate the requirement that ∂U_h must interpolate ∂U. Moreover, one could try to explicitly account for the fact that $U = \tau(U_r), U_h = \tau(U_{r,h})$, in these estimates

A. Functional spaces

Let us collect, for the convenience of the reader, some technical results that will be used throughout our work. Where appropriate, we give a short proof or a reference for one.

A.1. Sobolev spaces

Theorem A.1.1 (Integration by parts)
Let Ω be a bounded Lipschitz domain. Let $1 < p < \infty$ and $f, g \in W^{1,p}(\Omega), W^{1,q}(\Omega)$, $q = p'$, the dual Hölder exponent. Then:

$$\int_\Omega f \partial_i g = - \int_\Omega g \partial_i f + \int_{\partial\Omega} \operatorname{tr} u \nu_i d\mathcal{H}^{n-1}$$

Proof.

This follows from [45], theorem 18.1 at page 592, where g needs to be $C_c^1(\mathbb{R}^n)$. But [1], theorem 3.18 at page 54, says that (thanks to the smoothness of the boundary) the set of the restriction of such functions is dense in $W^{1,q}(\Omega)$, so that we can conclude by a density argument. $\square$

Proposition A.1.2 (Characterization of $W^{1,\infty}$)
Let Ω be a bounded Lipschitz domain, or $\mathbb{R}^n$. Then $W^{1,\infty}(\Omega) = C^{0,1}(\overline{\Omega}) \cap L^\infty(\Omega)$.
This means that $u \in W^{1,\infty}(\Omega)$ if and only if u has a (unique) representative that is bounded, Lipschitz continuous. Weak and classical derivatives coincide a.e.

Proof.

In any case, Ω is an extension domain for $W^{1,\infty}(\Omega)$ (see [45], theorem 13.17 at page 425, 13.13 at page 424, and definition 9.57 at page 273).

Let $u \in W^{1,\infty}(\Omega)$. By [45], 11.50 at page 339, because Ω is an extension domain, we obtain that u has a representative $\bar{u}$ that is bounded Lipschitz. Let $\phi \in C_c^\infty(\Omega)$. By The Kirszbraun theorem (see e.g. [5]), we can extend $\bar{u}$ to a Lipschitz on $\mathbb{R}^n$. Then, by Fubini's theorem and integration by parts for AC functions, we conclude $\int_\Omega \bar{u} \partial_i \phi = - \int_\Omega \partial_i \bar{u} \phi$, so that $\nabla \bar{u} = \nabla u$ almost everywhere.

Conversely, let u be bounded Lipschitz. The above reasoning shows that u has essentially bounded weak derivatives equal to the a.e. classical derivatives. $\square$

A.2. Bochner spaces

Proposition A.2.1 (Bochner integral and bounded operators)
Let X, Y be separable Banach, let $T \in L(X, Y)$ be a linear bounded operator. For $f \in L^1(I, X)$ define $Tf(t) := T(f(t))$. Then $Tf \in L^1(I, Y)$ with $T \int_I f = \int_I Tf$.

Proof.

Let f_n be simple, $f_n \to f$ a.e., with $\lim_n \int_I f_n = \int_I f$ and $\|f_n\|_X \leq C \|f\|_X$ (see page 6, and corollary 2.7 at page 8 of [44]).

For almost all t, $T(f_n(t)) \to T(f(t)) = Tf(t)$ in Y, so that Tf is measurable (strongly).

By dominated convergence (corollary 2.6 of [44]), Tf is integrable. Thus $\int_T Tf = \lim_n \int_I Tf_n = \lim_n T \int_I f_n$, because f_n is simple. And now, by the choice of f_n, $\int_T Tf = \lim_n T \int_I f_n = T \lim_n \int_I f_n = T \int_I f$. $\square$

Corollary A.2.2 (Derivations and bounded operators)
As before, let X, Y be separable Banach, let $T \in L(X, T)$ be a linear bounded operator.
For $k \geq 0$, $1 \leq p < \infty$, $f \in W^{k,p}(I, X) \implies Tf \in W^{k,p}(I, Y)$, with weak derivatives $\partial_{t^i} Tf = T \partial_{t^i} f$, $0 \leq i \leq k$.
The map $f \mapsto Tf$, $W^{k,p}(I, X) \to W^{k,p}(I, Y)$ is linear, and bounded by $\|T\|$.

Proposition A.2.3 (Continuous representatives)
Let X be separable Banach. $f \in L^1(I, X)$ has at most a continuous representative on $[0, T]$.

We now check that a vector valued test function has weak derivatives of all orders.

Proposition A.2.4 (Weak derivatives of test functions)
Let $\phi \in C^1([0,T], X)$, for X separable Banach. It means that the limit of the difference quotients exists for all points of I, that $t \mapsto \phi(t), \phi'(t)$ are continuous, and that they can be continuously extended to $[0,T]$.
Then these classical derivatives coincide a.e. with the weak derivatives of u.

Proof.

Apply proposition 3.8 of [44] at page 26, thanks to theorem 6 at page 146 of [31], a mean value theorem for vector valued function. □

We also need a time dependent trace lemma, which we provide in a space-time "tensor product" form, but under non-optimal regularity assumptions, for the sake of making some arguments more transparent.

Definition A.2.5 (Time dependent trace)
Let Ω be a bounded Lipschitz domain. For $k \geq 0$ we define $\mathrm{tr}_k : H^k(I, H^1(\Omega)) \to H^k(I, H^{1/2}(\partial\Omega))$ by $\mathrm{tr}(u)(t) := \mathrm{tr}(u(t))$

Below are some properties of this operator.

Proposition A.2.6 (Properties of trace operator)
The trace operator just defined:

1. is well posed, linear and bounded

2. admits a linear bounded right inverse, for instance, $E_k(g)(t) := E(g(t))$ (for E a right inverse of the "static" trace)

3. $\mathrm{tr}_k u = \mathrm{tr}_0 u$, for $u \in L^2(I, H^1(\Omega))$ and $E_k g = E_0 g$ gor $g \in L^2(I, H^{1/2}(\partial\Omega))$

Proof.
Proof of the proposition

We recall that the trace operator is bounded surjective onto $H^{1/2}(\partial\Omega)$, with a right inverse E (see theorem 3.37 at page 102 of [50]). The first two points are consequences of this fact and of proposition A.2.1.
The third property follows by the definition of tr, E and the fact that $H^l \subseteq H^k$, for $k \leq l$.

□

Lemma A.2.7 (Some interpolants)
Let X be a separable Banach space, and $u \in H^1(I, X)$. Discretize I into uniform subintervals $I_k := [t^k, t^{k+1}]$ of width δt. Call πu the function $\pi u(t) = u(t^k)$, for $t \in (t^k, t^{k+1})$, $\tilde{\pi} u(t) = u(t^{k+1})$ for $t \in (t^k, t^{k+1})$ and $\pi_1 u(t) = u(t^k)(t^{k+1} - t)/\delta t + u(t^{k+1})(t - t^k)/\delta t$ for $t \in (t^k, t^{k+1})$. Then:

- $\|u - \pi u\|_{L^2(I,X)}, \|u - \tilde{\pi} u\|_{L^2(I,X)} \leq C\delta t \|u'\|_{L^2(I,X)}$, for $C = 1/\sqrt{2}$

- for $v \in H^2(I, X)$, if X is Hilbert with $(\cdot, \cdot)_X$, there holds $\int_I ((u - \pi_1 u)', v)_X \leq \delta t^2 \|u\|_{H^2(I,X)} \|v\|_{H^1(I,X)}$

- if $u \in H^2(I, X)$, then $\|u - \pi_1 u\|_{L^2(I,X)} \leq C\delta t^2 \|u''\|_{L^2(I,X)}$, $C = 1/4\sqrt{3}$.

Proof.

There holds $\int_{I_k} \|\pi u - u(t)\|_X^2 \, dt = \int_{I_k} \left\| \int_{t^k}^t u'(s) ds \right\|_X^2 dt \leq \int_{I_k} \left(\int_{t^k}^t \|u'(s)\|_X \, ds \right)^2 dt$.

By Hölder's inequality we then see that $\int_{I_k} \|\pi u - u(t)\|_X^2 \, dt \leq \int_{I_k} \|u'(s)\|_X^2 \, ds \int_{I_k} (t - t^k) dt = \dfrac{\delta t^2}{2} \|u'\|_{L^2(I_k, X)}^2$. The result follows after summation. For $\tilde{\pi}$ the same reasonings work.

Now, on I_k there holds $(u - \pi_1 u)' = u' - \delta t^{-1} \int_{I_k} u'$, so that by a straightforward adaptation of lemma 3.2 of [41] one gets $\left\| u' - \delta t^{-1} \int_{I_k} u' \right\|_{L^2(I,X)}^2 \leq \delta t^2 \|u'\|_{H^1(I_k, X)}^2$. To conclude, note that $\int_{I_k} \left(u' - \delta t^{-1} \int_{I_k} u', v \right)_X = \int_{I_k} \left(u' - \delta t^{-1} \int_{I_k} u', v - \delta t^{-1} \int_{I_k} v \right)_X$ and apply the just derived $L^2(I, X)$ estimate to both arguments ot $(\cdot, \cdot)_X$.

For the last result, it suffices to note that $\pi_1 u(t) - u(t) = \int_{I_k} \dfrac{(t^{k+1} - \max(t, s))(\min(t, s) - t^k)}{\delta t} u''$ on I_k and suitably estimate the latter integral using the Cauchy-Schwarz inequality and some algebraic computations. □

34

B. Parabolic equations

Let us discuss the functional analytic setting for the various (parabolic) PDEs we are concerned with. We start with an abstract approach, which we then apply to a general boundary value problem.

B.1. Abstract theory

Assumption B.1.1 (Basic assumption for parabolic problems)
Let $V \subseteq H$ be real separable Hilbert spaces, V dense in H. Then $H \hookrightarrow V^*$ is also dense, as stated in [62] at page 147. This embedding is $H \ni f \mapsto (f, \cdot)_H$. We thus obtain a Gelfand triple, and we have $W(I, V) \subseteq C(I, H)$ (this is stated in [62], page 148).
Let $A : V \to V^*$ be linear bounded, $u \in W(I; V)$, $f \in L^2(I, V^*)$ and $u_0 \in H$.
We also assume that $\langle Av, v \rangle_{V^*, V} + \lambda \|v\|_H^2 \geq \alpha \|v\|_V^2$ for $\lambda \geq 0, \alpha > 0$.

We are interested in the following problem:

Problem B.1.2 (Abstract parabolic equation)

$$u_t + Au = f \text{ in } V^* \text{ and for a.e. } t \in (0, T) \tag{B.1.3}$$
$$u(0) = u_0 \tag{B.1.4}$$

Theorem B.1.5 (Basic well-posedness of problem B.1.2)
Under assumption B.1.1, problem B.1.2 has a unique solution u. Moreover u satisfies the stability estimate:

$$\|u\|_{W(I,V)} + \|u\|_{C([0,T],H)} \leq c(\lambda, \alpha, \|A\|_{V^*}, T)(\|u_0\|_H + \|f\|_{L^2(I,V^*)}) \tag{B.1.6}$$

Proof.
See [35] at page 19, theorem 26. □

We can also obtain additional regularity. Here are further assumptions to make this possible.

Assumption B.1.7 (Assumptions for additional regularity in time)
We assume $u_0 \in V$, $f = f_1 + f_2 \in L^2(I, H) + H^1(I, V^*)$. We also need A to be symmetric (i.e. $\langle Au, v \rangle_{V^*, V} = \langle Av, u \rangle_{V^*, V}$).

Proposition B.1.8 (Time regularity and tracking the costants)
With assumption B.1.1 there holds:

$$\|u\|_{C([0;T],H)}^2 + \alpha \|u\|_{L^2(I,V)}^2 \leq C \exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1} \|f\|_{L^2(I,V^*)}^2) \tag{B.1.9}$$
$$C \|u'\|_{L^2(I,V^*)} \leq \|A\|_{L(V,V^*)} \alpha^{-1/2} \sqrt{\exp(2\lambda T)} \|u_0\|_H + \left(\|A\|_{L(V,V^*)} \alpha^{-1} \sqrt{\exp(2\lambda T)} + 1 \right) \|f\|_{L^2(I,V^*)} \tag{B.1.10}$$

With additionally assumption B.1.7 we obtain $u \in H^1(I, H)$ with:

$$C \|u'\|_{L^2(I,H)}^2 \leq (1 + (1 + C_0)\alpha^{-1}) \|f_2\|_{H^1(I,V^*)}^2 + (1 + \|A\|_{L(V,V^*)}) \|u_0\|_V^2 + C_0 \|u_0\|_H^2 + \|f_1\|_{L^2(I,H)}^2 + C_0\alpha^{-1} \|f_1\|_{L^2(I,V^*)}^2 \tag{B.1.11}$$

with $C > 0$ a real number independent of problem data and solution, space dimension, and which need not to be the same for the three estimates.
Here $C_0 = 2^{-1} \max(1, \lambda) \max(1, \alpha^{-1}) \exp(2\lambda T)$.

Proof.
No regularity

From page 21 of [35] we obtain that $\|u\|_{C([0;T],H)}^2 + \alpha \|u\|_{L^2(I,V)}^2 \leq \exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1} \|f\|_{L^2(I,V^*)}^2)$, where from here onwards, in this proof, we leave out purely numeric constants that are independent of the solution, the space dimension, the data of the problem.
Moreover $\|u'\|_{L^2(I,V^*)} \leq \|Au\|_{L^2(I,V^*)} + \|f\|_{L^2(I,V^*)} \leq \|A\| \|u\|_{L^2(I,V)} + \|f\|_{L^2(I,V^*)}$.

All in all, we obtain:

$$\|u\|_{C([0;T],H)}^2 + \alpha \|u\|_{L^2(I,V)}^2 \leq \exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1} \|f\|_{L^2(I,V^*)}^2)$$

$$\|u'\|_{L^2(I,V^*)} \leq \|A\|_{L(V,V^*)} \alpha^{-1/2} \sqrt{\exp(2\lambda T)}(\|u_0\|_H + \alpha^{-1/2} \|f\|_{L^2(I,V^*)}) + \|f\|_{L^2(I,V^*)}$$

<u>More regularity</u>

We tie back to page 25 of [35]. In particular:

$$\int_0^t \|u_n'\|_H^2 + \int_0^t \langle Au_n, u_n' \rangle_{V^*,V} = \int_0^t (f_1, u_n')_H + \int_0^t \langle f_2, u_n' \rangle_{V^*,V}$$

Then:

$$\int_0^t \langle Au_n, u_n' \rangle_{V^*,V} \geq \frac{\alpha}{2} \|u_n(t)\|_V^2 - \frac{\lambda}{2} \|u_n(t)\|_H^2 - \frac{\|A\|}{2} \|u_{n0}\|_V$$

whereas, with integration by parts:

$$\left| \int_0^t \langle f_2, u_n' \rangle_{V^*,V} \right| \leq \frac{1}{2} \|f_2'\|_{L^2(I,V^*)}^2 + \frac{1}{2} \|u_n\|_{L^2(I,V)}^2 + \frac{\alpha}{4} \|u_n(t)\|_V^2 + \frac{4}{\alpha} \|f_2\|_{L^\infty(I,V^*)}^2 + \frac{1}{2} \|f_2\|_{L^\infty(I,V^*)}^2 + \frac{1}{2} \|u_{n0}\|_V^2$$

Also:

$$\int_0^t (f_1, u_n')_H \leq \frac{1}{2} \|f_1\|_{L^2(I,H)}^2 + \frac{1}{2} \int_0^t \|u_n'\|_H^2$$

This brings us to:

$$\frac{1}{2} \int_0^t \|u_n'\|_H^2 + \frac{\alpha}{4} \|u_n(t)\|_V^2 - \frac{\lambda}{2} \|u_n(t)\|_H^2 \leq \frac{1}{2} \|f_2'\|_{L^2(I,V^*)}^2 + \frac{1}{2} \|u_n\|_{L^2(I,V)}^2 + \frac{8+\alpha}{2\alpha} \|f_2\|_{L^\infty(I,V^*)}^2 + \frac{1+\|A\|}{2} \|u_{n0}\|_V^2 + \frac{1}{2} \|f_1\|_{L^2(I,H)}^2 \tag{B.1.12}$$

and thus, because norms are weakly lower semicontinuous and because we have weak convergence of the time derivative, and V-strong convergence of the initial data (see again [35] for this):

$$\int_0^T \|u'\|_H^2 \leq \|f_2'\|_{L^2(I,V^*)}^2 + (1+\alpha^{-1}) \|f_2\|_{L^\infty(I,V^*)}^2 + (1+\|A\|) \|u_0\|_V^2 + \|f_1\|_{L^2(I,H)}^2 + \limsup_n \left(\frac{\lambda}{2} \|u_n\|_{C([0,T],H)}^2 + \frac{1}{2} \|u_n\|_{L^2(I,V)}^2 \right)$$

For the last term, employing the exact argument as in the first part of the proof:

$$\limsup_n \left(\frac{\lambda}{2} \|u_n\|_{C([0,T],H)}^2 + \frac{1}{2} \|u_n\|_{L^2(I,V)}^2 \right) \leq C_0 \|u_0\|_H^2 + \alpha^{-1} \|f_1\|_{L^2(I,V^*)}^2 + \alpha^{-1} \|f_2\|_{L^2(I,V^*)}^2 \tag{B.1.13}$$

where $C_0 = 2^{-1} \max(1,\lambda) \max(1,\alpha^{-1}) \exp(2\lambda T)$.

Therefore:

$$\int_0^T \|u'\|_H^2 \leq \|f_2'\|_{L^2(I,V^*)}^2 + (1+\alpha^{-1}) \|f_2\|_{L^\infty(I,V^*)}^2 + (1+\|A\|) \|u_0\|_V^2 + \|f_1\|_{L^2(I,H)}^2 + C_0(\|u_0\|_H^2 + \alpha^{-1} \|f_1\|_{L^2(I,V^*)}^2 + \alpha^{-1} \|f_2\|_{L^2(I,V^*)}^2)$$

The embedding $H^1(I,V^*) \hookrightarrow C([0,T],V^*)$ has norm that only depends on T, which follows from the equality $f_2(t) = f_2(s) + \int_s^t f_2'$, for $0 \leq s \leq t \leq T$, a bound being $1 + T$.

Thus:

$$\int_0^T \|u'\|_H^2 \leq (1 + (1+C_0)\alpha^{-1}) \|f_2\|_{H^1(I,V^*)}^2 + (1+\|A\|) \|u_0\|_V^2 + C_0 \|u_0\|_H^2 + \|f_1\|_{L^2(I,H)}^2 + C_0 \alpha^{-1} \|f_1\|_{L^2(I,V^*)}^2$$

$\square$

Proving higher time regularity under additional compatibility assumptions and smoothness of the data can also be done as follows.

Proposition B.1.14 (Higher time regularity)
Let $k \geq 1$. Suppose $f \in H^k(I,V^*)$, together with:

- $g_j := f^{(j-1)}(0) - Ag_{j-1} \in H$, for $j = k$

- $g_{j-1} \in V$ for $1 \leq j \leq k$

where $g_0 = u_0$.

Then, there holds, for $1 \leq j \leq k$:

$$\begin{cases} u^{(j+1)} + Au^{(j)} = f^{(j)} \\ u^{(j)}(0) = f^{(j-1)}(0) - Ag_{j-1} \end{cases}$$

In particular $u \in H^k(I, V)$, and $u^{(k+1)} \in L^2(I, V^*)$. One can prove, with the help of theorem B.1.5, a-priori estimates on these successive derivatives.

Proof.

See [66], theorem 27.2, page 406.

□

B.2. Application to inhomogeneous parabolic problems

Here we apply the results of the last section to tackle a general inhomogeneous heat equation, which comprises e.g. the PDEs fo problem 2.1.1. We make the following assumption.

Assumption B.2.1 (Basic assumption for well-posedness of problem B.2.2)

1. $u_0 \in H^1(U)$

2. $\Omega \subset\subset D$ are bounded Lipschitz domains, so that $U := D \setminus \Omega$ is one as well

3. $g_D \in H^1(I, H^{1/2}(\Gamma_D))$. Here $\Gamma_D \neq \emptyset$ is either $\partial U, \partial D$ or $\partial\Omega$, with $g_D(0) = u_0$ on Γ_D

4. $g_N \in H^1(I, L^2(\Gamma_N))$, where $\Gamma_N = \partial U \setminus \Gamma_D$

5. $f \in L^2(I, H)$

Call $H = L^2(U)$, $V = \{v \in H^1(U), \mathrm{tr}\, u = 0 \text{ on } \Gamma_D\} =: H^1_{0,D}$. V is a closed subspace of H^1, which is Hilbert separable, hence also Hilbert separable. We norm it with the full H^1 norm. Because $H^1_0(U)$ is dense in H, so is V and we obtain a Gelfand triple.

We define A by $(Au)v := \int_u \nabla u \nabla v$. The general heat equation is then:

Problem B.2.2 (Inhomogeneous heat equation, general case)

$$\begin{aligned} u_t - \Delta u &= f \text{ in } (0,T) \times U \\ \partial_\nu u(\Sigma_N) &= g_N \\ u(\Sigma_D) &= g_D \\ u(0) &= u_0 \end{aligned}$$

By this we mean, upon calling $V := H^1_{0,D}(U)$ (H^1 functions of zero trace on the Dxirichlet boundary Γ_D), and $H = L^2(U)$:

$$\begin{aligned} u &\in W(I, H^1) \\ u_t + Au &= f + G \text{ in the sense of } V^* \text{ and for a.e. } t \in (0,T) \\ \mathrm{tr}\, u &= g_D \text{ on } \Sigma_D \\ u(0) &= u_0 \end{aligned}$$

where $\langle G(t), v \rangle_{V^*,V} := \int_{\Gamma_N} g(t)\mathrm{tr}\, v\, d\sigma$, σ the 1-codimensional Hausdorff measure.

It is known that global-in-time regularity of solutions to parabolic equations depends on the satisfaction of certain compatibility conditions by the boundary data and the source term, see [47], chapter 2, for instance. Taking these into account, in a situation of minimal regularity on the problem data, is beyond the scope of this work: we will see that by assuming slightly more regularity on the data, it is possible to obtain higher regularity of the solution in a fairly easy way.

Assumption B.2.3 (Time regularity assumption for problem B.2.2)

Let $k \geq 1$, consider any splitting $u = \bar{u} + \delta$, where, similarly to eq. (B.2.7), $\bar{u}$ extends the Dirichlet data.

We ask, aside from assumption B.2.1:

1. $g_D \in H^{k+1}(I, H^{1/2}(\Gamma_D))$

2. $g_N \in H^k(I, L^2(\Gamma_N))$

3. $f \in H^k(I, H)$

4. $g_j(\delta) \in V$, for $j = 0, ..., k-1$, where $g_j(\delta)$ are the terms g_j of proposition B.1.14, for the equation satisfied by δ

5. $g_j(\delta) \in H$

Assumption B.2.4 (Additional time regularity assumptions)
Apart from assumption B.2.1 and assumption B.2.3, suppose that, for $k \geq 1$, there holds:

- $g_N \in H^{k+1}(I, L^2(\Gamma_N))$

- $g_k(\delta) \in V$

Assumption B.2.5 (Spatial regularity assumptions)
Let assumption B.2.1 for $k = 0$, and also assumption B.2.3 and assumption B.2.4 hold for $k \geq 1$. Further assume:

- $\partial U \in C^{1,1}$

- $g_D \in H^k(I, H^{3/2}(\Gamma_D))$

- $g_N \in H^k(I, H^{1/2}(\Gamma_N))$

Theorem B.2.6 (Some results for problem B.2.2)
Under assumption B.2.1:

- there exists a unique $u \in W(I, H^1(U))$ solution to problem B.2.2

- for such u there holds $u' \in L^2(I, L^2(U))$ with:

$$\|u\|^2_{C([0,T];H)} + \|u\|^2_{L^2(I,H)} + \|\nabla u\|^2_{L^2(I,H)} + \|u'\|^2_{L^2(I,H)} \leq$$
$$C(T)\left(\|f\|^2_{L^2(I,H)} + \|g_N\|^2_{H^1(I,L^2(\Gamma_N))} + \|\bar{u}\|^2_{H^1(I,H^1(U))} + \|u_0\|^2_{H^1(U)}\right)$$
$$C(T)\left(\|f\|^2_{L^2(I,H)} + \|g_N\|^2_{H^1(I,L^2(\Gamma_N))} + C(U)\|g_D\|^2_{H^1(I,H^{1/2}(\Gamma_D))} + \|u_0\|^2_{H^1(U)}\right)$$

with $C > 1$, only dependent on T, smoothly, exploding for large T.

Under assumption B.2.3 we have that $u \in H^k(I, V) \cap (H^{k+1}(I, V) + H^{k+1}(I, V^*))$.
Under assumption B.2.4, $u^{k+1} \in H^1(I, H)$, or $u \in H^{(k+1)}(I, H)$, and, for $1 \leq j \leq k$:

$$\begin{cases} (u^{(j+1)}, v)_H + (\nabla u^{(j)}, \nabla v)_H = (f^{(j)}, v)_H + (g_N^{(j)}, v)_{L^2(\Gamma_N)} \\ u^{(j)}(0) \in H^1(U) \\ \mathrm{tr}u^{(j)}(\Sigma_D) = g_D^{(j)} \end{cases}$$

Finally, if assumption B.2.5 holds, then $u \in H^k(I, H^2(U)) \cap H^{k+1}(I, H)$.

Proof.

Well-posedness, stability

We remind that $V = H^1_{0,D}$. Now, we conjecture the splitting $u = \bar{u} + \delta$, $\delta = \delta(\bar{u})$.

Here $\bar{u}$ is (for a.e. t), an extension of g_D. $U := D \setminus \Omega$ is indeed bounded Lipschitz too and the trace operator is bounded surjective onto $H^{1/2}(\partial U)$, with a right inverse E (see theorem 3.37 at page 102 of [50]), $E : H^{1/2}(\partial U) \to H^1(U)$. We obtain by corollary A.2.2 that $\bar{u} := Eg_D \in H^1(I, H^1(U))$ (see also proposition A.2.6). Using the results of trace theory we know, in particular, that $\bar{u} \in H^1(U)$ with $\|\bar{u}\|_{H^1} \leq C(U)\|g_D\|_{H^{1/2}(U)}$, for almost every $t \in I$.

On the other hand, $\delta \in W(I, V) \cap H^1(I, H)$ is the unique solution (see theorem B.1.5) to:

$$\begin{cases} (\delta_t, v)_H + (\nabla \delta, \nabla v)_H = (f - \partial_t \bar{u}, v)_H + (g_N, v)_{L^2(\Gamma_N)} \text{ for all } v \in V \\ \delta(0) = u_0 - \bar{u}(0) \in V \end{cases} \tag{B.2.7}$$

Note that $\bar{u}(0)$ makes sense, being $g_D \in C([0,T], H^{1/2}(\Gamma_D))$, and that $u := \bar{u} + \delta$ solves problem B.2.2. By making use of the stability

estimates of theorem B.1.5 we can also conclude that problem B.2.2 is uniquely solvable, because the difference of two solutions satisfies a problem with zero boundary data, source and initial conditions.

It is also easy to see that eq. (B.2.7) and problem B.2.2 are in fact equivalent: if u, then $\delta := u - \bar{u}$ solves eq. (B.2.7), and if $\delta(\bar{u})$ solves eq. (B.2.7), then $\bar{u} + \delta(\bar{u})$ solves problem B.2.2.

By the splitting $u = \bar{u} + \delta$ and using proposition B.1.8 and the triangle inequality:

$$\|u\|^2_{C([0,T],H)} + \|u\|^2_{L^2(I,H)} + \|\nabla u\|^2_{L^2(I,H)} + \|u'\|^2_{L^2(I,H)} \leq$$
$$C(T) \left(\|f\|^2_{L^2(I,H)} + \|g_N\|^2_{H^1(I,L^2(\Gamma_N))} + \|\bar{u}\|^2_{H^1(I,H^1(U))} \right) \leq$$
$$C(T) \left(\|f\|^2_{L^2(I,H)} + \|g_N\|^2_{H^1(I,L^2(\Gamma_N))} + C(U) \|g_D\|^2_{H^1(I,H^{1/2}(\Gamma_D))} + \|u_0\|^2_{H^1(U)} \right)$$

with $C > 1$, only dependent on T, smoothly, exploding for large T.

Regularity: time smoothness

So, proposition B.1.14 ensures then that $\delta \in H^k(I,V)$, $\delta^{(k+1)} \in L^2(I,V^*)$. Because $\bar{u} \in H^{k+1}(I,H^1(U))$ by our assumptions and by corollary A.2.2, we obtain that $u = \bar{u} + \delta$ is in $H^{k+1}(I,H^1(U)) + H^{k+1}(I,V^*)$ and in $H^k(I,H^1(U))$.

Regularity: time smoothness again

By proposition B.1.14 we also have:

$$\begin{cases} \langle \partial_t \delta^{(k)}, v \rangle_{V^*,V} + (\nabla \delta^{(k)}, \nabla v)_H = \langle F^{(k)}, v \rangle_{V^*,V} \\ \delta^{(k)}(0) = g_k \in H \end{cases}$$

The right hand side $F^{(k)} = (f^{(k)} - G_D^{(k+1)}, \cdot)_H + (g_N^{(k)}, \text{tr}(\cdot))_{L^2(\Gamma_N)}$ is now an element of $L^2(I,H) + H^1(I,V^*)$, meaning that we can apply proposition B.1.8 to obtain $\delta \in H^{k+1}(I,H)$, provided that we ask for $g_k \in V$. We conclude that $u \in H^{(k+1)}(I,H)$, and, for $1 \leq j \leq k$:

$$\begin{cases} (u^{(j+1)}, v)_H + (\nabla u^{(j)}, \nabla v)_H = (f^{(j)}, v)_H + (g_N^{(j)}, v)_{L^2(\Gamma_N)} \\ u^{(j)}(0) = g_k + \bar{u}^{(j)}(0) \in V \\ \text{tr} u^{(j)}(\Sigma_D) = g_D^{(j)} \end{cases}$$

Spatial regularity

This last equation reads also:

$$\begin{cases} -\Delta u^{(j)} = f^{(j)} - u^{(j+1)} \\ u^{(k)}(\Gamma_D) = g_D^{(k)} \\ \partial_\nu u^{(j)}(\Gamma_N) = g_N^{(j)} \end{cases}$$

This holds for $0 \leq j \leq k$, and for a.e. $t \in I$.

H^2 regularity results that can be found in chapter 2 of [36] let us conclude the proof. $\square$

B.3. Alternative reformulations

By the last section, the two parabolic equations of interest contained in problem 2.1.1 can be recast into problem B.2.2 and in particular, into finding $u \in W(I,V)$, $u(0) = 0$, $u_t + Au = F$ for a.e. t in V^*, a proper right hand side $F \in L^2(I,V^*)$ and $V := H^1_{0,m}$, the space of H^1 functions vanishing on the moving boundary Γ_m. If inhomogeneous Dirichlet data are present, we always refer to the equivalent form B.2.7.

Here, $Au \in L^2(I,V^*)$ too (because $A \in L(V,V^*)$, and by corollary A.2.2). Call then $\mathcal{E}(u) := u_t + Au - F \in L^2(I,V^*)$ and $W_0(I,V)$ the $W(I,V)$ functions with zero initial value. Then, the differential equation reads $\langle \mathcal{E}(u)(t), v \rangle_{V^*,V} = 0$ for all $v \in V$, for a.a. t, equivalently, $\mathcal{E}(u) = 0$ for a.a. t. Thus, we are interested in the abstract problem:

> **Problem B.3.1** (Even more abstract parabolic equation)
> Given a function $\mathcal{E} : W(I,V) \to L^2(I,V^*)$, find $u \in W_0(I,V)$, such that $\mathcal{E}(u) = 0$ for a.a. t.

We can view $L^2(I,V^*) \cong L^2(I,V)^*$. Hence $\langle \mathcal{E}(u), v \rangle_{L^2(I,V)^*,L^2(I,V)} = \int_I \langle \mathcal{E}(u)(t), v(t) \rangle_{V^*,V} dt$ (see [39], theorem 1.31 at page 39). We are now ready to restrict both state and adjoint space, in view of the proof of proposition 2.2.10.

> **Definition B.3.2** ($Q(I,V)$)
> We define $Q(I,V) = H^{1,1} = L^2(I,V) \cap H^1(I,H)$, with the norm $\|v\|^2_Q = \|v\|^2_{L^2(I,V)} + \|v_t\|^2_{L^2(I,H)}$.

Proposition B.3.3 (Properties of Q)
There holds:

- $Q = Q(I, V)$ is Hilbert with $(v, w)_{L^2(I,V)} + (v_t, w_t)_{L^2(I,H)}$

- $Q(I, V)$ is dense in $L^2(I, V)$

- $Q(I, V) \hookrightarrow C([0, T], H)$

- $Q_0(I, V)$ is dense in $L^2(I, V)$, $Q_0(I, V)$ the space of $Q(I, V)$ function with zero initial value

- $Q(I, V) = W(I, V) \cap H^1(I, H)$, $Q_0(I, V) = W_0(I, V) \cap H^1(I, H)$ as sets

- integration by parts in time holds: $\displaystyle\int_I (v_t, w)_H = -\int_I (w_t, v)_H + (v(T), w(T))_H - (v(0), w(0))_H$

- if q_n is bounded in $Q(I, V)$, then there exists a weakly convergent subsequence q_k such that $q_k \rightharpoonup q$ in $L^2(I, H)$, $\partial_i q_k \rightharpoonup \partial_i q$ in $L^2(I, H)$ and $q'_k \rightharpoonup q'$ in $L^2(I, H)$

Proof.

Continuity

Follows from the embedding $H^1(I, H) \hookrightarrow C([0, T], H)$, as seen in [29], theorem 2 of page 286.

Density

We have $C_c^\infty(I, V) \subseteq Q(I, V) \subseteq L^2(I, V)$. The first inclusion holds because of proposition A.2.4, so that $C_c^\infty(I, V) \subseteq H^1(I, V)$. Moreover $H^1(I, V) \subseteq Q(I, V)$ trivially, where the $H^1(I, H)$ derivative is the $H^1(I, V)$ derivative. $C_c^\infty(I, V)$ is dense in $L^2(I, V)$ by [39], page 39, lemma 1.9. In particular, $C_c^\infty(I, V) \subseteq Q_0(I, V) \subseteq L^2(I, V)$, and as before, the density result follows.

Integration by parts

We note that $v, w \in Q(I, V) \subseteq W(I, V)$: we can now apply theorem 3.11 at page 148 of [62].

Weak convergence

At first we note that ∂_i, ∂_t are linear bounded operators from $Q(I, V)$ to $L^2(I, H)$. Remember that in any case, V is a closed subspace of H^1. Then, $\partial_i : V \to H$ is linear and bounded, because we chose V to be normed by the full H^1 norm. By corollary A.2.2, ∂_i extends to a linear bounded map from $L^2(I, V)$ to $L^2(I, H)$, therefore, to a linear bounded map on $Q(I, V)$, in the sense of:

$$Q(I, V) \xhookrightarrow{\ i\ } L^2(I, V) \xrightarrow{\ \partial_i\ } L^2(I, H)$$

Here, i is the natural injection. Because q_n is bounded in the Hilbert space $Q(I, V)$, it has a weakly convergent subsequence $q_k \rightharpoonup q \in Q(I, V)$. Therefore, $\partial_i(i(q_k)) \rightharpoonup \partial_i(i(q))$ in $L^2(I, H)$. By the Hilbert space property of $L^2(I, H)$ we conclude that $(\partial_i q_k, p)_{L^2(I,H)} \to (\partial_i q, p)_{L^2(I,H)}$ for all $p \in L^2(I, H)$.

For the time derivative, and the convergence $(q_k, p)_{L^2(I,H)} \to (q, p)_{L^2(I,H)}$ for all $p \in L^2(I, H)$, we can reason analogously. $\qquad\square$

We can now restrict the testing space.

Proposition B.3.4 (Equivalent testing)
Let $\mathcal{E} : W(I, V) \to L^2(I, V^*)$, and $u \in W_0(I, V)$. Then:

$$\mathcal{E}(u) = 0 \iff \langle \mathcal{E}(u), v \rangle_{L^2(I,V)^*, L^2(I,V)} = 0 \quad \forall v \in L^2(I, V) \text{ or } \forall v \in W^0(I, V) \text{ or } \forall v \in Q^0(I, V)$$

We have also seen that with smoothness assumption on data (assumption B.2.1) we obtain that the solution problem B.2.2 has $Q_0(I, V)$ smoothness.

We can therefore formulate the two partial differential equations of problem 2.1.1 in equivalent form directly on $Q_0(I, V)$ as follows.

$$w \in W_0(I, H^1_{0,m}), \bar{u} + v_0 \in W_0(I, H^1_{0,m}), v_0 \in W_0(I, H^1_0)$$
$$w' + Aw = (g, \cdot)_{L^2(\Gamma_f)} \text{ in } H^{1*}_{0,m} \text{ and for a.e. } t \in (0, T)$$
$$v'_0 + Av_0 = -((\bar{u}', \cdot)_H + A\bar{u}) \text{ in } H^{-1} \text{ and for a.e. } t \in (0, T)$$

with $\bar{u}$ any given $\bar{u} \in H^1(I, H^1_{0,m})$ such that $\mathrm{tr}\bar{u} = f$ on Σ_f, and with $\bar{u}(0) = 0$. We are working under assumption B.2.1. Thanks to proposition B.3.5, by the regularity ensured by assumption B.2.1 and thanks to proposition B.3.3, we get:

$$w \in Q_0(I, H^1_{0,m}), \bar{u} + v_0 \in Q_0(I, H^1_{0,m}), v_0 \in Q_0(I, H^1_0)$$
$$\int_I (w', q)_H + (\nabla w, \nabla q)_H = \int_I (g, \mathrm{tr}q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, H^1_{0,m})$$
$$\int_I (v'_0, p)_H + (\nabla v_0, \nabla p)_H = -\int_I (\bar{u}', p)_H + (\nabla \bar{u}, \nabla p)_H, \quad \forall p \in Q^0(I, H^1_0)$$

where now the derivatives are in the $H^1(I, H)$ sense.

Conversely, a solution $w \in Q_0(I, H_{0,m}^1), \bar{u} + v_0 \in Q_0(I, H_{0,m}^1), v_0 \in Q_0(I, H_0^1)$ to the above problem satisfies $w \in W_0(I, H_{0,m}^1), \bar{u} + v_0 \in W_0(I, H_{0,m}^1), v_0 \in W_0(I, H_0^1)$, see proposition B.3.3, and the proof of theorem B.2.6 . And by proposition B.3.3 at first, and then by proposition B.3.4 we obtain back:

$$w \in W_0(I, H_{0,m}^1), \bar{u} + v_0 \in W_0(I, H_{0,m}^1), v_0 \in W_0(I, H_0^1)$$
$$w' + Aw = (g, \cdot)_{L^2(\Gamma_f)} \text{ in } H_{0,m}^{1*} \text{ and for a.e. } t \in (0, T)$$
$$v_0' + Av_0 = -((\bar{u}', \cdot)_H + A\bar{u}) \text{ in } H^{-1} \text{ and for a.e. } t \in (0, T)$$

Therefore:

Proposition B.3.5 (Equivalent formulation)
Under assumption B.2.1, the PDEs of problem 2.1.1 can be equivalently formulated as:

$$w \in Q_0(I, H_{0,m}^1), \bar{u} + v_0 \in Q_0(I, H_{0,m}^1), v_0 \in Q_0(I, H_0^1)$$
$$\int_I (w', q)_H + (\nabla w, \nabla q)_H = \int_I (g, \operatorname{tr} q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, H_{0,m}^1)$$
$$\int_I (v_0', p)_H + (\nabla v_0, \nabla p)_H = -\int_I (\bar{u}', p)_H + (\nabla \bar{u}, \nabla p)_H, \quad \forall p \in Q^0(I, H_0^1)$$

Existence, uniqueness and stability proved already in theorem B.2.6, carry over to this new formulation.

C. Domains transformations

C.1. Transforming domains

Throughout, D is a bounded Lipschitz domain. We define as in [57] the following spaces of transformations:

Definition C.1.1 (Spaces of transformations)
We define:

- $\mathcal{V}^k = \{\tau \in \mathcal{M}, \tau - \mathrm{Id} \in W^{k,\infty}(\mathbb{R}^n, \mathbb{R}^n)\}$, $k \geq 1$

- $\mathcal{T}^k = \{\tau \in \mathcal{V}^k \text{ with an } \eta \in \mathcal{V}^k, \tau \circ \eta = \eta \circ \tau = \mathrm{Id}\}$. Any such η is unique, we denote it by τ^{-1} and we have that $U(\tau)$ is a Lipschitz homeomorphism with $U(\tau^{-1}) = U(\tau)^{-1}$

Proposition C.1.2 (Chain rule for $k = 1$)
Let $f \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ or $\mathcal{V}^1$, together with $\psi \in \mathcal{T}^1$. Then:

- $f \circ \psi$ has essentially bounded weak derivatives, and $D(f \circ \psi) = Df \circ \psi D\psi$.

- $D(\psi^{-1}) = (D\psi)^{-1} \circ \psi^{-1}$, where $(D(\psi^{-1}))^{-1} := [(DU(\psi^{-1}))^{-1}]$

- $|\det(D\psi)|$ is an essentially bounded measurable function with $|\det(D\psi)| \geq \delta > 0$ a.e..

Proof.
See [57], lemme 2.1 at page II-6, lemme 4.2, pag. IV-7.

$\square$

We go on to define the space of admissible transformations.

Definition C.1.3 (Admissible transformations)
We define $\Theta := \{\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \text{ with } \theta = 0 \text{ on } \mathbb{R}^n \setminus D\}$, a Banach subspace of $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$.
We also define $\mathcal{T} := \{\tau \in \mathcal{T}^1, \tau^{\pm 1}|_{\mathbb{R}^n \setminus D} = \mathrm{Id}\}$.

Proposition C.1.4 (Some group properties of $\mathcal{T}$)
Let $\eta, \tau \in \mathcal{T}, \theta \in \Theta$. Then:

- $\eta \circ \tau \in \mathcal{T}$

- $\theta \circ \tau \in \Theta$

- Id is the neutral element

- $\eta^{-1} \in \mathcal{T}$

Proposition C.1.5 (Small perturbations of $\mathcal{T}$)
Let $\theta \in \Theta$ with small enough $\|\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$. Then, $\mathrm{Id} + \theta \in \mathcal{T}$.
Let $\delta\theta \in \Theta$ with small enough $\|\delta\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$, and $\tau \in \mathcal{T}$. Then, $\tau + \delta\theta \in \mathcal{T}$.

Proof.

Perturbation of identity

We only need to check the properties of the inverse map.

τ^{-1} exists and is Lipschitz, see the proof of lemme 2.4 of [57], page II-16, so that $\tau \in \mathcal{T}^1$. The fact that $\tau = \mathrm{Id}$ outside of D automatically implies $\tau^{-1} = \mathrm{Id}$ outside of D.

Perturbation, not of identity

We solve the equation $\tau + \delta\theta = \eta \circ \tau$, i.e., we define $\eta := \mathrm{Id} + \delta\theta \circ \tau^{-1}$. Because $\tau^{-1} \in \mathcal{T}$ and $\delta\theta \in \Theta$ we observe that $\delta\theta \circ \tau^{-1} \in \Theta$, thanks to proposition C.1.4.

We only need to prove that $\delta\theta \circ \tau^{-1}$ is small, and then use the first part.

But by proposition C.1.2 this follows immediately.

$\square$

Theorem C.1.6
Small perturbations of identity, Lipschitz property Let $U \subset\subset D$ be Lipschitz bounded. There exists $0 < C(U) < 1$ such that, for $\tau \in W^{1,\infty}(\mathbb{R}^n; \mathbb{R}^n)$ and $\|\tau - \mathrm{Id}\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \leq C(U)$, then $T(U)$ is also bounded Lipschitz, where T is $U(\tau)$, the unique Lipschitz continuous representative of τ (see proposition A.1.2).
This result can be applied to, e.g., $\tau \in \mathcal{T}$ which is a small perturbation of identity in the $W^{1,\infty}$ topology.

Proof.
It is done in [3], lemma 3, page 629. □

Proposition C.1.7 (Some boundedness and continuity results)
Let $\delta\theta \in W^{1,\infty}(\mathbb{R}^n; \mathbb{R}^n)$, $\tau \in \mathcal{T}$. Then:

- $\|\delta\theta \circ \tau\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \leq \|\delta\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \leq C \|\delta\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \left(1 + \|\tau - \mathrm{Id}\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}\right)$

- the map $\eta \mapsto \eta \circ \tau$ is affine and continuous $\mathcal{V}^1 \to \mathcal{V}^1$

- the maps $\tau \mapsto \|\det(D\tau)\|_{L^\infty(\mathbb{R}^n;\mathbb{R})}, \tau \mapsto \|\det((D\tau)^{-1})\|_{L^\infty(\mathbb{R}^n;\mathbb{R})}, \tau \mapsto \|D\tau\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})}, \tau \mapsto \|(D\tau)^{-1}\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})}$ are continuous at every $\tau \in \mathcal{T}$, with respect to the $\mathcal{V}^1$ topology (given by the affine structure)

Proof.
These are exacly lemme 2.2 at page II .8 and (4.12) of remarque 4.1, page IV.6 of [57]. □

C.2. Transforming Sobolev spaces

Theorem C.2.1 (Change of variables)
Let U be open and $\tau = U(\tau)$ for $\tau \in \mathcal{T}^1$, and let $p \in [1, \infty]$. Then:

1. $f \in L^p(T(U)) \iff f \circ \tau \in L^p(U)$ and there holds, for $f \in L^p(\tau(U))$:

$$\|f\|_{L^p(\tau(Q))} \leq \left(\|\det D\tau\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \|f \circ \tau\|_{L^p(Q)}$$

2. $f \in W^{1,p}(\tau(U)) \iff f \circ \tau \in W^{1,p}(U)$ and there holds, for $f \in W^{1,p}(\tau(U))$:

$$Df \circ \tau = (Df)^{-t} D(f \circ \tau)$$

$$\|Df\|_{L^p(\tau(Q);\mathbb{R}^n)} \leq \left(\|\det D\tau\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \|(D\tau)^{-1}\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})} \|D(f \circ \tau)\|_{L^p(Q;\mathbb{R}^n)}$$

3. if $p \in (1, \infty)$, $f \in W_0^{1,p}(\tau(U)) \iff f \circ \tau \in W_0^{1,p}(U)$

4. therefore, composition by τ is a linear isomorphism between $W^{k,p}(\tau(U)) \to W^{k,p}(U)$ for $k = 0, 1$, and between $W_0^{1,p}(\tau(U)) \to W_0^{1,p}(U)$ for $k = 0, 1$, $p \in (1, \infty)$

5. for D a bounded Lipschitz domain and $\mathcal{T}, \Theta$ defined before, we get, for $f \in H^1(D)$, that $\mathrm{tr}_D f = \mathrm{tr}_D(f \circ \tau)$

6. if moreover, $\Omega, \tau(\Omega) \subset\subset D$ are also bounded Lipschitz domains, letting $U := D \setminus \Omega$, another bounded Lipschitz domain, for $f \in H^1(\tau(U))$ and $\mathrm{tr}_{\tau(U)} f = 0$ on $\partial\tau(\Omega)$, then $\mathrm{tr}_U f \circ \tau = 0$ on $\partial\Omega$ and $\mathrm{tr}_{\tau(U)} f = \mathrm{tr}_U f \circ \tau$ on ∂D

7. so, $\circ\tau$ is a linear isomorphism of $H_{0,m}^1(U)$ and $H_{0,m}^1(\tau(U))$ ($H_{0,m}^1$ is defined in appendix B.2 as $\{u \in H^1, u(\Gamma_m) = 0\}$)

Proof.
We need to prove only the last points, for the other ones are proved in [57], pages IV.4, IV.5, IV.6.

<u>Static strace</u>

Let $f_n \in C(\overline{D}) \cap H^1(D)$ converging in $H^1(D)$ to f (see theorem 3.18 of [1], page 54). By point 4, we have $f_n \circ \tau \to f \circ \tau$ in $H^1(D)$ (rememeber, $\tau(D) = D$ by invertibility of τ and the fact that $\tau(x) = x$ outside of D). Therefore we have:

$$\mathrm{tr}_D f \leftarrow_{L^2(\partial D)} \mathrm{tr}(f_n) = f_n|_{\partial D} = (f_n \circ \tau)|_{\partial D} = \mathrm{tr}(f_n \circ \tau) \rightarrow_{L^2(\partial D)} \mathrm{tr}_D(f \circ \tau)$$

<u>Moving trace</u>

First of all, as τ is a homeomorphism of $\mathbb{R}^n$, $\tau U = D \setminus \tau(\Omega)$, $\tau\partial U = \partial D \sqcup \partial\Omega$, $\tau\partial\Omega = \partial\tau\Omega$. Now, an application of theorem A.1.1 yields that the zero extension to $\tau\Omega$ of f, call it $\bar{f}$, is $H^1(D)$, with $\partial_i \bar{f} = \partial_i f$ in τU, 0 in $\tau(\Omega)$.

We have moreover $\mathrm{tr}_D \bar{f} = \mathrm{tr}_{\tau(U)} f|_{\partial D}$ (using approximation arguments based on theorem 3.18 of [1], page 54).

Using this: $\mathrm{tr}_{\tau(U)}f|_{\partial D} = \mathrm{tr}_D \bar f = \{\text{ point 5 }\} = \mathrm{tr}_D(\bar f \circ \tau) = \mathrm{tr}_D(\overline{f \circ \tau}) = \mathrm{tr}_U(f \circ \tau)|_{\partial D}$, where we used that $\bar f \circ \tau$ is zero in $\tau^{-1}\tau\Omega = \Omega$ (because τ maps Lebesgue null sets into null sets, being bi-Lipschitz), so it is the zero extension $\overline{f \circ \tau}$ of $f \circ \tau$, and applied the same reasoning as above to conclude $\mathrm{tr}_D(\overline{f \circ \tau}) = \mathrm{tr}_U(f \circ \tau)|_{\partial D}$. Both $\bar f \circ \tau$ and $f \circ \tau$ are H^1 functions by point 2.

Now that we know that $\mathrm{tr}_{\tau(U)}f|_{\partial D} = \mathrm{tr}_U(f \circ \tau)|_{\partial D}$, it is left to show $\mathrm{tr}_U f \circ \tau = 0$ on $\partial\Omega$, via some additional steps.

Multiplication by a $W^{1,\infty}$ function

For $\psi \in W^{1,\infty}(\mathbb{R}^n; \mathbb{R})$ and $f \in H^1(U)$, $f\psi$ has the same trace as f as long as $\psi = 1$ in a neighbourhood of ∂U. This follows again by an approximation argument on f by smooth functions and by proposition A.1.2.

Reducing to a function of 0 trace

Let η be a smooth cut-off function which is 1 close to ∂D and 0 close to $\partial\tau\Omega$, $\beta = 0$ close to ∂D and 1 close to $\partial\tau\Omega$. They can be found by e.g. building a suitable partition of unity of the compact sets $\partial\Omega$ and ∂D. $f\beta$ has zero trace, as it can be verified by approximating f by suitable smooth functions f_n: $\mathrm{tr}_{\tau(U)}f\beta \leftarrow_{L^2(\partial\tau(U))} \mathrm{tr}_{\tau(U)}f_n\beta$, where the latter quantity is $\mathrm{tr}_{\tau(U)}f_n$ on $\partial\tau(\Omega)$ and 0 on ∂D.

Domain transformation

We have that $\beta \circ \tau + \eta \circ \tau$ is $W^{1,\infty}$ and 1 near ∂U. So, $\mathrm{tr}_U f \circ \tau = \mathrm{tr}_U f \circ \tau(\beta \circ \tau + \eta \circ \tau) = \mathrm{tr}_U((f \circ \tau)(\beta \circ \tau)) + \mathrm{tr}_U((f \circ \tau)(\eta \circ \tau))$.

Approximate $f \circ \tau$ by g_n smooth as seen above. Then, $\mathrm{tr}_U(g_n\eta \circ \tau)$ is 0 on $\partial\Omega$, and selecting an almost everywhere convergent subsequence, we conclude $\mathrm{tr}_U(f \circ \tau\eta \circ \tau) = 0$ on $\partial\Omega$.

Finally, $\mathrm{tr}_U f \circ \tau|_{\partial\Omega} = tr_U(f \circ \tau)(\beta \circ \tau)|_{\partial\Omega} = tr_U((f\beta) \circ \tau)|_{\partial\Omega} = 0$, where at last we used point 3 (zero trace functions in $H^1(\tau(U))$, since $\tau(U)$ is assumed to be bounded Lipschitz, are exactly the functions $H_0^1(\tau(U))$ (theorem 18.7 at page 595 of [45])). $\qquad\square$

C.3. Transforming Bochner spaces

> **Proposition C.3.1** (Isomorphism between Q spaces)
> Let $\tau \in \mathcal{T}$. Then:
>
> $$\circ\tau : Q(I, V_\tau) \to Q(I, V), Q_0(I, V_\tau) \to Q_0(I, V)$$
>
> are linear isomorphisms. In particular, $(u \circ \tau)' = u' \circ \tau$.

Proof.

From theorem C.2.1, with the help of corollary A.2.2 and thanks to the properties of Q listed in proposition B.3.3, we obtain that $\circ\tau \circ \tau : Q(I, V_\tau) \to Q(I, V)$ is linear bounded, and by the inverse function theorem, an isomorphism. Reasoning by continuous representatives (in time), we get $(\circ\tau)(Q_0(I, V_\tau)) \subseteq Q_0(I, V)$, and the same goes for $\circ\tau^{-1}$. $\qquad\square$

C.4. Transforming partial differential equations

We consider again the two parabolic equations of interest from proposition B.3.5. We stress that we need:

> **Assumption C.4.1**
> We have $\tau \in \mathcal{T}$, $U \subset\subset D$ bounded Lipschitz domains and we also assume that $\tau(U)$ is bounded Lipschitz.

Suppose the problem is formulated on $\tau(U)$. To ease the notation, call $H_{0,m}^1(\tau(U)) = \mathtt{W}_\tau$, $H_{0,m}^1(U) = \mathtt{W}$, $H_0^1(U) = \mathtt{V}$ and analogously for the other spaces. We continue from proposition B.3.5. Applying a change of variables, and noting that:

- $\mathrm{tr}_{\tau(U)}q = \mathrm{tr}_U(q \circ \tau)$ on Σ_f by theorem C.2.1
- $w_t^\tau \circ \tau = (w^\tau \circ \tau)_t$ by proposition C.3.1 and analogously for v_0
- by proposition C.3.1, $\circ\tau$ is a bijection between $Q^0(I, \mathtt{W}_\tau)$ and $Q^0(I, \mathtt{W})$ and analogously for $\mathtt{V}$
- $\bar u \in H^1(I, \mathtt{W}_\tau)$ and that $\bar u'$ denoted the weak derivative in the $H^1(I, \mathtt{W}_\tau)$ sense, so that proposition A.2.1 yields $\bar u \circ \tau \in H^1(I, \mathtt{W})$ and $(\bar u \circ \tau)' = \bar u' \circ \tau$

we get, equivalently:

$$w^\tau \in Q_0(I, \mathtt{W}_\tau), v_0^\tau \in Q_0(I, \mathtt{V}_\tau)$$

$$\int_I ((w^\tau \circ \tau)_t, q|\det(D\tau)|)_H + (A_\tau \nabla(w^\tau \circ \tau), \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W})$$

$$\int_I ((v_0^\tau \circ \tau)_t, p|\det(D\tau)|)_H + (A_\tau \nabla(v_0^\tau \circ \tau), \nabla p)_H =$$

$$-\int_I ((\bar u \circ \tau)', p|\det(D\tau)|)_H + (A_\tau \nabla(\bar u \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V})$$

and by proposition C.3.1, we also get $w^\tau \circ \tau \in Q_0(I, \mathtt{W}), v_0^\tau \circ \tau \in Q_0(I, \mathtt{V})$. Here $A_\tau = |\det(D\tau)|D\tau^{-1}(D\tau)^{-t}$.

On the other hand, consider:

$$w \in Q_0(I, \mathtt{W}), v_0 \in Q_0(I, \mathtt{V})$$

$$\int_I (w_t, q| \det(D\tau)|)_H + (A_\tau \nabla w, \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W})$$

$$\int_I (v_{0t}, p| \det(D\tau)|)_H + (A_\tau \nabla v_0, \nabla p)_H =$$

$$-\int_I ((\bar{u} \circ \tau)', p| \det(D\tau)|)_H + (A_\tau \nabla(\bar{u} \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V})$$

Then, we note the following:

- by proposition C.3.1, $w \circ \tau^{-1} \in Q_0(I, \mathtt{W}_\tau), v_0 \circ \tau^{-1} \in Q_0(I, \mathtt{V}_\tau)$, and as seen above, $((w \circ \tau^{-1}) \circ \tau)_t = (w \circ \tau^{-1})_t \circ \tau$ and the same goes for $v_0 \circ \tau^{-1}$

Therefore we obtain, equivalently:

$$w \circ \tau^{-1} \in Q_0(I, \mathtt{W}_\tau), v_0 \circ \tau^{-1} \in Q_0(I, \mathtt{V}_\tau)$$

$$\int_I ((w \circ \tau^{-1})_t, q^\tau)_{H_\tau} + (\nabla(w \circ \tau^{-1}), \nabla q^\tau)_{H_\tau} = \int_I (g, \mathrm{tr}_{\tau(U)} q^\tau)_{L^2(\Gamma_f)}, \quad \forall q^\tau \in Q^0(I, \mathtt{W}_\tau)$$

$$\int_I ((v_0 \circ \tau^{-1})_t, p^\tau)_{H_\tau} + (\nabla(v_0 \circ \tau^{-1}), \nabla p^\tau)_{H_\tau} = -\int_I (\bar{u}', p^\tau)_{H_\tau} + (\nabla \bar{u}, \nabla p^\tau)_{H_\tau}, \quad \forall p^\tau \in Q^0(I, \mathtt{V}_\tau)$$

and $w \circ \tau^{-1} \in Q_0(I, \mathtt{W}_\tau), v_0 \circ \tau^{-1} \in Q_0(I, \mathtt{V}_\tau)$.

These findings can be summarized as follows.

Theorem C.4.2 (Equivalent formulations with transported domain)
Let assumption B.2.1, assumption C.4.1 hold.
Consider the following problems, where $\tau \in \mathcal{T}$.

Problem C.4.3 (Joint parabolic problem, moving domain)

$$w^\tau \in Q_0(I, \mathtt{W}_\tau), v_0^\tau \in Q_0(I, \mathtt{V}_\tau)$$

$$\int_I (w_t^\tau, q^\tau)_{H_\tau} + (\nabla w^\tau, \nabla q^\tau)_{H_\tau} = \int_I (g, \mathrm{tr}_{\tau(U)} q^\tau)_{L^2(\Gamma_f)}, \quad \forall q^\tau \in Q^0(I, \mathtt{W}_\tau)$$

$$\int_I (v_{0t}^\tau, p^\tau)_{H_\tau} + (\nabla v_0^\tau, \nabla p^\tau)_{H_\tau} = -\int_I (\bar{u}', p^\tau)_{H_\tau} + (\nabla \bar{u}, \nabla p^\tau)_{H_\tau}, \quad \forall p^\tau \in Q^0(I, \mathtt{V}_\tau)$$

Problem C.4.4 (Joint parabolic problem, reference domain)

$$w \in Q_0(I, \mathtt{W}), v_0 \in Q_0(I, \mathtt{V})$$

$$\int_I (w_t, q| \det(D\tau)|)_H + (A_\tau \nabla w, \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W})$$

$$\int_I (v_{0t}, p| \det(D\tau)|)_H + (A_\tau \nabla v_0, \nabla p)_H =$$

$$-\int_I ((\bar{u} \circ \tau)', p| \det(D\tau)|)_H + (A_\tau \nabla(\bar{u} \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V})$$

We have the following:

- consider $w^\tau \in Q_0(I, \mathtt{W}_\tau), v_0^\tau \in Q_0(I, \mathtt{V}_\tau)$. They solve problem C.4.3 $\iff w^\tau \circ \tau, v_0^\tau \circ \tau$ solve problem C.4.4

- consider $w \in Q_0(I, \mathtt{W}), v_0^\tau \in Q_0(I, \mathtt{V})$. They solve problem C.4.4 $\iff w \circ \tau^{-1}, v_0 \circ \tau^{-1}$ solve problem C.4.3

Here, $A_\tau := (D\tau)^{-1}(D\tau)^{-t}| \det(D\tau)|$.

D. FEM and smooth domains

Handling smooth geometries in finite element analysis is not a trivial task. On one hand, finite element discretizations is naturally set up on polygonal/polyhedral domains, whereas the smoothness of the analytical solution required to obtain optimal order error estimates, can only be achieved with a smooth boundary (or more generally, when U is convex, which it isn't, in our case). An apparent contradiction therefore arises, and many authors simply conduct theoretical analysis on the polyhedral domains, but assuming enough smoothness of the solutions (this is the contradiction of "polygonal smooth" domains, mentioned in [61]): an example of this in a setting close to ours, is contained in [40].

There are few different ways to go about this dilemma, many of them are only a partially satisfactory answer to the problem. For instance, finite elements formulated directly on arbitrarily curved simplices have been studied, see [67]. This requires complete knowledge of the (curved) boundary of the computational domain. Optimal order estimates are also observed in [11]. Their techniques work with smooth and rough data, but also require complete knowledge of a parametrization of the boundary, and are not easily extendable to a dimension higher than 2. Interestingly, shape optimization techniques can be applied to analyze the discrepancy between discrete and smooth geometry in the solution process, see [61]: the techniques therein presented only yield optimal order estimates in the H^1 norm.

The presence of Dirichlet boundary conditions further complicates the analysis. The Dirichlet values might be imposed strongly, i.e. enforced at the boundary nodes, or weakly (see e.g. [19] for the elliptic case, or, more generally, the discussion in [20], and that in [9] for the parabolic case). The latter solution is viable only if one can extend to the whole volume the boundary data.

We chose an approach that was as little intrusive as possible with regards to the exact geometry and data: it only requires the knowledge of the smooth domain and boundary data at some points of the smooth boundary. It is straightforward to implement, both from a meshing point of view and from a finite element code point of view. Standard meshing tools can be used without modification, GMSH being our choice ([33]), and powerful finite element libraries can be directly used to simulate the partial differential equations, we used Fenics ([49]).

In short, the discrete solution is computed on a polygonal/polyhedral approximation Ω_h of the smooth domain Ω, where the nodes of $\partial\Omega_h$ lie on $\partial\Omega$, and the Dirichlet conditions are imposed strongly. The boundary data is substituted by its Langrange interpolant, thus requiring its knowledge only on the boundary nodes of $\partial\Omega_h$.

The drawback is that we ask "unnatural" smoothness to the boundary data, because we evaluate it pointwise ("unnatural" is compared to he hypothesis necessary to obtain H^2 regularity in the elliptic case, i.e. $H^{1/2}$ smoothness for Neumann data and $H^{3/2}$ smoothness for Dirichlet data: we will require both to be H^2 on the boundary). Such surplus of smoothness is however present in the majority of the other works that analyze the change in geometry in detail. Strong imposition of Dirichlet boundary conditions, on the other hand, may not me the best solution for all PDEs, see e.g. [8].

The approach we took is based on the work of [27], [26], [10] and [25].

We mention that one might alternatively solve the PDEs resulting from shape optimization, on the reference domain, rather than on the moving domain. This however complicates the variational formulation, and in the case of more difficult equations (more than a Poisson, or a heat equation in our case), already existing high performance solvers may be unavailable.

D.1. Preliminaries

> **Assumption D.1.1** (Geometric assumptions)
> Consider a domain $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$, with C^2 boundary.
> We define a polygonal/polyhedral meshing made of triangles/tetrahedra Ω_h (open) of Ω, which has boundary nodes on $\partial\Omega$. The family of meshes for Ω_h must be regular and quasi-uniform in the sense of [13].
> Denoting by $\Gamma_D, \Gamma_N \subseteq \partial\Omega$ subsets of $\partial\Omega$ where Dirichlet and Neumann boundary conditions will be imposed, we call their discretizations $\Gamma_{D_h}, \Gamma_{N_h}$.
> We assume $\Gamma_D \neq \emptyset$ for simplicity (but many of the following arguments work with suitable adaptations otherwise), and $\overline{\Gamma_D} \cap \overline{\Gamma_N} = \emptyset$.

Call $S^1_{h,0,D_h}$ the space of piecewise linear lagrangian FEM S^1_h which are zero on Γ_{D_h}.

We collect some useful tools to relate Ω and Ω_h.

> **Proposition D.1.2** (Deformation into smooth boundary)
> Assume we have a shapre regular and quasi-uniform mesh (see [13] for a definition). There exists, for h small enough, $G_h : \overline{\Omega_h} \to \overline{\Omega}$ satisfying:
>
> - $G_h|_T = \text{Id}$ on interior simplices T (those with at most one node on $\partial\Omega$)
>
> - $G_h(\partial\Omega_h) = \partial\Omega$, $G_h|_e = p$, where e is an edge/face of $\partial\Omega_h$ and p is the closest point operator to $\partial\Omega$ (so that $G_h|_{\partial\Omega_h}$ coincides with the boundary lift in definition 4.12 of [27])
>
> - G_h is bi-Lipschitz, with $\|\text{Id} - G_h\|_{W^{1,\infty}(\Omega_h)} \lesssim h$, and $\||\det(DG_h)| - 1\|_{L^\infty(\Omega_h)} \lesssim h$

- given $G_h(K)$, all the facets are at least C^1 smooth

- $G_h|_T$ is of class $C^1(T)$ for all closed simplices T composing Ω_h

Proof.

See section 4.1 of [27] for the first two points, which follow from the definition of G_h. See also Lemma 8.16 of [26].

The last one is contained in Lemma 8.12, [26]. We give more detail for the third and fourth point, which are not addressed in [26], [27].

$\underline{G_h \text{ is a bi-Lipschitz homeomorphism}}$

We first note that $G_h|_K$ agrees with $G_h|_{K'}$ for $K \cap K' \neq \emptyset$. Therefore G_h is continuous on $\overline{\Omega_h}$.

Then, we also note that G_h has $DG_h \in L^\infty(\Omega_h)$ as weak derivative, where the gradient is defined element-wise. To see this, pick $\phi \in C_c^\infty(\Omega_h)$.

Then, applying theorem A.1.1:

$$\int_{\Omega_h} G_h \partial_i \phi = \sum_K \int_{\partial K} G_h|_K \phi \nu_{K,i} - \int_{\Omega_h} \partial_i G_h \phi$$

The first integral on the right is zero, because G_h is continuous, the normal on the same interior facet is equal of opposite sign when referred to the two parent simplices it belongs to, and because $\phi = 0$ on exterior facets.

Thus, $G_h \in W^{1,\infty}(\Omega_h)$, and lemma 8.12 of [26] shows that $\|\text{Id} - G_h\|_{W^{1,\infty}(\Omega_h)} \lesssim h$. Thanks to proposition A.1.2, we obtain that G_h has a bounded Lipschitz representative, i.e., G_h is bounded and Lipschitz on Ω_h. Then G_h is Lipschitz on all of $\overline{\Omega_h}$, and $\text{Lip}(\text{Id} - G_h) \lesssim \|\text{Id} - G_h\|_{W^{1,\infty}(\Omega_h)}$.

So, G_h is a Lipschitz perturbation of identity, on $\overline{\Omega_h}$. An application of the reverse triangle inequality also shows that $|G_h(x) - G_h(y)| \geq (1 - \text{Lip}(G_h))|x - y|$, which yields that G_h is bijective (for small h), with a Lipschitz inverse.

$\underline{\text{Smooth facets of curved simplex}}$

From the last point we know that G_h is of class C^1 when restricted to K, a closed simplex. By Whitney's extension theorem on simplices (see [64]) we can conclude that $G_h|_K$ extends to a C^1 function on a neighbourhood of K. This extension is injective on K as we saw before, and by Lemma 8.16 of [26] (the determinant of G_h is small), it has invertible jacobian on K. An application of a global version of the inverse function theorem (see e.g. [37], chapter 1) yields that G_h extends to a C^1 diffeomorphism around K, so that the smoothness of ∂K follows. $\square$

Given G_h, we can define pullbacks and pushforwards of functions defined on Ω or Ω_h.

Proposition D.1.3 (Lift)
We define, for $u : \Omega \to \mathbb{R}$, $u^{-l} := u \circ G_h : \Omega_h \to \mathbb{R}$, and analogously for $u_h : \Omega_h \to \mathbb{R}$ we define $u_h^l := u_h \circ G_h^{-1}$. Again, we need the mesh to be quasi-uniform (see proposition 4.7 of [27]).
There holds:

- $v \in H^m(Q)$ if and only if $v^{-l} \in H^m(G_h(Q))$, for $m = 0, 1$, and $Q \subseteq \Omega_h$ open

- for $v_h \in S^1_{h,0,D_h}$, we have $v_h^l \in H^1(\Omega)$, with zero trace on Γ_D

- for $v_h \in S^1_h$, one has the following norm equivalences, which don't depend on h:

  1. $\|v_h\|_{L^2(\partial\Omega_h)} \sim \|v_h^l\|_{L^2(\partial\Omega)}$

  2. $\|v_h\|_{L^2(\Omega_h)} \sim \|v_h^l\|_{L^2(\Omega)}$

  3. $\|\nabla v_h\|_{L^2(\Omega_h)} \sim \|\nabla v_h^l\|_{L^2(\Omega)}$

- consequently, the lifting operator $S^1_{h,0,D_h} \to H^k_{0,D}(\Omega)$ is bounded, for the L^2 norms if $k = 0$, and H^1 norms if $k = 1$

Proof.

The first point follows by the fact that G_h is bi-Lipschitz, see proposition D.1.2, and theorem 11.53 of [45].

The second point follows by applying the arguments about conformity outlined in section 5 of [10]. Following example 2 therein, we discover that we can apply proposition and corollary 5.1.

The last point can be found in [27], see e.g proposition 4.9 and 4.13. $\square$

Proposition D.1.4 (Interpolation on curved domains)
Let $u \in H^2(\Omega)$, let $g \in H^2(\partial\Omega)$.
Let $u \in H^2(\Omega)$ and define $\Pi_c u = (\Pi_h u)^l$, where Π_h is the usual pointwise Lagrange interpolator on S^1_h.
We can also define $\Pi_c g$ for $g \in H^2(\partial\Omega)$ in the same fashion.
It follows that:

- $\|u - \Pi_c u\|_{L^2(\Omega)} + h \|u - \Pi_c u\|_{H^1(\Omega)} \lesssim h^2 \|u\|_{H^2(\Omega)}$

- $\|g - \Pi_c g\|_{L^2(\partial\Omega)} + h \|g - \Pi_c g\|_{H^1(\partial\Omega)} \lesssim h^2 \|g\|_{H^2(\partial\Omega)}$

Here $a \lesssim b$ means $a \leq Cb$ for $C \geq 0$ not depending on h.

Proof.

See proposition 5.4 of [27]. □

Proposition D.1.5 (Approximation of linear and bilinear forms)
Let $v_h, w_h \in S_h^1$, $v, w \in H^2(\Omega)$, $\delta\theta_h \in (S_h^1)^n$ (n is the dimension of Ω), $\delta\theta \in W^{1,\infty}(\Omega; \mathbb{R}^d)$, $\delta\theta_h \in W^{1,\infty}(\Omega_h; \mathbb{R}^d)$. Then:

1. $\left| \int_\Omega v_h^l w_h^l - \int_{\Omega_h} v_h w_h \right| \lesssim h^{k+1} \|v_h\|_{H^k(\Omega_h)} \|w_h\|_{H^k(\Omega_h)}, \ k = 0, 1$

2. $\left| \int_{\partial\Omega} v_h^l w_h^l - \int_{\partial\Omega_h} v_h w_h \right| \lesssim h^2 \|v_h\|_{L^2(\partial\Omega_h)} \|w_h\|_{L^2(\partial\Omega_h)}$

3. $\left| \int_\Omega \nabla v_h^l \nabla w_h^l - \int_{\Omega_h} \nabla v_h \nabla w_h \right| \lesssim h \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)}$

4. $\left| \int_\Omega \nabla v \nabla w - \int_{\Omega_h} \nabla v^{-l} \nabla w^{-l} \right| \lesssim h^2 \|v\|_{H^2(\Omega)} \|w\|_{H^2(\Omega)}$

5. $\left| \int_\Omega v_h^l w_h^l \mathrm{div}(\delta\theta_h^l) - \int_{\Omega_h} v_h w_h \mathrm{div}(\delta\theta_h) \right| \lesssim h^{k+1} \|v_h\|_{H^k(\Omega_h)} \|w_h\|_{H^k(\Omega_h)} \|\mathrm{div}(\delta\theta_h)\|_{L^\infty(\Omega_h)}, \ k = 0, 1$

6. $\left| \int_\Omega (A'(\delta\theta_h^l)\nabla v_h^l)\nabla w_h^l - \int_{\Omega_h} (A'(\delta\theta_h)\nabla v_h)\nabla w_h \right| \lesssim h \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)} \|D\delta\theta_h\|_{L^\infty(\Omega_h)}$

7. $\left| \int_\Omega (A'(\delta\theta)\nabla v)\nabla w - \int_{\Omega_h} (A'(\delta\theta^{-l})\nabla v^{-l})\nabla w^{-l} \right| \lesssim h^2 \|v\|_{H^2(\Omega)} \|w\|_{H^2(\Omega)} \|D\delta\theta\|_{L^\infty(\Omega)}$

Proof.

See [25], and in particular, for the second point, lemma 5.6 of [43]. Only the last three points are not already present in the literature, but they follow with very similar arguments as the others. See for instance, section 6 of [27]: one needs to apply a change of variables to the integrals on Ω_h, and then use the approximation properties in proposition D.1.2. To obtain $O(h^2)$ estimates, the "narrow band" inequality lemma 6.3, [27], as suggested in lemma 6.4 of [27], has to be used. □

Proposition D.1.6 (Uniform coercivity)
For h small enough, $a_h(v_h, w_h) := \int_{\Omega_h} \nabla v_h \nabla w_h$ is coercive, uniformly with respect to h.

Proof.

For C not depending on h:

$$a_h(v_h, v_h) \geq C \left\| v_h^l \right\|_{H^1(\Omega)}^2 - |a_h(v_h, v_h) - a(v_h^l, v_h^l)| \geq C \|v_h\|_{H^1(\Omega_h)}^2 - Ch \left\| v_h^l \right\|_{H^1(\Omega)}^2 \geq C(1-h) \|v_h\|_{H^1(\Omega_h)}^2$$

We used the $h-$uniform coercivity of a (descending from the Poincaré inequality in which functions vanish only on part of the boundary, Γ_D, see e.g. lemma 1 of [24]), proposition D.1.3 on $\left\| v_h^l \right\|_{H^1(\Omega)}^2$ and proposition D.1.5. □

D.2. Semidiscrete estimates

We partly build upon the previous section, to deal with problems of the following form.

Problem D.2.1 (Inhomogeneous parabolic problem)
With reference to problem B.2.2, we define:

$$\begin{cases} \partial_t u - \Delta u = f & \text{on } \Omega \times I \\ u = g_D & \text{on } \Gamma_D \times I \\ \partial_\nu u = g_N & \text{on } \Gamma_N \times I \\ u(0) = u_0 \end{cases}$$

We ask assumption B.2.1.

We provide a semidiscrete estimate, in the sense that only space is discretized. To do so we follow a classical argument involving the use of Ritz projections, see [60] in e.g. theorem 1.2. To deal with the polygonal/polyhedral domain approximation we adapt some arguments contained in [26], where parabolic problems are treated on moving domains, but with homogeneous boundary conditions. The inhomogeneous Dirichlet boundary conditions require special care.

We start indeed from the Ritz projection, by keeping the same notation as in the last section for the lift.

Throughout this section, $\lesssim$ means $\leq C$, for C independent of both the discretization parameter h, and time.

Definition D.2.2 (Inhomogeneous Ritz projection)
Consider $z \in H^2(\Omega)$. We define $R_h z \in S_h^1$ by:

$$a_h(R_h z, v_h) = a(z, v_h^l), v_h \in S_{h,0,D_h}^1$$

$$R_h z = \Pi_h z \text{ on } \partial \Omega_h$$

We denote $R_c z := (R_h z)^l$.

Here are some useful properties of such projection.

Proposition D.2.3 (Properties of the Ritz projection)
The following facts hold true about R_h, where we assume that h is small enough:

1. R_h is well defined

2. R_h is continuous, uniformly in h, from $H^2(\Omega)$, to S_h^1, i.e., $\|R_h z\|_{H^1(\Omega_h)} \lesssim \|z\|_{H^2(\Omega)}$

3. $\|R_c z - z\|_{H^1(\Omega)} \lesssim h \|z\|_{H^2(\Omega)}$

4. $\|R_c z - z\|_{L^2(\Omega)} \lesssim h^2 \|z\|_{H^2(\Omega)} + \|z - \Pi_c z\|_{L^2(\Gamma_D)}$

5. for $z \in H^1(I, H^2(\Omega))$, $R_c \frac{d}{dt} = \frac{d}{dt} R_c$ and we can therefore use the above properties also for z_t

Proof.

Existence, uniqueness and stability

The splitting $\delta_h := R_h z - \Pi_h z$, the fact that a_h is (h-uniformly) coercive on $S_{h,0,D_h}^1$ by proposition D.1.6 and the Lax-Milgram lemma yield existence, uniqueness follows as in **??**

Now, for the stability: by uniform coercivity and the definition of R_h: $\|R_h z\|_{H^1(\Omega_h)}^2 \lesssim a_h(R_h z, R_h z) = a_h(\delta_h, R_h z) + a_h(\Pi_h z, R_h z)$, so that $\|R_h z\|_{H^1(\Omega_h)} \lesssim \|\delta_h\|_{H^1(\Omega_h)} + \|\Pi_h z\|_{H^1(\Omega_h)}$. We only need now to apply proposition D.1.3, proposition D.1.4, proposition D.1.5.

Error bounds

For the H^1 error bound, we refer to [26], in particular to the proof of lemma 3.8 at page 1720. Note that H^2 stability of R_h is sufficient, instead of the stronger H^1 stability they use.

For the L^2 error bound, we apply a variant of the Aubin-Nitsche trick. Call $e := z - R_c z \in H^1(\Omega)$ (this holds by proposition D.1.3), and define w by:

$$\begin{cases} -\Delta w = e & \text{on } \Omega \\ w = 0 & \text{on } \Gamma_D \\ \partial_\nu w = 0 & \text{on } \Gamma_N \end{cases}$$

Now, by H^2 regularity:

$$\|e\|_{L^2(\Omega)}^2 = a(w, e) - \int_{\partial \Omega} e \partial_\nu w$$

and:

$$\|e\|_{L^2(\Omega)}^2 \leq a(w, e) + C \|e\|_{L^2(\Gamma_D)} \|e\|_{L^2(\Omega)} = F_h(w) + C \|e\|_{L^2(\Gamma_D)} \|e\|_{L^2(\Omega)}$$

The first term is bounded as in the proof of lemma 3.8 of [26], whereas, using H^2 regularity for w we are able to conclude:

$$\|z - R_c z\|_{L^2(\Omega)} \lesssim h^2 \|z\|_{H^2(\Omega)} + \|z - \Pi_c z\|_{L^2(\Gamma_D)}$$

Commutation with time derivative

Follows from corollary A.2.2, and the fact that R_c is linear and bounded. The latter is true as lifting a finite element function is a linear bounded map, see proposition D.1.3. $\square$

Note, for the parabolic problems arising from shape optimization (problem 2.1.1), theorem B.2.6 suffices.

We can now attempt an error estimate for problem D.2.1, for the following spatial semidiscrete formulation.

Proof.

Existence and uniqueness

A function $\delta_h \in H^1(I, S_{h,0,D_h}^1)$ can be written as $\delta_h = \sum_j d_{hj}(t) v_{hj}$, for the usual finite element basis $\{v_{hj}\}_j$ of $S_{h,0,D_h}^1$. We employ the splitting technique $\delta_h = u_h - G_{D,h}$. By testing with the equation of problem D.2.5 with the basis functions v_{hj} we obtain the problem:

$$M_h d_h'(t) + A_h d_h(t) = F_h(t), \text{ a.e. } t \tag{D.2.8}$$

$$d_h(0) = d_{h,0} \tag{D.2.9}$$

Here, $M_{h,ij} = (v_{hi}, v_{hj})_{L^2(\Omega_h)}$, $A_{h,ij} = a(v_{hi}, v_{hj})$ are the so called mass and stiffness matrices, both invertible, with respect to the nodal basis of $S_{h,0,D_h}^1$. We also have $F_{h,j}(t) := -(\partial_t G_{D,h}, v_{hj})_{L^2(\Omega_h)} - a_h(G_{D,h}, v_{hj}) + (f_h, v_{hj})_{L^2(\Omega_h)} + (g_{N,h}, v_{hj})_{L^2(\Gamma_{N_h})}$, together with $d_{h,0} := u_{0h} - G_{D,h}$, in the sense of the non-Dirichlet nodal values (we are able to come to this problem thanks to the assumed compatibility between $u_{0h}, g_{D,h}$).

Thanks to the smoothness assumptions on the data, we have that F has $L^2(I)$ entries.

Hence, by basic theory of ordinary differential equations (theorem 3.4 of [54], for instance), we conclude the existence (and uniqueness) of $d \in H^1(I)$ solving the problem above. The function $u_h := \sum_j d_j(t) v_{hj} + G_{D,h}$ is therefore a solution to the original problem.

Uniqueness (and hence, independence on the particular extension $G_{D,h}$) follows by usual stability estimates. Stability

Following [35], page 20, 21, we can prove stability estimates for δ_h and then, by triangle inequality:

$$\|u_h\|_{C([0,T],L^2(\Omega_h))} + \|u_h\|_{L^2(I,H^1(\Omega_h))} \lesssim$$

$$\|f_h\|_{L^2(I,(S^1_{h,0,D_h})^*)} + \|g_{N,h}\|_{L^2(I,L^2(\Gamma_{N_h}))} + \|G_{D,h}\|_{H^1(I,H^1(\Omega_h)))} + \|u_{0h}\|_{L^2(\Omega_h)}$$

Now, thanks to assumption D.2.6:

- $\|g_{N,h}\|_{L^2(I,L^2(\Gamma_{N_h}))} \lesssim \|g_N\|_{L^2(I,H^2(\Gamma_N))}$ (here is suffices to use proposition D.1.4))

- because the Lagrange interpolator is linear bounded $H^2(\Omega) \to S^1_h$ there holds, by proposition D.1.4: $\partial_t G_{D,h} = \Pi_h \partial_t G_D$, so that $\|\partial_t G_{D,h}\|_{H^1(\Omega_h)} = \|\Pi_h \partial_t G_D\|_{H^1(\Omega_h)} \lesssim \|\partial_t G_D\|_{H^2(\Omega))}$, where we used proposition D.1.4 and proposition D.1.3. Thanks to the properties of G_D, and the fact that the extension E of proposition A.2.6 commutes with Π_h (by corollary A.2.2), there holds $\|\partial_t G_{D,h}\|_{H^1(\Omega_h)} \lesssim \|\partial_t g_D\|_{H^{3/2}(\Gamma_D)}$. With analogous reasonings we can conclude that $\|G_{D,h}\|_{H^1(I,H^1(\Omega_h)))} \lesssim \|g_D\|_{H^1(I,H^{3/2}(\Gamma_D)))}$

- similarly, $\|u_{0h}\|_{L^2(\Omega_h)} \lesssim \|u_0\|_{H^2(\Omega)}$

All in all:

$$\|u_h\|_{C([0,T],L^2(\Omega_h))} + \|u_h\|_{L^2(I,H^1(\Omega_h))} \lesssim \|f_h\|_{L^2(I,(S^1_{h,0,D_h})^*)} + \|g_N\|_{L^2(I,H^2(\Gamma_N))} + \|g_D\|_{H^1(I,H^{3/2}(\Gamma_D)))} + \|u_0\|_{H^2(\Omega)}$$

$\square$

Theorem D.2.10 (Semidiscrete error bound)
There holds:

$$\left\|u(t) - u_h^l(t)\right\|_{L^2(\Omega)}^2 + h^2 \int_0^T \left\|u - u_h^l\right\|_{H^1(\Omega)}^2 \lesssim$$
$$h^4 A^2$$

where $A^2 := \|u\|_{H^1(I,H^2(\Omega))}^2 + \|g_D\|_{H^1(I,H^2(\Gamma_D))}^2 + \|u_0\|_{H^2(\Omega)}^2 + \int_0^T C_f^2 + \int_0^T \|f_h\|_{H^1(\Omega_h)}^2 + \int_0^T \|g_N\|_{H^2(\Gamma_N)}^2$.
For this to hold, assumption D.2.4, assumption D.2.6 and assumption B.2.1 must be fulfilled.

Proof.

Also here, we adapt the argument from [26], in particular, those of pages 1727, 1728, 1729, which are modifications of standard techniques that can be traced in e.g. [60], theorem 1.2.

Error split

We want to bound $e := u - u_h = u - R_c u + R_c u - u_h^l =: \rho + \theta_h^l$. We already have the needed bounds on ρ by proposition D.2.3.

An equation for θ_h

Consider then $\theta_h := R_h u - u_h$. It is an element of $H^1(I, S^1_{h,0,D_h})$ (i.e. it is 0 on the Dirichlet boundary), making it a suitable test function: this is the primary reason to impose boundary conditions on R_h.

So, we have, for $v_h \in S^1_{h,0,D_h}$:

$$(\partial_t R_h u, v_h)_{L^2(\Omega_h)} + a_h(R_h u, v_h) = \{ \text{ definition of Ritz projection } \} =$$
$$(\partial_t R_h u, v_h)_{L^2(\Omega_h)} + a(u, v_h^l) =$$
$$(\partial_t R_h u, v_h)_{L^2(\Omega_h)} - (\partial_t u, v_h^l)_{L^2(\Omega)} + (f, v_h^l)_{L^2(\Omega)} + (g_N, v_h^l)_{L^2(\Gamma_N)}$$

Adding the equation for u_h, and then adding and subtracting $(\partial_t R_c u, v_h^l)_{L^2(\Omega)}$:

$$(\partial_t \theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h) = (\partial_t R_h u, v_h)_{L^2(\Omega_h)} - (\partial_t R_c u, v_h^l)_{L^2(\Omega)} \tag{D.2.11}$$
$$- (\partial_t \rho, v_h^l)_{L^2(\Omega)} \tag{D.2.12}$$
$$+ (f, v_h^l)_{L^2(\Omega)} - (f_h, v_h)_{L^2(\Omega_h)} \tag{D.2.13}$$
$$+ (g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})} \tag{D.2.14}$$

This means that we can estimate the right hand sides of the above equation to quantify the size of θ_h.

Estimating the size of θ_h: right hand sides

By corollary A.2.2 we can write $\partial_t R_h u = R_h \partial_t u, \partial_t R_c u = (R_h \partial_t u)^l$.

Hence, $|(\partial_t R_h u, v_h)_{L^2(\Omega_h)} - (\partial_t R_c u, v_h^l)_{L^2(\Omega)}| \lesssim h^2 \|\partial_t u\|_{H^2(\Omega)} \|v_h\|_{H^1(\Omega_h)}$, where we used proposition D.1.5, and proposition D.2.3.

Similarly, we have $\partial_t \rho = \partial_t u - R_c \partial_t u$.

Thus $|(\partial_t \rho, v_h^l)_{L^2(\Omega)}| \lesssim h^2 \|\partial_t u\|_{H^2(\Omega)} \|v_h\|_{H^1(\Omega_h)} + \|\partial_t(g_D - g_{D,h})\|_{L^2(\Gamma_D)} \|v_h\|_{H^1(\Omega_h)}$ by proposition D.2.3. By the choice of $g_{D,h}$ and by proposition D.1.4, $|(\partial_t \rho, v_h^l)_{L^2(\Omega)}| \lesssim h^2 (\|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \|v_h\|_{H^1(\Omega_h)}$.

Moreover:

$$|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \leq$$

$$|(g_N - g_{N,h}^l, v_h^l)_{L^2(\Gamma_N)}| + |(g_{N,h}^l, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}|$$

By proposition D.1.5 and trace theorems there holds:

$$|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \lesssim$$

$$\left\| g_N - g_{N,h}^l \right\|_{L^2(\Gamma_N)} \left\| v_h^l \right\|_{H^1(\Omega)} + h^2 \left\| g_{N,h} \right\|_{L^2(\Gamma_{N_h})} \left\| v_h \right\|_{H^1(\Omega_h)}$$

Using the choice of $g_{N,h}$ and also proposition D.1.4, proposition D.1.3, we obtain:

$$|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \lesssim h^2 \left\| g_N \right\|_{H^2(\Gamma_N)} \left\| v_h \right\|_{H^1(\Omega_h)}$$

Analogously:

$$|(f, v_h^l)_{L^2(\Omega)} - (f_h, v_h)_{L^2(\Omega_h)}| \lesssim$$

$$\left\| f - f_h^l \right\|_{L^2(\Omega)} \left\| v_h \right\|_{H^1(\Omega_h)} + h^2 \left\| f_h \right\|_{H^1(\Omega_h)} \left\| v_h \right\|_{H^1(\Omega_h)} \lesssim (C_f + \left\| f_h \right\|_{H^1(\Omega_h)}) h^2 \left\| v_h \right\|_{H^1(\Omega_h)}$$

We used throughout assumption D.2.6.

Calling $E_h(v_h) := (\partial_t \theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h)$, we discovered that:

$$|E_h(v_h)| \lesssim h^2 \left\| v_h \right\|_{H^1(\Omega_h)} (C_f + \left\| f_h \right\|_{H^1(\Omega_h)} + \left\| g_N \right\|_{H^2(\Gamma_N)} + \left\| \partial_t u \right\|_{H^2(\Omega)} + \left\| \partial_t g_D \right\|_{H^2(\Gamma_D)}) \tag{D.2.15}$$

Estimating the size of θ_h: stability estimate

By the equation of θ_h, and by the possibility of testing with $v_h = \theta_h$ itself, we obtain:

$$\frac{1}{2} \frac{d}{dt} \left\| \theta_h \right\|_{L^2(\Omega_h)}^2 + \left\| \theta_h \right\|_{H^1(\Omega_h)}^2 - \left\| \theta_h \right\|_{L^2(\Omega_h)}^2 = E_h(\theta_h)$$

Hence, calling $Q := C_f + \left\| f_h \right\|_{H^1(\Omega_h)} + \left\| g_N \right\|_{H^2(\Gamma_N)} + \left\| \partial_t u \right\|_{H^2(\Omega)} + \left\| \partial_t g_D \right\|_{H^2(\Gamma_D)}$, by Young's inequality, some algebraic manipulations and by using Gronwall's inequality (25, page 19 of [35]), for all $t \in [0, T]$ we have:

$$\left\| \theta_h(t) \right\|_{L^2(\Omega_h)}^2 + \int_0^T \left\| \theta_h \right\|_{H^1(\Omega_h)}^2 \lesssim 8h^4 \int_0^T Q^2 + 2 \left\| \theta_h(0) \right\|_{L^2(\Omega_h)}^2 \tag{D.2.16}$$

We can also apply proposition D.1.3 to obtain an estimate in spaces that don't depend on h:

$$\left\| \theta_h^l(t) \right\|_{L^2(\Omega)}^2 + \int_0^T \left\| \theta_h^l \right\|_{H^1(\Omega)}^2 \lesssim h^4 \int_0^T Q^2 + \left\| \theta_h^l(0) \right\|_{L^2(\Omega)}^2$$

Conclusion

We have, for $e = u - u_h^l = \rho + \theta_h^l$, and h small, by combining eq. (D.2.16) and proposition D.2.3:

$$\left\| e(t) \right\|_{L^2(\Omega)}^2 + h^2 \int_0^T \left\| e \right\|_{H^1(\Omega)}^2 \lesssim$$

$$h^4 \left\| u(t) \right\|_{H^2(\Omega)}^2 + h^4 \left\| g_D(t) \right\|_{L^2(\Gamma_D)}^2 + h^2 h^2 \int_0^T \left\| u \right\|_{H^2(\Omega)}^2 + h^4 \int_0^T Q^2 + \left\| \theta_h^l(0) \right\|_{L^2(\Omega)}^2$$

A triangle inequality applied to $\left\| \theta_h^l(0) \right\|_{L^2(\Omega)}^2$, an application of proposition D.2.3 and the definition of Q allow us to conclude. □

We can also prove convergence of the derivatives in a rather strong norm.

Corollary D.2.17 (Refined error estimate)
Apart from assumption D.2.4, assumption D.2.6 and assumption B.2.1, further assume that $g_N \in H^1(I, H^2(\Gamma_N))$. Then, for all $t \in (0, T)$:

$$\int_0^T \left\| \partial_t u - (\partial_t u_h)^l \right\|_{L^2(\Omega)}^2 + \left\| u(t) - u_h^l(t) \right\|_{H^1(\Omega)}^2 \lesssim h^2 B^2$$

where $B := \|u\|_{H^1(I,H^2(\Omega))}^2 + \|g_D\|_{H^1(I,H^2(\Gamma_D))}^2 + \int_0^T C_f^2 + \|f_h\|_{L^2(I,L^2(\Omega_h))}^2 + \|g_N\|_{H^1(H^2(\Gamma_N))}^2 + \|u_0\|_{H^2(\Omega)}^2.$

Proof.

We employ again the error decomposition $e = \rho + \theta_h^l$.

Another estimate for θ_h

Consider again eq. (D.2.11). We intend to test by $\partial_t \theta_h \in L^2(I, S_{h,0,D_h}^1)$. This is possible also by the reasonings in [39], (1.61), page 42. Integrate from 0 to t to obtain:

$$\int_0^t \|\partial_t \theta_h\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\left(a_h(\theta_h(t),\theta_h(t)) - a_h(\theta_h(0),\theta_h(0))\right) = \int_0^t (\partial_t R_h u, \partial_t \theta_h)_{L^2(\Omega_h)} - \int_0^t (\partial_t R_c u, \partial_t \theta_h^l)_{L^2(\Omega)}$$
$$- \int_0^t (\partial_t \rho, \partial_t \theta_h^l)_{L^2(\Omega)}$$
$$+ \int_0^t (f, \partial_t \theta_h^l)_{L^2(\Omega)} - \int_0^t (f_h, \partial_t \theta_h)_{L^2(\Omega_h)}$$
$$+ \int_0^t (g_N, \partial_t \theta_h^l)_{L^2(\Gamma_N)} - \int_0^t (g_{N,h}, \partial_t \theta_h)_{L^2(\Gamma_{N_h})}$$

By suitable estimations of the left hand side (involving proposition D.1.6), using integration by parts for the terms with $g_N, g_{N,h}$ and proposition D.1.5 on the right hand side, plus the Young inequality, we get:

$$\int_0^t \|\partial_t \theta_h\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\|\theta_h(t)\|_{H^1(\Omega_h)}^2 \leq \frac{1}{2}\|\theta_h(t)\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\|\theta_h(0)\|_{H^1(\Omega_h)}^2$$
$$+ Ch^2\int_0^t \|\partial_t u\|_{H^2(\Omega)}^2 + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|_{L^2(\Omega_h)}^2$$
$$+ Ch^2\int_0^t (\|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)})^2 + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|_{L^2(\Omega_h)}^2$$
$$+ Ch^2\int_0^t C_f^2 + Ch^2\int_0^t \|f_h\|_{L^2(\Omega_h)}^2 + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|_{L^2(\Omega_h)}^2$$
$$+ Ch^2\int_0^t \|\partial_t g_N\|_{H^2(\Gamma_N)}^2 + \int_0^t \|\theta_h\|_{H^1(\Omega_h)}^2$$
$$+ Ch^2\|g_N(t)\|_{H^2(\Gamma_N)}^2 + \frac{1}{4}\|\theta_h(t)\|_{H^1(\Omega_h)}^2$$
$$+ Ch^2\|g_N(0)\|_{H^2(\Gamma_N)}^2 + \frac{1}{2}\|\theta_h(0)\|_{H^1(\Omega_h)}^2$$

where C is independent of h and t. We re-arrange, and apply eq. (D.2.16) to the term $\|\theta_h(t)\|_{L^2(\Omega_h)}^2 + \int_0^t \|\theta_h\|_{H^1(\Omega_h)}^2$.

Calling $q = \int_0^T \left[\|\partial_t u\|_{H^2(\Omega)}^2 + \|\partial_t g_D\|_{H^2(\Gamma_D)}^2 + C_f^2 + \|f_h\|_{L^2(\Omega_h)}^2 + Q^2 + \|g_N\|_{H^2(\Gamma_N)}^2 + \|\partial_t g_N\|_{H^2(\Gamma_N)}^2\right]$, and upon using proposition D.1.3, proposition D.2.3 and proposition D.1.4:

$$\int_0^T \left\|\partial_t \theta_h^l\right\|_{L^2(\Omega)}^2 + \left\|\theta_h(t)^l\right\|_{H^1(\Omega)}^2 \lesssim \|\theta_h(0)\|_{H^1(\Omega_h)}^2 + h^4 q \lesssim h^2 \|u_0\|_{H^2(\Omega)}^2 + h^4 q$$

Conclusion

There holds:

$$\|e(t)\|_{H^1(\Omega)}^2 + \int_0^T \|\partial_t e\|_{L^2(\Omega)}^2 \leq$$
$$\int_0^T \|\partial_t \rho\|_{L^2(\Omega)}^2 + h^2\|\rho(t)\|_{H^1(\Omega)}^2 + \int_0^T \left\|\partial_t \theta_h^l\right\|_{L^2(\Omega)}^2 + \left\|\theta_h^l(t)\right\|_{H^1(\Omega)}^2 \leq \{\text{ above, and proposition D.2.3 }\} \leq$$
$$h^2\int_0^T (\|\partial_t u\|_{H^2(\Omega)}^2 + \|\partial_t g_D\|_{H^2(\Gamma_D)}^2) + h^2\|u(t)\|_{H^2(\Omega)}^2 + h^2\|u_0\|_{H^2(\Omega)}^2 + h^4 q$$

$\square$

If however we content ourselves with estimating the convergence of the derivatives in a weaker norm, we can actually obtain $O(h^2)$ convergence, in every case. To do so, it will be crucial to establish the H^1 stability of the L^2 projection in our context. This fact is known for polyhedral domains with some assumptions on the meshes, see e.g. [7].

> **Corollary D.2.18** (Order two convergence of derivatives in dual norm)
> Under assumption D.2.4, assumption D.2.6 and assumption B.2.1 we have, for all $w \in L^2(I, H^1_{0,D}(\Omega))$:
>
> $$\left| \int_I (\partial_t(u - u^l_h), w)_{L^2(\Omega)} \right| \lesssim h^2 A \|w\|_{L^2(I, H^1(\Omega))}$$

Proof.

We introduce the L^2 projection $\pi_h : L^2(\Omega) \to S^1_{h,0,D_h}$, given by:

$$(\pi_h w, v_h)_{L^2(\Omega_h)} = (w, v^l_h)_{L^2(\Omega)}, \quad \forall v_h \in S^1_{h,0,D_h}$$

The definition is remimniscent of that of the Ritz projection. We will prove well-posedness and H^k stability of such projection, i.e. $\|\pi_h w\|_{H^k(\Omega_h)} \lesssim \|w\|_{H^k(\Omega)}$, for $k = 0, 1$. First, let us show how this projection helps in the estimate.

Conclusion

For $w \in H^1_{0,D}(\Omega)$ we estimate $(\partial_t(\theta^l_h), w)_{L^2(\Omega)} = (w, (\partial_t \theta^l_h))_{L^2(\Omega)} = (\pi_h w, \partial_t \theta_h)_{L^2(\Omega_h)}$. We have also used that lifting and the time derivative commute, by proposition D.1.3 and corollary A.2.2. We can now apply eq. (D.2.11):

$$(\partial_t(\theta^l_h), w)_{L^2(\Omega)} = a_h(\theta_h, \pi_h w) - E_h(\pi_h w) \lesssim \{ \text{ eq. (D.2.15) } \} \lesssim$$

$$\|\theta_h\|_{H^1(\Omega_h)} \|\pi_h w\|_{H^1(\Omega_h)} + h^2(\|\pi_h w\|_{H^1(\Omega_h)} C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \lesssim$$

$$\|\theta_h\|_{H^1(\Omega_h)} \|w\|_{H^1(\Omega)} + h^2 \|w\|_{H^1(\Omega)} (C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)})$$

where in the last step we used the assumed stability of π_h. Integrating in time and using the Cauchy-Schwarz inequality:

$$\left| \int_I (\partial_t(\theta^l_h), w)_{L^2(\Omega)} \right|^2 \lesssim$$

$$\left(\int_I \|\theta_h\|^2_{H^1(\Omega_h)} + h^4 \int_I (C_f^2 + \|f_h\|^2_{H^1(\Omega_h)} + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}) \right) \int_I \|w\|^2_{H^1(\Omega)} \lesssim \{ \text{ eq. (D.2.16) } \} \lesssim$$

$$h^4 \left(\int_I Q^2 + \|u_0\|^2_{H^2(\Omega)} + \int_I (C_f^2 + \|f_h\|^2_{H^1(\Omega_h)} + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}) \right) \|w\|^2_{L^2(I, H^1(\Omega))}$$

We can also estimate:

$$\left| \int_I (\rho_t, w)_{L^2(\Omega)} \right| \lesssim \{ \text{ as in the proof of theorem D.2.10 } \} \lesssim$$

$$\int_I h^2(\|\partial_t w\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \|w\|_{H^1(\Omega_h)} \lesssim \{ \text{ Cauchy-Schwarz } \} \lesssim$$

$$h^2 \sqrt{\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}} \|w\|_{L^2(I, H^1(\Omega))}$$

and by the usual splitting $e = \rho + \theta^l_h$ we can conclude.

L^2 projection: well-posedness

From the definition of π_h we obtain:

$$(\pi_h w, v_h)_{L^2(\Omega_h)} = (w, v^l_h)_{L^2(\Omega)} = (w^{-l} \xi, v_h)_{L^2(\Omega_h)}$$

where $\xi \in L^\infty(\Omega_h)$ is a term originating from the change of variables. We therefore recognize that $\pi_h w$ is the usual L^2 projection of $w^{-l} \xi \in L^2(\Omega_h)$ onto the closed subspace $S^1_{h,0,D_h}$, for which we know existence and uniqueness.

L^2 projection: stability

L^2 stability of π_h follows by testing with $\pi_h w$ itself and using proposition D.1.3. Also, denote by π_h^* the usual L^2 projector:

$$(\pi_h^* v - v, v_h)_{L^2(\Omega_h)} = 0, \quad \forall v_h \in S^1_{h,0,D_h}$$

We have, for $w \in L^2(\Omega)$, that $(\pi_h w - \pi_h^* w^{-l}, v_h)_{L^2(\Omega_h)} = (w, v^l_h)_{L^2(\Omega)} - (w^{-l}, v_h)_{L^2(\Omega_h)}$. An application of proposition D.1.5 and of proposition D.1.3 yields:

$$\left\| \pi_h w - \pi_h^* w^{-l} \right\|^2_{L^2(\Omega_h)} \lesssim h \|w\|_{L^2(\Omega)} \left\| \pi_h w - \pi_h^* w^{-l} \right\|_{L^2(\Omega_h)}$$

Now, we can adapt the original proof of [6] to our case, see in particular (A.1). In fact: $|\pi_h w|_{H^1(\Omega_h)} \leq |\pi_h w - \pi^* w^{-l}|_{H^1(\Omega_h)} + |\pi_h^* w^{-l}|_{H^1(\Omega_h)}$.

We can apply an inverse inequality to the first member: $|\pi_h w - \pi^* w^{-l}|_{H^1(\Omega_h)} \lesssim h^{-1} \left\| \pi_h w - \pi^* w^{-l} \right\|_{L^2(\Omega_h)} \lesssim \|w\|_{L^2(\Omega)}$.

For the second term, consider a suitable $w_h \in S^1_{h,0,D_h}$. We have: $|\pi_h^* w^{-l}|_{H^1(\Omega_h)} \leq |\pi_h^*(w^{-l} - w_h)|_{H^1(\Omega_h)} + |\pi_h^* w_h|_{H^1(\Omega_h)} \lesssim h^{-1} \left\| \pi_h^*(w^{-l} - w_h) \right\|_{L^2(\Omega_h)} + \|w_h\|_{H^1(\Omega_h)}$, where we again applied inverse inequalities, together with the fact that $\pi_h^* w_h = w_h$ for $w_h \in S^1_{h,0,D_h}$ (i.e. π_h^* is really a projection, unlike π_h). Moreover, $\|\pi_h^* v\|_{L^2(\Omega_h)} \leq \|v\|_{L^2(\Omega_h)}$, so that $|\pi_h^* w^{-l}|_{H^1(\Omega_h)} \lesssim h^{-1} \left\| w^{-l} - w_h \right\|_{L^2(\Omega_h)} + \|w_h\|_{H^1(\Omega_h)}$. So, if there holds $\left\| w^{-l} - w_h \right\|_{L^2(\Omega_h)} \lesssim h \|w\|_{H^1(\Omega)}$ and $\|w_h\|_{H^1(\Omega_h)} \lesssim \|w\|_{H^1(\Omega)}$, then we are done.

Finding w_h

Such w_h will be the optimal order interpolator with boundary conditions described in (5.9) at page 1230, [10]. We need to check that our framework matches that of [10] to apply such a result.

But this is ensured by the construction outlined in [26], sections 8.5 and 8.6. The assumptions of theorem 5.1, in particular, are all satisfied: that the triangulations satisfy the so called 1-regularity is proved in lemma 8.13 or [26], whereas all the other properties are already discussed in [10] following example 2 (see pages 1216, 1221, 1228, and remark 5.2 at page 1230).

Applying corollary 5.1 of [10] to $\Gamma_0 = \Gamma_D$ (Γ_0 is in the notation of [10]) we find $w_h \in S^1_{h,0,D_h}$ (true by proposition and corollary 5.1, [10]), with:

- $\left\| w - w_h^l \right\|_{L^2(\Omega)} \lesssim h \|w\|_{H^1(\Omega)}$

- $\left| w - w_h^l \right|_{H^1(\Omega)} \lesssim \|w\|_{H^1(\Omega)}$

Therefore we also get $\left\| w_h^l \right\|_{H^1(\Omega)} \lesssim (C(1 + h) + 1) \|w\|_{H^1(\Omega)}$.

Applying proposition D.1.3 we see that w_h satisfies all the requirements. Note, is is essential here that $w = 0$ on Γ_D.

$\square$

D.3. Fully discrete estimates

Here, we attempt at deriving fully discrete estimates given the semidiscrete results just above.

Assumption D.3.1 (Assumptions for full discretization)

We discuss the implicit Euler method ($\theta = 1$) and the Crank-Nicolson method ($\theta = 1/2$).
We ask assumption D.2.6.
We further assume:

- $g_N \in H^{1/\theta+1}(I, H^{3/2}(\Gamma_N))$

- $g_D \in H^{1/\theta+1}(I, H^{3/2}(\Gamma_D))$

- $f_h \in H^{1/\theta}(I, S_h^1)$

- $\left\| \delta_h(0)^{(1/\theta)} \right\|_{L^2(\Omega_h)}$ is bounded uniformly for small h

---

We consider f_h^k to be a suitable approximation of $f_h(t^k)$, i.e. $f_h^k \simeq f_h(t^k)$ (suitable in a way that will be further specified later on)ò

Problem D.3.2 (Numerical scheme)
Under assumption D.3.1, it is:

$$\left(\frac{u_h^{k+1} - u_h^k}{\delta t}, v_h \right)_{L^2(\Omega_h)} + a_h(\theta u_h^{k+1} + (1 - \theta) u_h^k, v_h) =$$
$$(\theta f_h^{k+1} + (1 - \theta) f_h^k, v_h)_{L^2(\Omega_h)} + (\theta g_{N,h}^{k+1} + (1 - \theta) g_{N,h}^k, v_h)_{L^2(\Gamma_{N_h})}, \quad v_h \in S^1_{h,0,D_h}, 1 \leq k \leq K$$
$$u_h^{k+1} = g_{D,h}^{k+1}, \quad 1 \leq k \leq K, \text{ on } \Gamma_{D_h}$$
$$u_h^0 = u_{0h}$$

Proposition D.3.3 (Discrete versus semidiscrete)
We are working under assumption D.3.1.
Call $e_h^k := u_h^k - u_h(t^k)$ and $\delta f_h^k := f_h^k - f_h(t^k)$. Then, for $\theta = 1, 1/2$, we have $u_h \in H^{1/\theta+1}(I, S_h^1)$ and, for $1 \leq n \leq K$:

$$\delta t \sum_{k=0}^{n-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{(H^1_{0,D_h}(\Omega_h))^*} + \|e_h^n\|^2_{L^2(\Omega_h)} + \delta t \sum_{k=0}^{n-1} \left\| \theta e_h^{k+1} + (1 - \theta) e_h^k \right\|^2_{H^1(\Omega_h)} \lesssim D^2 + (\delta t)^{2/\theta} C^2$$

Note, the difference quotient is estimated in the dual norm of $H^1_{0,D_h} = \{u \in H^1, u(\Gamma_{D_h}) = 0\}$.

Proof.

Recall the semidiscrete problem, problem D.2.5, for $u_h \in H^1(I, S_h^1)$. For the L^2, H^1 estimate we refer to [55], page 385 and following, in particular, theorem 11.3.1 and 11.3.2. In particular, calling $e_h^k := u_h^k - u_h(t^k)$, and $\delta f_h^k := f_h^k - f_h(t^k)$:

$$\left(\frac{e_h^{k+1} - e_h^k}{\delta t}, v_h \right)_{L^2(\Omega_h)} + a_h(\theta e_h^{k+1} + (1-\theta)e_h^k, v_h) = (\theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k, v_h)_{L^2(\Omega_h)} \tag{D.3.4}$$

$$e_h^{k+1} = 0, \text{ on } \Gamma_{D_h} \tag{D.3.5}$$

$$e_h^0 = 0 \tag{D.3.6}$$

where we defined $Q_h^k := \frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} - \theta \partial_t u_h(t^{k+1}) - (1-\theta)\partial_t u_h(t^k)$. The proof now consists in deriving discrete stability estimates for eq. (D.3.4), exactly how it is done in [55]. We only remark a few facts that will be referenced in other proofs.

<u>Estimating Q_h^k</u>

We provide estimates of Q_h^k in a suitable norm. In the case $\theta = 1/2$, from the smoothness assumptions on the data we obtain $u_h \in H^3(I, S_h^1)$ and, exactly as in [55]:

$$\delta t \sum_{k=0}^{n-1} \left\| Q_h^k \right\|_{-1,h}^2 \lesssim \delta t^4 \int_I \left\| u_h''' \right\|_{-1,h}^2$$

Differentiating problem D.2.5 twice we obtain:

$$\left\| u_h'''(t) \right\|_{-1,h} \le \left\| f_h'' \right\|_{-1,h} + \left\| g_{N,h}'' \right\|_{L^2(\Gamma_{N_h})} + \left\| u_h'' \right\|_{H^1(\Omega_h)}$$

By stability estimates, as in proposition D.2.7, through the splitting $u_h = \delta_h + G_{D,h}$ (see assumption D.2.6):

$$\left\| u_h'' \right\|_{L^2(I,H^1(\Omega_h))} \lesssim \left\| f_h'' \right\|_{L^2(I,(S_{h,0,D_h}^1)^*)} + \left\| g_{N,h}'' \right\|_{L^2(I,L^2(\Gamma_{N_h}))} + \left\| G_{D,h}''' \right\|_{L^2(I,H^1(\Omega_h))} + \left\| \delta_h(0)'' \right\|_{L^2(\Omega_h)} \tag{D.3.7}$$

Under our hypothesis assumption D.3.1, we have that $\left\| \delta_h''(0) \right\|_{L^2(\Omega_h)}^2 \lesssim C$. This, and assumption D.2.6, yield a bound, uniform on h, on $\int_I \left\| u_h''' \right\|_{-1,h}^2$.

This bound is:

$$\int_I \left\| u_h'''(t) \right\|_{-1,h}^2 \lesssim \int_I \left\| f_h'' \right\|_{-1,h}^2 + \int_I \left\| g_{N,h}'' \right\|_{L^2(\Gamma_{N_h})}^2 + \int_I \left\| G_{D,h}''' \right\|_{H^1(\Omega_h)}^2 + \left\| \delta_h(0)'' \right\|_{L^2(\Omega_h)}^2$$

But $\left\| g_{N,h}'' \right\|_{L^2(\Gamma_{N_h})} = \left\| \Pi_h g_N'' \right\|_{L^2(\Gamma_{N_h})}$, where Π_h is the nodal interpolator (see assumption D.2.6). By proposition D.1.5, $\left\| g_{N,h}'' \right\|_{L^2(\Gamma_{N_h})} \lesssim \left\| \Pi_c g_N'' \right\|_{L^2(\Gamma_N)} \le (1+h) \left\| g_N'' \right\|_{H^{3/2}(\Gamma_N)}$, where we also used proposition D.1.4.

Moreover $\left\| G_{D,h}''' \right\|_{H^1(\Omega_h)} = \left\| \Pi_h G_D''' \right\|_{H^1(\Omega_h)} \lesssim \left\| \Pi_c G_D''' \right\|_{H^1(\Omega)} \lesssim (1+h) \left\| G_D''' \right\|_{H^2(\Omega)} \lesssim \left\| g_D''' \right\|_{H^{3/2}(\Gamma_D)}$. Therefore:

$$\int_I \left\| u_h'''(t) \right\|_{-1,h}^2 \lesssim \int_I \left\| f_h'' \right\|_{-1,h}^2 + \int_I \left\| g_N'' \right\|_{H^2(\Gamma_N)}^2 + \int_I \left\| g_D''' \right\|_{H^{3/2}(\Gamma_D)}^2 + \left\| \delta_h(0)'' \right\|_{L^2(\Omega_h)}^2$$

The proof for $\theta = 1$ is very similar.

<u>Estimates for the difference quotient</u>

We go back to eq. (D.3.4). We employ the L^2 projection π_h^* as in the proof of corollary D.2.18, where we proved its stability properties. Consider then any $v \in H^1_{0,D}(\Omega)$, so that $v^{-l} \in H^1_{0,D_h}(\Omega_h)$ (i.e. $v^{-l} = 0$ on Γ_{D_h}).

Then:

$$\left(\frac{e_h^{k+1} - e_h^k}{\delta t}, v^{-l} \right)_{L^2(\Omega_h)} = \left(\frac{e_h^{k+1} - e_h^k}{\delta t}, \pi_h^* v^{-l} \right)_{L^2(\Omega_h)} = \tag{D.3.8}$$

$$-a_h(\theta e_h^{k+1} + (1-\theta)e_h^k, \pi_h^* v^{-l}) + (\theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k, \pi_h^* v^{-l})_{L^2(\Omega_h)} \tag{D.3.9}$$

which leads us to:

$$\left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{(H_{0,D_h}^1(\Omega_h))^*} \lesssim \left\| \theta e_h^{k+1} + (1-\theta)e_h^k \right\|_{H^1(\Omega_h)} + \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k \right\|_{-1,h}$$

and we can conlude by the above estimates on Q_h^k and the H^1 estimate. $\qquad\square$

Theorem D.3.10 (Fully discrete estimates)
With the hypothesis and notation of theorem D.2.10, proposition D.3.3, corollary D.2.17, corollary D.2.18, there holds:

$$\left\| u(t^k) - (u_h^k)^l \right\|_{L^2(\Omega)} \lesssim h^2 A + D + (\delta t)^{1/\theta} C$$

$$\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - (u_h^{k+1})^l) + (1-\theta)(u(t^k) - (u_h^k)^l) \right\|_{H^1(\Omega)}^2} \lesssim hB + D + (\delta t)^{1/\theta} C$$

$$\left| \int_I (\partial_t u, w_K)_{L^2(\Omega)} - \delta t \sum_{k=0}^{K-1} \left(\frac{(u_h^{k+1})^l - (u_h^k)^l}{\delta t}, w_{K,k} \right)_{L^2(\Omega)} \right| \lesssim \left(h^2 A + D + (\delta t)^{1/\theta} C \right) \| w_K \|_{L^2(I, H_{0,D}^1(\Omega))}$$

where $D^2 := \delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)}^2$. Here w_K is assumed to be piecewise constant on the time discretization, and with values $w_{K,k}$, on $[t^k, t^{k+1}]$, that belong to $H_{0,D}^1(\Omega)$.

Proof.

$\underline{L^2 \text{ norm}}$
By theorem D.2.10, $\left\| u(t) - u_h^l(t) \right\|_{L^2(\Omega)}^2 \lesssim h^4 A^2$. Combining this with the L^2 estimates proved in proposition D.3.3 we see, thanks to proposition D.1.3:

$$\left\| u(t^k) - (u_h^k)^l \right\|_{L^2(\Omega)} \lesssim \left\| u(t^k) - u_h^l(t^k) \right\|_{L^2(\Omega)} + \left\| u_h(t^k) - u_h^k \right\|_{L^2(\Omega)} \lesssim Ah^2 + \sqrt{\delta t \sum_{k=0}^{n-1} \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)}^2} + C(\delta t)^{1/\theta}$$

$\underline{H^1 \text{ norm}}$
Using proposition D.3.3 and proposition D.1.3:

$$\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h^{k+1})^l) + (1-\theta)(u(t^k) - u_h^k)^l) \right\|_{H^1(\Omega)}^2 \lesssim$$

$$\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h(t^{k+1})^l) + (1-\theta)(u(t^k) - u_h(t^k)^l) \right\|_{H^1(\Omega)}^2 + \delta t \sum_{k=0}^{K-1} \left\| \theta e_h^{k+1} + (1-\theta)e_h^k \right\|_{H^1(\Omega)}^2$$

By employing corollary D.2.17:

$$\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h(t^{k+1})^l) + (1-\theta)(u(t^k) - u_h(t^k)^l) \right\|_{H^1(\Omega)}^2 \leq 2\delta t \sum_{k=0}^{K} \left\| u(t^k) - u_h(t^k)^l \right\|_{H^1(\Omega)}^2 \lesssim 2\delta t K h^2 B^2$$

$\underline{\text{Estimate for the derivative}}$
Let $w \in L^2(I, H_{0,D}^1(\Omega))$ be piecewise constant in time, with values w_k on $[t^k, t^{k+1}]$. We can then write:

$$\int_I (\partial_t u, w)_{L^2(\Omega)} - \delta t \sum_{k=0}^{K-1} \left(\frac{(u_h^{k+1})^l - (u_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)} = \int_I (\partial_t(u - u_h^l), w)_{L^2(\Omega)} + \delta t \sum_{k=0}^{K-1} \left(\frac{(e_h^{k+1})^l - (e_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)}$$

For the first term we can use corollary D.2.18. For the second one we can write, thanks to proposition D.1.5:

$$\left| \delta t \sum_{k=0}^{K-1} \left(\frac{(e_h^{k+1})^l - (e_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)} \right| \lesssim$$

$$\delta t h \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)} \|w_k\|_{H^1(\Omega)} + \delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{-1,h} \|w_k\|_{H^1(\Omega)} \leq$$

$$\left(h \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2} + \sqrt{\sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{-1,h}^2} \right) \|w\|_{L^2(I, H^1(\Omega))}$$

If we can control $\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2$ we are done, also by the estimates in proposition D.3.3. We test eq. (D.3.4) by $\frac{e_h^{k+1} - e_h^k}{\delta t}$. Then, applying an additional Young's inequality in the case $\theta = 1$ this reads:

$$\left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2 + \frac{\|\nabla e_h^{k+1}\|_{L^2(\Omega_h)}^2}{2\delta t} - \frac{\|\nabla e_h^k\|_{L^2(\Omega_h)}^2}{2\delta t} \leq \left(\left\| \theta \delta f_h^{k+1} + (1-\theta) \delta f_h^k \right\|_{L^2(\Omega_h)} + \left\| Q_h^k \right\|_{-1,h} \right) \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{H^1(\Omega_h)}$$

or also, as $e_h^0 = 0$:

$$\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2 \leq \left(\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta) \delta f_h^k \right\|_{L^2(\Omega_h)}^2} + \sqrt{\delta t \sum_{k=0}^{K-1} \left\| Q_h^k \right\|_{-1,h}^2} \right) \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{H^1(\Omega_h)}^2}$$

Applying inverse inequalities and by the proof of proposition D.3.3, for h small:

$$h \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2} \leq \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta) \delta f_h^k \right\|_{L^2(\Omega_h)}^2} + (\delta t)^{1/\theta} C$$

$\square$

Proposition D.3.11 (Estimate for derivative in a stronger norms)
With the hypothesis and notation of theorem D.2.10, proposition D.3.3, corollary D.2.17, there holds:

$$\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{u(t^{k+1}) - u(t^k)}{\delta t} - \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|_{L^2(U)}^2} \lesssim hB + \delta t^{1/\theta} E + \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta) \delta f_h^k \right\|_{L^2(\Omega_h)}^2}$$

where B comes from corollary D.2.17 and $E^2 := \left\| g_D^{(2+1/\theta)} \right\|_{L^2(I, H^{3/2}(U))}^2 + \left\| g_N^{(2+1/\theta)} \right\|_{L^2(I, H^{3/2}(\Gamma_N))}^2 + \left\| \delta_h^{(1/\theta)}(0) \right\|_{H^1(U_h)}^2 +$
$\left\| f_h^{(1/\theta)} \right\|_{L^2(I, L^2(U_h))}^2$.

Proof.
We again perform a separation into semidiscretization in space, and then full discretization, and adopt the notation u to represent either one of the two state variables. In this proof $\theta = 1$, but the same ideas hold for $\theta = 1/2$.

Estimating Q_h^k in the L^2 norm

With reference to the proof of proposition D.3.3, let us bound Q_h^k in the stronger L^2 norm. From the definitions of Q_h^k (also see [55], pages 388, 389), there holds $\delta t \sum_{k=0}^{K-1} \left\| Q_h^k \right\|_{L^2(U_h)}^2 \leq \delta t^{2/\theta} \left\| u_h^{(1+2/\theta)} \right\|_{L^2(I, L^2(U_h))}^2$, also by an application of the Cauchy-Schwarz inequality. The latter norm can be bounded uniformly on h. This is achieved by the same reasonings as in the proof of proposition B.1.8:

$$\left\| u_h^{(1+2/\theta)} \right\|_{L^2(I, L^2(U_h))}^2 \lesssim \left\| G_{D,h}^{(2+1/\theta)} \right\|_{L^2(I, H^1(U_h))}^2 + \left\| g_{N,h}^{(2+1/\theta)} \right\|_{L^2(I, L^2(\Gamma_{N,h}))}^2 + \left\| \delta_h^{(1/\theta)}(0) \right\|_{H^1(U_h)}^2 + \left\| f_h^{(1/\theta)} \right\|_{L^2(I, L^2(U_h))}^2$$

$$\lesssim \left\| g_D^{(2+1/\theta)} \right\|_{L^2(I, H^{3/2}(U))}^2 + \left\| g_N^{(2+1/\theta)} \right\|_{L^2(I, H^{3/2}(\Gamma_N))}^2 + \left\| \delta_h^{(1/\theta)}(0) \right\|_{H^1(U_h)}^2 + \left\| f_h^{(1/\theta)} \right\|_{L^2(I, L^2(U_h))}^2 =: E^2$$

We see that we need the stronger compatibility condition that $\delta_h'(0)$ is bounded in H^1.

Semidiscrete bound

Consider eq. (D.3.4), where we remind that $e_h^k = u_h^k - u_h(t^k)$. We can test it by $\dfrac{e_h^{k+1} - e_h^k}{\delta t}$, and employing Young and Cauchy-Schwarz inequalities we obtain:

$$\left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(U_h)}^2 + \frac{1}{2\delta t} \left(\left\| \nabla e_h^{k+1} \right\|_{L^2(U_h)}^2 - \left\| \nabla e_h^k \right\|_{L^2(U_h)}^2 \right) \leq \left(\left\| Q_h^k \right\|_{L^2(U_h)} + \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)} \right) \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(U_h)}$$

Passing to summations, because $e_h^0 = 0$ and by the Cauchy-Schwarz inequality:

$$\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(U_h)}^2} \lesssim \delta t^{1/\theta} E + \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)}^2}$$

where we used the first part of the proof.

Fully discrete bound

We have, denoting with $(\cdot)^l$ the lifting of finite element functions defined in proposition D.1.3, and using proposition D.1.3 itself:

$$\delta t \sum_{k=0}^{K-1} \left\| \frac{u(t^{k+1}) - u(t^k)}{\delta t} - \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|_{L^2(U)}^2 \lesssim \delta t \sum_{k=0}^{K-1} \left\| \frac{e(t^{k+1}) - e(t^k)}{\delta t} \right\|_{L^2(U)}^2 + \delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(U_h)}^2$$

The second term on the right is $O(\delta t^2)$ by above, so that we need to concentrate only on the first one, where $e = u - u_h^l$. But by a suitable modification of Lemma 3.2 of [41], we can reason as follows:

$$\delta t \sum_{k=0}^{K-1} \left\| \frac{e(t^{k+1}) - e(t^k)}{\delta t} \right\|_{L^2(U)}^2 = \delta t \sum_{k=0}^{K-1} \left\| \frac{1}{\delta t} \int_{I_k} e' \right\|_{L^2(U)}^2 \lesssim \left\| e' \right\|_{L^2(I, L^2(U))}^2 \lesssim h^2 B^2$$

where we also used corollary D.2.17. $\qquad\square$

Bibliography

[1] R.A. Adams. *Sobolev Spaces. Adams.* Pure and applied mathematics. Academic Press, 1975. URL: `https://books.google.it/books?id=JxzpSAAACAAJ`.

[2] G. Allaire, C. Dapogny, and F. Jouve. "Shape and topology optimization". In: *Geometric partial differential equations, part II.* Ed. by Andrea Bonito and Ricardo H. Nochetto. Vol. 22. Handbook of Numerical Analysis. Jan. 2021. DOI: `10.1016/bs.hna.2020.10.004`. URL: `https://hal.archives-ouvertes.fr/hal-02496063`.

[3] J. F. Almagro Bello et al. "The Differentiability of the Drag with Respect to the Variations of a Lipschitz Domain in a Navier–Stokes Flow". In: *Siam Journal on Control and Optimization* 35 (1997), pp. 626–640.

[4] T. Aubin. *Some Nonlinear Problems in Riemannian Geometry.* Springer Monographs in Mathematics. Springer Berlin Heidelberg, 1998. ISBN: 9783540607526. URL: `https://books.google.it/books?id=l2nEoSxpHfoC`.

[5] D. Azagra, E. Le Gruyer, and C. Mudarra. "Kirszbraun's Theorem via an Explicit Formula". In: *Canadian Mathematical Bulletin* 64.1 (2021), 142–153. DOI: `10.4153/S0008439520000314`.

[6] R. E. Bank and T. Dupont. "An Optimal Order Process for Solving Finite Element Equations". In: *Mathematics of Computation* 36.153 (1981), pp. 35–51. ISSN: 00255718, 10886842. URL: `http://www.jstor.org/stable/2007724` (visited on 09/09/2022).

[7] R. E. Bank and H. Yserentant. "On the H1-stability of the L2-projection onto finite element spaces". In: *Numerische Mathematik* 126.2 (2014), pp. 361–381. ISSN: 0945-3245. DOI: `10.1007/s00211-013-0562-4`. URL: `https://doi.org/10.1007/s00211-013-0562-4`.

[8] Y. Bazilevs and T.J.R. Hughes. "Weak imposition of Dirichlet boundary conditions in fluid mechanics". In: *Computers and Fluids* 36.1 (2007). Challenges and Advances in Flow Simulation and Modeling, pp. 12–26. ISSN: 0045-7930. DOI: `https://doi.org/10.1016/j.compfluid.2005.07.012`. URL: `https://www.sciencedirect.com/science/article/pii/S0045793005001258`.

[9] P. Benner and J. Heiland. "Time-dependent Dirichlet Conditions in Finite Element Discretizations". In: *ScienceOpen Research* (Oct. 2015). DOI: `10.14293/S2199-1006.1.SOR-MATH.AV2JW3.v1`.

[10] C. Bernardi. "Optimal Finite-Element Interpolation on Curved Domains". In: *SIAM Journal on Numerical Analysis* 26.5 (1989), pp. 1212–1240. DOI: `10.1137/0726068`. eprint: `https://doi.org/10.1137/0726068`. URL: `https://doi.org/10.1137/0726068`.

[11] J. H. Bramble and J. T. King. "A Robust Finite Element Method for Nonhomogeneous Dirichlet Problems in Domains with Curved Boundaries". In: *Mathematics of Computation* 63.207 (1994), pp. 1–17. ISSN: 00255718, 10886842. URL: `http://www.jstor.org/stable/2153559` (visited on 10/06/2022).

[12] C. Brandenburg et al. "A Continuous Adjoint Approach to Shape Optimization for Navier Stokes Flow". In: *Optimal Control of Coupled Systems of Partial Differential Equations.* Basel: Birkhäuser Basel, 2009, pp. 35–56.

[13] S. Brenner and L.R. Scott. *The Mathematical Theory of Finite Element Methods.* Texts in Applied Mathematics. Springer New York, 2002. ISBN: 9780387954516. URL: `https://books.google.it/books?id=YhPJf\_4pu8kC`.

[14] R. Brügger, H. Harbrecht, and J. Tausch. "On the Numerical Solution of a Time-Dependent Shape Optimization Problem for the Heat Equation". In: *SIAM Journal on Control and Optimization* 59.2 (2021), pp. 931–953. DOI: `10.1137/19M1268628`. eprint: `https://doi.org/10.1137/19M1268628`. URL: `https://doi.org/10.1137/19M1268628`.

[15] V.I. Burenkov. *Sobolev Spaces on Domains.* Rechtswissenschaftliche Veroffentlichungen. Vieweg+Teubner Verlag, 1998. ISBN: 9783815420683. URL: `https://books.google.it/books?id=vr0ie4uxh3YC`.

[16] J. Cea. "Conception optimale ou identification de formes, calcul rapide de la dérivée directionnelle de la fonction coût". fr. In: *ESAIM: Mathematical Modelling and Numerical Analysis - Modélisation Mathématique et Analyse Numérique* 20.3 (1986), pp. 371–402. URL: `http://www.numdam.org/item/M2AN_1986__20_3_371_0/`.

[17] R. Chapko, R. Kress, and J.-R. Yoon. "An inverse boundary value problem for the heat equation: the Neumann condition". In: *Inverse Problems* 15.4 (1999), pp. 1033–1046. DOI: `10.1088/0266-5611/15/4/313`. URL: `https://doi.org/10.1088/0266-5611/15/4/313`.

[18] R. Chapko, R. Kress, and J.-R. Yoon. "On the numerical solution of an inverse boundary value problem for the heat equation". In: *Inverse Problems* 14.4 (1998), pp. 853–867. DOI: `10.1088/0266-5611/14/4/006`. URL: `https://doi.org/10.1088/0266-5611/14/4/006`.

[19] Y. Chiba and N. Saito. *Nitsche's method for a Robin boundary value problem in a smooth domain.* 2019. DOI: `10.48550/ARXIV.1905.01605`. URL: `https://arxiv.org/abs/1905.01605`.

[20] F. Chouly. "A review on some discrete variational techniques for the approximation of essential boundary conditions". In: (Aug. 2022).

[21] Cruz-Uribe D. and Neugebauer C. J. "An Elementary Proof of Error Estimates for the Trapezoidal Rule". In: *Mathematics Magazine* 76.4 (2003), pp. 303–306. URL: `http://www.jstor.org/stable/3219088`.

[22] K. Deckelnick, P. J. Herbert, and M. Hinze. "A novel W 1,infty approach to shape optimisation with Lipschitz domains". In: *ESAIM: Control, Optimisation and Calculus of Variations* 28 (2022), p. 2. DOI: `10.1051/cocv/2021108`. URL: `https://doi.org/10.1051%2Fcocv%2F2021108`.

[23] J. S. Dokken, S. Mitusch, and S. Funke. "Automatic shape derivatives for transient PDEs in FEniCS and Firedrake". In: (Jan. 2020).

[24] W. Dörfler and M. Rumpf. "An Adaptive Strategy for Elliptic Problems Including a Posteriori Controlled Boundary Approximation". In: *Mathematics of Computation* 67.224 (1998), pp. 1361–1382. ISSN: 00255718, 10886842. URL: http://www.jstor.org/stable/2584853 (visited on 08/23/2022).

[25] D. Edelmann. "Isoparametric finite element analysis of a generalized Robin boundary value problem on curved domains". en. In: *The SMAI journal of computational mathematics* 7 (2021), pp. 57–73. DOI: 10.5802/smai-jcm.71. URL: https://smai-jcm.centre-mersenne.org/articles/10.5802/smai-jcm.71/.

[26] C. M. Elliott and T. Ranner. "A unified theory for continuous-in-time evolving finite element space approximations to partial differential equations in evolving domains". In: *IMA Journal of Numerical Analysis* 41.3 (Nov. 2020), pp. 1696–1845. ISSN: 0272-4979. DOI: 10.1093/imanum/draa062. eprint: https://academic.oup.com/imajna/article-pdf/41/3/1696/38983520/draa062.pdf. URL: https://doi.org/10.1093/imanum/draa062.

[27] Charles M. Elliott and Thomas Ranner. "Finite element analysis for a coupled bulk–surface partial differential equation". In: *IMA Journal of Numerical Analysis* 33.2 (2013), pp. 377–402. DOI: 10.1093/imanum/drs022.

[28] K. Eppler and H. Harbrecht. "A regularized Newton method in electrical impedance tomography using shape Hessian information". eng. In: *Control and Cybernetics* 34.1 (2005), pp. 203–225. URL: http://eudml.org/doc/209343.

[29] L.C. Evans. *Partial Differential Equations*. Graduate studies in mathematics. American Mathematical Society, 2010. ISBN: 9780821849743. URL: https://books.google.it/books?id=Xnu0o_EJrCQC.

[30] T. Flaig. *Discretization strategies for optimal control problems with parabolic partial differential equations*. Jan. 2013. ISBN: 9783843911023.

[31] T. M. Flett. "Mean value theorems for vector-valued functions". In: *Tohoku Mathematical Journal, Second Series* 24.2 (1972), pp. 141–151.

[32] S. Funke and P. Farrell. "A framework for automated PDE-constrained optimisation". In: (Feb. 2013).

[33] C. Geuzaine and J.-F. Remacle. "Gmsh: A 3-D finite element mesh generator with built-in pre- and post-processing facilities". In: *International Journal for Numerical Methods in Engineering* 79.11 (2009), pp. 1309–1331. DOI: https://doi.org/10.1002/nme.2579. eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/nme.2579. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/nme.2579.

[34] G. Gilardi. *Analisi matematica di base*. Collana di istruzione scientifica. McGraw-Hill Companies, 2011. ISBN: 9788838666599. URL: https://books.google.it/books?id=H-0nuQAACAAJ.

[35] G. Gilardi. "Equazioni paraboliche astratte: impostazione variazionale".

[36] P. Grisvard. *Elliptic Problems in Nonsmooth Domains*. Classics in Applied Mathematics. Society for Industrial and Applied Mathematics, 2011. ISBN: 9781611972023. URL: https://books.google.it/books?id=lJTtujsZSgkC.

[37] V. Guillemin and A. Pollack. *Differential Topology*. AMS Chelsea Publishing. AMS Chelsea Pub., 2010. ISBN: 9780821851937. URL: https://books.google.it/books?id=FdRhAQAAQBAJ.

[38] H. Harbrecht and J. Tausch. "On the Numerical Solution of a Shape Optimization Problem for the Heat Equation". In: *SIAM Journal on Scientific Computing* 35.1 (2013), A104–A121. DOI: 10.1137/110855703. eprint: https://doi.org/10.1137/110855703. URL: https://doi.org/10.1137/110855703.

[39] M. Hinze et al. *Optimization with PDE Constraints*. Mathematical Modelling: Theory and Applications. Springer Netherlands, 2008. ISBN: 9781402088391. URL: https://books.google.it/books?id=PFbqxa2uDS8C.

[40] R. Hiptmair, A. Paganini, and S. Sargheini. "Comparison of approximate shape gradients". In: *BIT Numerical Mathematics* 55.2 (2015), pp. 459–485. ISSN: 1572-9125. DOI: 10.1007/s10543-014-0515-z. URL: https://doi.org/10.1007/s10543-014-0515-z.

[41] L. S. Hou and W. Zhu. "Error Estimates Under Minimal Regularity for Single Step Finite Element Approximations of Parabolic Partial Differential Equations". In: *International Journal of Numerical Analysis and Modeling* 3.4 (2006), pp. 504–524. ISSN: 2617-8710. DOI: https://doi.org/. URL: http://global-sci.org/intro/article_detail/ijnam/915.html.

[42] A. Kirsch. *An Introduction to the Mathematical Theory of Inverse Problems*. Applied Mathematical Sciences. Springer New York, 2013. ISBN: 9781461428510. URL: https://books.google.it/books?id=IWhSmwEACAAJ.

[43] B. Kovács. "High-order evolving surface finite element method for parabolic problems on evolving surfaces". In: *IMA Journal of Numerical Analysis* 38.1 (Mar. 2017), pp. 430–459. ISSN: 0272-4979. DOI: 10.1093/imanum/drx013. eprint: https://academic.oup.com/imajna/article-pdf/38/1/430/23651609/drx013.pdf. URL: https://doi.org/10.1093/imanum/drx013.

[44] M. Kreuter. "Sobolev Spaces of Vector-Valued Functions". MA thesis. Ulm University, 2015.

[45] G. Leoni. *A First Course in Sobolev Spaces*. Graduate studies in mathematics. American Mathematical Society, 2017. ISBN: 9781470429218. URL: https://books.google.it/books?id=qoA8DwAAQBAJ.

[46] F. Lindemann. "Theoretical and Numerical Aspects of Shape Optimization with Navier-Stokes Flows". PhD thesis. 2012.

[47] J.L. Lions, P. Kenneth, and E. Magenes. *Non-Homogeneous Boundary Value Problems and Applications: Volume II*. Grundlehren der mathematischen Wissenschaften. Springer Berlin Heidelberg, 2012. ISBN: 9783642652172. URL: https://books.google.it/books?id=xD71CAAAQBAJ.

[48] J. Liu and Z. Wang. "Non-commutative discretize-then-optimize algorithms for elliptic PDE-constrained optimal control problems". In: *Journal of Computational and Applied Mathematics* 362 (2019), pp. 596–613. ISSN: 0377-0427. DOI: https://doi.org/10.1016/j.cam.2018.07.028. URL: https://www.sciencedirect.com/science/article/pii/S0377042718304485.

[49] J. Hake A. Johansson B. Kehlet A. Logg C. Richardson J. Ring M. E. Rognes M. S. Alnaes J. Blechta and G. N. Wells. "The FEniCS Project Version 1.5". In: *Archive of Numerical Software* 3 (2015). DOI: 10.11588/ans.2015.100.20553.

[50] W. McLean and W.C.H. McLean. *Strongly Elliptic Systems and Boundary Integral Equations*. Cambridge University Press, 2000. ISBN: 9780521663755. URL: `https://books.google.it/books?id=RILqjEeMfKOC`.

[51] D. Meidner and B. Vexler. "A Priori Error Estimates for Space-Time Finite Element Discretization of Parabolic Optimal Control Problems Part I: Problems Without Control Constraints". In: *SIAM Journal on Control and Optimization* 47.3 (2008), pp. 1150–1177. DOI: `10.1137/070694016`. URL: `https://doi.org/10.1137/070694016`.

[52] S. Mitusch, S. Funke, and J. S. Dokken. "dolfin-adjoint 2018.1: automated adjoints for FEniCS and Firedrake". In: *Journal of Open Source Software* 4 (June 2019), p. 1292. DOI: `10.21105/joss.01292`.

[53] J.R. Munkres and Karreman Mathematics Research Collection. *Topology; a First Course*. Prentice-Hall, 1974. ISBN: 9780139254956. URL: `https://books.google.it/books?id=LtEPAQAAMAAJ`.

[54] D. O'Regan. *Existence Theory for Nonlinear Ordinary Differential Equations*. Mathematics and Its Applications. Springer Netherlands, 2013. ISBN: 9789401715171. URL: `https://books.google.it/books?id=ijjpCAAAQBAJ`.

[55] A. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations*. Springer Series in Computational Mathematics. Springer Berlin Heidelberg, 2009. ISBN: 9783540852681. URL: `https://books.google.it/books?id=nfdDAAAAQBAJ`.

[56] T. Schwedes et al. "Mesh dependence in PDE-constrained optimisation". In: July 2017, pp. 53–78. ISBN: 978-3-319-59482-8. DOI: `10.1007/978-3-319-59483-5_2`.

[57] J. Simon. *Sur le contrôle par un domaine géométrique*. Jan. 1976.

[58] G. Strang and G.J. Fix. *An Analysis of the Finite Element Method*. Prentice-Hall Series in Electronic Technology. Prentice-Hall, 1973. ISBN: 9780130329462. URL: `https://books.google.it/books?id=VZRRAAAAMAAJ`.

[59] K. Sturm and A. Laurain. "Distributed shape derivative via averaged adjoint method and applications". In: *ESAIM Mathematical Modelling and Numerical Analysis* 50 (Sept. 2015). DOI: `10.1051/m2an/2015075`.

[60] V. Thomee. *Galerkin Finite Element Methods for Parabolic Problems*. Springer Series in Computational Mathematics. Springer Berlin Heidelberg, 2013. ISBN: 9783662033593. URL: `https://books.google.it/books?id=nfHrCAAAQBAJ`.

[61] T. Tiihonen. "Shape Calculus And Finite Element Method In Smooth Domains". In: *Mathematics of Computation* 70 (Dec. 1997). DOI: `10.1090/S0025-5718-00-01323-5`.

[62] F. Tröltzsch and J. Sprekels. *Optimal Control of Partial Differential Equations: Theory, Methods, and Applications*. Graduate studies in mathematics. American Mathematical Society, 2010. ISBN: 9780821849040. URL: `https://books.google.it/books?id=O4yDAwAAQBAJ`.

[63] N. Weaver. *Lipschitz Algebras*. World Scientific, 1999. ISBN: 9789810238735. URL: `https://books.google.it/books?id=45rnwyVjg\_QC`.

[64] H. Whitney. "Functions Differentiable on the Boundaries of Regions". In: *Annals of Mathematics* 35.3 (1934), pp. 482–485. ISSN: 0003486X. URL: `http://www.jstor.org/stable/1968745` (visited on 09/12/2022).

[65] A. Wirgin. "The inverse crime". In: *arXiv: Mathematical Physics* (2004).

[66] J. Wloka, C.B. Thomas, and M.J. Thomas. *Partial Differential Equations*. Cambridge University Press, 1987. ISBN: 9780521277594. URL: `https://books.google.it/books?id=Eix7JA9VVyOC`.

[67] M. Zlamal. "Curved Elements in the Finite Element Method. I". In: *SIAM Journal on Numerical Analysis* 10.1 (1973), pp. 229–240. ISSN: 00361429. URL: `http://www.jstor.org/stable/2156389` (visited on 10/06/2022).