Technical University of Munich

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Finite element error in parabolic shape gradients

Master's Thesis

von

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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

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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 extend such observations in two ways: 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 semidiscrete estimates in a spatially semidiscrete setting, and fully discrete estimates when the implicit Euler method is adopted for the time discretization.

We conduct numerical tests to support these observations, and we conjecture that our conclusions should apply as well to when the more accurate Crank-Nicolson method is employed.

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.

Zusammenfassung

Im Zusammenhang mit elliptischer, PDG-gebundener Formoptimierung wurde bereits festgestellt, dass ein verteilter Ausdruck für die Formableitung genauer ist als das Gegenstück am Rand, wenn finite Elemente zur Diskretisierung der entstehenden PDGs verwendet werden.

Wir erweitern diese Beobachtungen in zweierlei Hinsicht: Erstens arbeiten wir in einem parabolischen Umfeld und zweitens berücksichtigen wir explizit die Tatsache, dass Finite-Elemente-Lösungen auf Polygonen/Polyedern leben, aber sie approximieren Funktionen, die auf glatten Gebieten definiert sind. Wir beweisen daher semidiskrete Schätzungen in einem räumlich semidiskreten Umfeld und vollständig diskrete Schätzungen, wenn die implizite Euler-Methode für die zeitliche Diskretisierung verwendet wird.

Wir führen numerische Tests durch, um diese Beobachtungen zu untermauern, und wir nehmen an, dass unsere Schlussfolgerungen auch gelten sollten, wenn die genauere Crank-Nicolson-Methode verwendet wird.

Unsere Analyse basiert auf einem modellhaften Formoptimierungsproblem für die Wärmeleitungsgleichung, bei dem das Ziel darin besteht, die Form eines Nulleinschlusses zu bestimmen, wenn die Temperatur und der Wärmestrom an einem äußeren Rand gegeben sind. Für ein solches Problem wird die Formableitung abgeleitet, ein sternförmiger Ansatz angewendet und numerische Ergebnisse werden vorgestellt und diskutiert.

Contents

1. Introduction

To obtain approximate estimates of solutions to PDE constrained shape optimization problems, a discretization of several "continuous" quantities has to be made. 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 true 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 as good of an approximation as possible to the continuous counterpart. There is actually one major design choice playing a role here, which is whether a boundary or distributed/volumetric approach is taken, when treating the shape optimization problem. There are of course advantages and disadvantages to both views (see e.g. [61]), 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 [42]. 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, but only a first order one in the boundary approach. Finite elements are employed, being a popular, widespread and general method that provides much flexibility for engineering applications.

Such conclusions are however only drawn in an elliptic setting, but parabolic shape optimization has important applications too, and deserves further analysis (see e.g. [12], [40] to mention a few). With this in mind, we try to extend the observations of [42] in two ways:

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

To this end, we borrow a model parabolic shape optimization problem from [40] and center our arguments around it. In [40], 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 converted to boundary integral equations). We take, in contrast, a distributed/volumetric approach and employ finite elements for the partial differential equations. As a by-product, we obtain a very easy implementation that is amenable to high-performance and already existing software packages, such as FEniCS ([51]) and dolfin-adjoint ([34], [24], [54]).

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 the shapes that we adopted for simplicity in the implementation
- chapter 3 is then about the finite element discretization of the problem 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. The analysis is satisfactory when the implicit Euler method is adopted in time, where we can even show that optimization and discretization commute. However, we only give some theoretical hints to some conjectures we made for the case where the Crank-Nicolson method is adopted
- in chapter 4 we discuss our implementation and conduct two sets of experiments are included: on one hand we illustrate results for the overall shape optimization algorithm for our model problem, and on the other hand we provide numerical evidence for the error estimates of chapter 2
- chapter 5 contains a brief summary of the thesis and lists some future research directions

For exposition purposes, we delegated many technicalities to appendices:

- some useful results from functional analysis are collected in appendix A
- all the details about parabolic equations that appear in the thesis can be found in appendix B
- several facts about domains deformations are to be 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 for our computer implementation
- in section 2.4 we further justify our implementation, that is discussed in section 4.1, with respect to the scalar product in which shape 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 $I = (0, T)$, $\Sigma_f = I \times \Gamma_f$, $\Sigma_m = I \times \Gamma_m$.

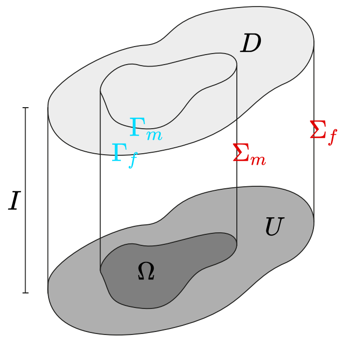

Figure 2.1.: Space-time cylinder with labels

Let us interpret D as a certain uniform and isotropic body, inside which a solid/liquid inclusion of zero temperature Ω is present. The temperature u inside $D \setminus \Omega = U$ evolves over time according to the heat equation, at least approximately. What one might do, is to access the outer boundary ∂D and measure its surface temperature and heat flux, and wonder about the actual shape of the inaccessible inclusion Ω. We ask ourselves how to reconstruct such information from the knowledge of the boundary data only. This is a non-linear and ill-posed inverse problem (according to e.g. [40]).

Our problem is therefore, given the outer temperature and outer heat flux, how to reconstruct the shape of Ω that induced, through heat diffusion, those boundary quantities.

In a more mathematical language, let us consider a heat equation on $U \times I$, with zero initial condition and no volumetric forcing term. On Σ_f are prescribed smooth enough Dirichlet and Neumann data, simultaneously, call them f and g, whereas on Σ_m, homogeneous Dirichlet conditions are imposed.

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:

$$\begin{cases} v_t - \Delta v = 0 & \text{on } U \times I \\ v(0) = 0 & \\ v = f & \text{on } \Sigma_f \\ v = 0 & \text{on } \Sigma_m \end{cases}, \quad \begin{cases} w_t - \Delta w = 0 & \text{on } U \times I \\ w(0) = 0 & \\ \partial_\nu w = g & \text{on } \Sigma_f \\ w = 0 & \text{on } \Sigma_m \end{cases}$$

This overdetermined partial differential equation for u need not to have a solution. It can be however shown that, for given f, g, there exists at most one Ω such that problem 2.1.1 is solvable (see [18], [17]).

Our aim is to find a numerical approximation for such domain. We are therefore trying to solve a shape identification problem. 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 tackle it is therefore, given data f, g, a guess Ω of the sought domain, to simulate v, w, measure their discrepancy $\|v - w\|$ and use this knowledge to improve the iterate Ω.

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 [40] using a different approach than ours, 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.

As already mentioned, some uniqueness results are already available. We are not concerned with the problem of existence of Ω, likewise this aspect is not addressed in the aforementioned work [40]. Some advances in this direction are done 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.

Definition 2.2.2 (Admissible transformations)
Given D, we consider the set $\mathcal{T}$ of bi-Lipschitz homeomorpshisms of $\mathbb{R}^n$ that fix D^c, endowed the perturbation space Θ, i.e. Lipschitz deformation fields null on D^c. See also definition C.1.3.
We will consider transformations of U 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 existence of $C(U_r)$ is guaranteed by theorem C.1.6. This is to ensure that $\tau(U_r) \subset\subset D$ is also bounded Lipschitz.

We remark that there exists a unique Lipschitz continuous representive 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 recast problem 2.1.2 in a new form, akin to shape optimization. To do so, we must at first analyze the well posedness of the equations for v, w of problem 2.1.1. This is done in detail in the appendix for the sake of presentation. What we remark is that such well-posedness holds, and that, given any extension $\bar{u}$ to f onto $U \times I$, then $v = v_0 + \bar{u}$, where v_0 solves the heat equation with homogeneous Dirichlet boundary conditions, but a non trivial source term. We write $v^\tau = v_0^\tau + \bar{u}$, and v_0^τ, w_τ to emphasize the dependence on τ, and refer to problem C.4.3 and problem B.2.1.12 for additional details. The adequate conditions for well-posedness are assumption B.2.1.1, assumption B.2.2.1.

Problem 2.2.3 (Shape optimization problem)
Suppose that assumption 2.2.1, assumption B.2.1.1, assumption B.2.2.1 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 a space defined on the moving domain, $H = L^2, \mathtt{V} = H^1_0, \mathtt{W} = H^1_{0,m} = \{v \in H^1, v(\Gamma_m) = 0\}$ (see also appendix B.2.1 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 (Well-posedness of J).
We know from theorem B.2.1.11 that $v_0^\tau + \bar{u}$ doesn't depend on the particular choice of $\bar{u}$, therefore, for different τ yielding the same domain U, $J(\tau)$ doesn't change.

Observation 2.2.5 (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 [40], the heat equations for the adjoint states (see proposition 2.2.11) 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. We are hence interested in finding the form $J'(\tau) \in \Theta^*$ such that, for all $\delta\theta_k \to 0$ in Θ, we have:

$$\lim_k \frac{|J(\tau+\delta\theta_k) - J(\tau) - J'(\tau)(\delta\theta_k)|}{\|\delta\theta_k\|_\Theta}$$

We have set $\|\theta\|_\Theta = \|\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} = \|\theta\|_{W^{1,\infty}(D;\mathbb{R}^n)}$.

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, yields an element $\tau + \delta\theta \in \mathcal{T}_a$: it will be this the way in which an initial guess for the sought domain $\Omega = \tau(\Omega_r)$ will be refined, i.e. by iteratively adding to τ, small perturbations $\delta\theta$. We remark that for k large enough, $\tau + \delta\theta_k \in \mathcal{T}_a$.

Observation 2.2.6.
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. We will see a more transparent way of obtaining $\tau(U_r) \subset\subset D$ Lipschitz, in section 2.3.
Note, we need τ to have a Lipschitz inverse to conclude $\tau(U_r) \subset\subset D$: for $x \in D$, we have $0 < \delta = \inf_{d\in\partial D} |x-d| \leq \|\tau^{-1}\|_{W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n)} \inf_{d\in\partial D} |\tau(x) - d|$.

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:

$$\lim_k \frac{|J((\mathrm{Id} + \delta\theta_k \circ \tau^{-1}) \circ \tau) - J(\tau) - J'(\tau)[\delta\theta_k]|}{\|\delta\theta_k\|_\Theta}$$

This amounts to setting the reference domain to $\tau(U_r)$ instead of U_r and perturbing the former, at least for the sake of computing derivatives.

We now introduce a Lagrangian functional, so as to derive the gradient expression of J. There are several ways to compute the so called "shape gradient" dJ, in the literature. We will adopt that contained in [61], but a valid alternative, at least formally, is the method of Cea, see [16]. The former requires the PDEs of $v = v^\tau$, $w = w^\tau$ to be reformulated on a non-moving domain, the reference domain U_r. We can perform such operation by considering the variational formulations of v^τ and w^τ and then applying a change of variables to the appearing integrals. This is precisely the content of 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:

$$\begin{aligned} L_\tau(k, w, v_0, q, p) = \\ \frac{1}{2}\int_I \int_{\tau(U_r)} |v_0 + \bar{u}\circ\tau_k - w|^2 |\det(D\tau_k)| + \\ \int_I (w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla w, \nabla q)_{H_\tau} - \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)} + \\ \int_I (v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla v_0, \nabla p)_{H_\tau} + \int_I ((\bar{u}\circ\tau_k)', p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla(\bar{u}\circ\tau_k), \nabla p)_{H_\tau} \end{aligned}$$

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 means 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, the variational formulation of v_0^τ and that of w^τ, all 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 problem B.2.1.12) of the Dirichlet datum f, on the moving domain $\tau_k(\tau(U_r))$. Because of this, let's fix $\bar{u}_\tau$ with this property on $\tau(U_r)$. We show that $\bar{u} := \bar{u}_\tau \circ \tau_k^{-1}$ satisfies the conditions stated in problem B.2.1.12.

In particular:

- composition with τ preserves the smoothness of the extension, as seen in corollary A.2.2, given that $\circ\tau_k^{-1}$ is a linear bounded operator between $\mathtt{W}_\tau$ and $\mathtt{W}_{\tau_k\circ\tau}$ (see theorem C.2.1)
- the initial value is preserved, as seen in the proof of proposition C.3.1
- the trace on Σ_f is preserved, because the trace on $\Gamma_f = \partial D$ is preserved, see theorem C.2.1

Therefore we can state the following definition.

Definition 2.2.7 (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:

$$
\begin{aligned}
L_\tau(k, w, v_0, q, p) = \\
\frac{1}{2}\int_I \int_{\tau(U_r)} |v_0 + \bar{u}_\tau - w|^2 |\det(D\tau_k)| + \\
\int_I (w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla w, \nabla q)_{H_\tau} - \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)} + \\
\int_I (v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla v_0, \nabla p)_{H_\tau} + \int_I (\bar{u}'_\tau, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla \bar{u}_\tau, \nabla p)_{H_\tau}
\end{aligned}
$$

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 $u = (w, v_0)$, $\pi = (q, p)$, $G(k, u, \pi) = L_\tau(k, w, v_0, q, p)$ 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 rest of this section is devoted to applying the averaged adjoint method [61] to our problem, so as to identify the shape gradient. To this end we will have to understand which properties the Lagrangian L_τ enjoys.

Proposition 2.2.8 (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 $\displaystyle\int_0^1 d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]ds = 0$ 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 2.2.9 (Averaged adjoint equations)

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

Proof.
We give some comments on the non trivial points.
Proof of 3
We get back the state equations, thanks to linearity, and by testing separately with $\delta\psi = (\delta q, 0)$ and $\delta\psi = (0, \delta p)$, so that a unique solution exists by theorem C.4.2.
Proof of 7
Is is easily seen that:

$$
\begin{aligned}
\int_0^1 d_\phi G(k, su^k + (1-s)u^0, \psi)[\delta\phi]ds = \\
\int_I (((v_0^k + \bar{u}_\tau - w^k) + (v_0^0 + \bar{u}_\tau - w^0))/2|\det(D\tau_k)|, \delta v_0 - \delta w)_{H_\tau} + \\
\int_I (\delta w_t, q|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla \delta w, \nabla q)_{H_\tau} + \\
\int_I (\delta v_{0t}, p|\det(D\tau_k)|)_{H_\tau} + (A_{\tau_k}\nabla \delta v_0, \nabla p)_{H_\tau}
\end{aligned}
$$

As in proposition C.3.1, $\delta w_t = (\delta w \circ \tau_k^{-1})_t \circ \tau_k$, where $\delta w \circ \tau_k^{-1} \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau})$ 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:

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

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

Here, as we saw in proposition C.3.1, we have $\delta w \circ \tau_k^{-1}, w \circ \tau_k^{-1} \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau})$, $\delta v_0 \circ \tau_k^{-1}, v_0 \circ \tau_k^{-1} \in Q_0(I, \mathtt{V}_{\tau_k \circ \tau})$, $q \circ \tau_k^{-1} \in Q^0(I, \mathtt{W}_{\tau_k \circ \tau})$ and $p \circ \tau_k^{-1} \in Q^0(I, \mathtt{V}_{\tau_k \circ \tau})$.
Because $\circ \tau_k^{-1}$ is a bijection of $Q_0(I, \mathtt{V}_{\tau_k \circ \tau})$ and $Q_0(I, \mathtt{V}_{\tau_k})$ as we saw in proposition C.3.1 (and analogously for $\mathtt{W}$), 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:

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

for all $\delta W \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau})$, $\delta V_0 \in Q_0(I, \mathtt{V}_{\tau_k \circ \tau})$.
We wish to find a (unique) solution $(q^k, p^k) \in Q^0(I, \mathtt{W}_\tau) \times Q^0(I, \mathtt{V}_\tau)$ of this problem. We can equivalently (by proposition C.3.1) find $(Q^k, P^k) \in Q^0(I, \mathtt{W}_{\tau_k \circ \tau}) \times Q^0(I, \mathtt{V}_{\tau_k \circ \tau})$ 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 $\delta W, \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau})$, $\delta V_0 \in Q_0(I, \mathtt{V}_{\tau_k \circ \tau})$.
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.2.1.12, problem B.2.2.2) of the PDEs:

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

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 proposition B.3.5).
By calling then $\pi^k = (Q^k \circ \tau^k, P^k \circ \tau^k)$ we conclude the proof. □

We now turn to the verification of Gateaux differentiability of J, applying the techniques proposed in [61].

Proposition 2.2.10 (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, [61].

□

Proposition 2.2.11 (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:

$$\begin{aligned} J'(\tau)[\delta\theta] = \\ \int_I (w_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), q^\tau)_{L^2(\tau(U_r))} + \int_I (A'(\delta\theta \circ \tau^{-1}) \nabla v^\tau, \nabla p^\tau)_{L^2(\tau(U_r))} + \\ \int_I (v_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), p^\tau)_{L^2(\tau(U_r))} + \int_I (A'(\delta\theta \circ \tau^{-1}) \nabla w^\tau, \nabla q^\tau)_{L^2(\tau(U_r))} + \\ \frac{1}{2} \int_I \int_{\tau(U_r)} |v^\tau - w^\tau|^2 \operatorname{div}(\delta\theta \circ \tau^{-1}) \end{aligned}$$

where p^τ, q^τ solve:

$$\begin{cases} -q_t^\tau - \Delta q^\tau = v^\tau - w^\tau \\ q^\tau(T) = 0 \\ \partial_\nu q^\tau = 0 \text{ on } \Sigma_f \\ q^\tau = 0 \text{ on } \Sigma_m \end{cases}, \qquad \begin{cases} -p_t^\tau - \Delta p^\tau = -v^\tau + w^\tau \\ p^\tau(T) = 0 \\ p^\tau = 0 \text{ on } \Sigma_f \\ p^\tau = 0 \text{ on } \Sigma_m \end{cases}$$

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 $\delta\theta$:

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

where in the last step we applied point i) of lemme 2.2, [59].
Conclusion
Assume at first that $p^k \rightharpoonup p^0$ in $Q(I, \mathtt{V}_\tau)$ and $q^k \rightharpoonup q^0$ in $Q(I, \mathtt{W}_\tau)$, something which will be later verified.
Now, using that $u^0 = (w^\tau, v_0^\tau)$, and cancelling the boundary integral:

$$\begin{aligned} G(k, u^0, \pi^k) - G(0, u^0, \pi^k) = \\ \frac{1}{2} \int_I \int_{\tau(U_r)} |v^\tau - w^\tau|^2 (|\det(D\tau_k)| - 1) + \\ \int_I (w_t^\tau (|\det(D\tau_k)| - 1), q^k)_{H_\tau} + ((A_{\tau_k} - I) \nabla w^\tau, \nabla q^k)_{H_\tau} + \\ \int_I (v_t^\tau (|\det(D\tau_k)| - 1), p^k)_{H_\tau} + ((A_{\tau_k} - I) \nabla v^\tau, \nabla p^k)_{H_\tau} \end{aligned}$$

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 by point i) of lemme 2.2, [59]. Note, we needed here $\tau \in \mathcal{T}^1$.
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 [48]. 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:

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

where $o_1^k \in L^\infty(\mathbb{R}^n; \mathbb{R})$ and $o_k^2 \in L^\infty(\mathbb{R}^n; \mathbb{R}^{n \times n})$ being 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:

$$\begin{aligned} a_k := \\ \frac{1}{2} \int_I \int_{\tau(U_r)} |v^\tau - w^\tau|^2 \operatorname{div}(\delta\theta \circ \tau^{-1}) + \\ \int_I (w_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), q^k)_{H_\tau} + (A'(\delta\theta \circ \tau^{-1}) \nabla w^\tau, \nabla q^k)_{H_\tau} + \int_I (v_t^\tau \operatorname{div}(\delta\theta \circ \tau^{-1}), p^k)_{H_\tau} + (A'(\delta\theta \circ \tau^{-1}) \nabla v^\tau, \nabla p^k)_{H_\tau} \end{aligned}$$

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 othe properties of o_k^1, o_k^2.

<u>Weak convergence of states</u>

We assumed $p^k \rightharpoonup p^0$ in $Q(I, \mathtt{V}_\tau)$ and $q^k \rightharpoonup q^0$ in $Q(I, \mathtt{W}_\tau)$. We now prove these claims. We show at first $v_0^k \rightharpoonup v_0^0$ in $Q(I, \mathtt{V}_\tau)$ and $w^k \rightharpoonup w^0$ in $Q(I, \mathtt{W}_\tau)$. We do this by uniformly estimating these quantities on k. To do this, 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.2.1.11, theorem B.2.2.10, to obtain the stability estimates:

$$\begin{aligned}
\left\|V^k\right\|^2_{C([0;T],H_{\tau_k\circ\tau})} + \left\|V^k\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} + \left\|\nabla V^k\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} + \left\|(V^k)_t\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} &\le C\left\|U^k\right\|^2_{H^1(I,\mathtt{W}_{\tau_k\circ\tau})} \\
\left\|W^k\right\|^2_{C([0;T],H_{\tau_k\circ\tau})} + \left\|W^k\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} + \left\|\nabla W^k\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} + \left\|W_t^k\right\|^2_{L^2(I,H_{\tau_k\circ\tau})} &\le C\left\|g\right\|^2_{H^1(I,L^2(\Gamma_f))}
\end{aligned}$$

where C is independent of k.

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

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

and a similar estimate we have for the first derivative.

This bound is uniform on k because of the continuity of the bound, with respect to k, as seen in 4.12, page IV.6, [59].

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

Now, for almost all times, using 4.11, page IV.6 of [59], we obtain that, for instance:

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

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 becase 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 $(v_{0t}^?, p)_{L^2(I,H_\tau)}$, see proposition B.3.3 for details on why we can write the time derivative of the limit. 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 4.12, page IV.6 of [59]. 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 $v^? = v^0$.

<u>Weak convergence of averages adjoint states</u>

So, $v_0^k \rightharpoonup v_0^0, w^k \rightharpoonup w^0$ in the sense of the $Q(I, \mathtt{V}_\tau)$ and $Q(I, \mathtt{W}_\tau)$ weak convergence. We now claim that $p^k \rightharpoonup p^0, q^k \rightharpoonup q^0$, in a similar style as 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 $\dfrac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1}$ 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 4.12 of [59] at page IV.6, it suffices to have an $L^2(I,H)$ bound on $\dfrac{v_0^k+w^k+v_0^0+w^0}{2}\circ\tau_k^{-1}\circ\tau_k = \dfrac{v_0^k+w^k+v_0^0+w^0}{2}$ 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:

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

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

Observation 2.2.12 (Fréchet differentiability).
A promising track to show Fréchet differentiability is to start from the Gateaux differentiability of proposition 2.2.11, after showing continuity of $\tau \mapsto dJ(\tau)$. Stronger smoothness assumptions on the transformations τ must however be made. Yet another way would be to apply implicit function theorems.

2.3. Star-shaped reparametrization

Here we reparametrize the problem assuming the domains $D, \Omega = \tau(\Omega_r)$ to be star-shaped with respect to the origin. We do this to justify the computer implementation of the solution algorithm. In particular, we define and analyze certain maps that convert functions on a sphere to radial deformation fields (see below for details), and based on those, detail the expression of the shape gradient of proposition 2.2.11. This is the result of proposition 2.3.6.

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], a fact that was not discussed in [23]. Note that the definition of Lipschitz domain of [15] is completely equivalent to that of [3] (and at least implies that of [52], [38], [47], [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 [55]. □

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 is taken to be $\Omega_{f_D} \setminus \overline{B}_\epsilon$, 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. $A_f(D \setminus \overline{B_\epsilon}) = D \setminus \overline{\Omega_f}$, $A_f(\partial D) = \mathrm{Id}$, $A_f(\epsilon\mathbb{S}^{n-1}) = \partial\Omega_f$
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 $\overline{D} \setminus \Omega_f \to \overline{D} \setminus B_\epsilon$

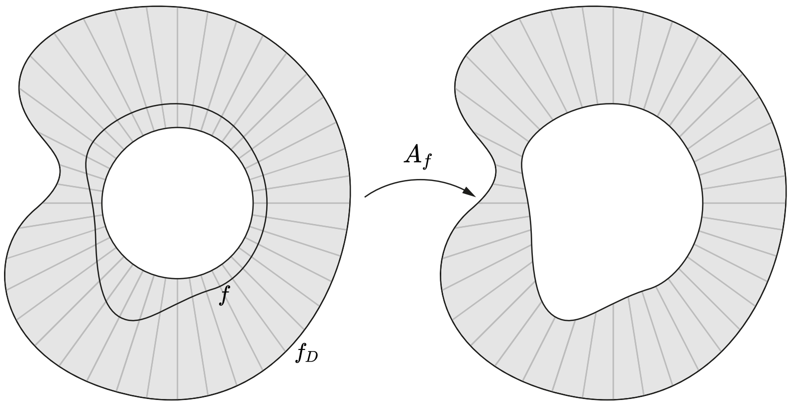

Figure 2.2.: Illustration of the action of A_f

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 $\overline{\Omega_{f_D}} \setminus \Omega_f = \{f(\hat{x}) \leq |x| \leq f_D(\hat{x})\}$ □

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 [23] in a weaker for, 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 [23]) 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 sums 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 $f_D(\hat{x}) - \epsilon$. Is is a bounded Lipschitz function that is uniformly above δ, so that its reciprocal is also a bounded Lipschitz function.

Analogous reasonings let us prove also the Lipschitz property of A_f^{-1}. □

We now try to glue H_f, A_f together and still obtain a bi-Lipschitz function. Even the Lipschitz property need not to hold in general, see page 7 of [65] 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 Lipshitz function on $\mathbb{S}^{n-1}$ produces a Lipschitz function, which would also yield the claim for τ_f, 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 $g : A \to \mathbb{R}^n$ and $h : \overline{B_\epsilon} \to \mathbb{R}^n$ are Lipschitz and 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.

□

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 $\tau_f \in \mathcal{T}$.

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 0 on ∂D, so that we are considering the zero extension outside D of a Lipschitz function, null on ∂D. This extension is Lipschitz. □

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

We finally have a look at shape derivatives in this radial framework. The cost functional will be $j(q) := J(\tau_{\epsilon+q})$, 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 [23]. The ansatz $\tau_{q+th} = (\mathrm{Id} + tV_h \circ \tau_q^{-1}) \circ \tau_q$ brings us to $V_h = \dfrac{\tau_q + th - \tau_q}{t}$, 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 $\epsilon\mathbb{S}^{n-1}$ by h and radially damping this movement to 0 close to ∂D. We can therefore conclude:

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 $W^{1,\infty}(\mathbb{S}^{n-1}) \to \Theta$. 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 proposition 2.3.4 shows that it is sufficient to bound the Lipschitz constants of the two branches, separately.

These bounds are respectively: $C(\epsilon)(\|h\|_\infty + 2\|D_T h\|_\infty)$ and $[2\epsilon^{-1}(\|D_T h\|_\infty + \|h\|_\infty)]C(f_D,\epsilon) + C(f_D,\epsilon)\|h\|_\infty$, which concludes the proof. □

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, neglecting the ϵ factor. It has gradient (see [23]) $DH_f(x) = f(\hat{x})I + \hat{x} \otimes D_T f(\hat{x})$, and $DH_f^{-1}(y) = 1/f(\hat{y})I - 1/f(\hat{y})^2 \hat{y} \otimes D_T f(\hat{y})$. They are C^o away from the origin. In particular H_f is C^o outside of $B_\delta(0)$, $\delta < 1$. $H_f(B_\delta)$ also contains a ball around the origin, and the complement 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 right set is open by H_f being a homeomorphism of $\mathbb{R}^n$. The Lischitz regularity of the gradients follows from the Lipschitz and boundedness of every factor, and the fact that we are setting ourselves 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 [36]), 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, $z \in V' \times I, z_n = \eta_n(z) \iff z \in (V' \times I) \cap \partial\Omega$)

Conclusion

Let a radial function $f > 0$ be of class C^o. Thanks to H_f, a punctured diffeomorphism of class C^o, we 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 [38]. □

2.4. Hilbertian regularization framework

Solving the optimization problem problem 2.2.3 cannot be done at the continous level: one must apply a discretization strategy and solve an optimization problem in finite dimensions isntead. We will adopt derivative based algorithms, where we compute search directions from the knowledge of the discretized shape derivative. It is important at this stage to respect the properties of the continuos problem when developing a discretization strategy. 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 [23], where descent directions are directly searched in $W^{1,\infty}$. 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, we are doing something 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 to descent directions that are too "squiggly" (see section 4.2 for an example), or to mesh-dependence effects, where finer and finer meshes require more and more optimization iterations to converge (see [58]).

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 $h \in H^1(\mathbb{S}^{n-1})$ by:

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

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) and $r(q) \in H^1(\mathbb{S}^{n-1})$: $q - \alpha r(q)$ 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 $j'(q)$ 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 2.2.11. We identify three different terms. We write u for a state v or w, and a for the corresponding adjoint, leaving 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 $H^1(\mathbb{S}^{n-1})$.

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 account for the fact the non-discretized domain is smooth and the computational one is polygonal/polyhedral.

We are not focusing here on optimization algorithms to solve the shape identification problem, nor on the specific domain 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 is required (compatible, for instance, with the case where only finite number of measurements are realized)
- implicit Euler or Crank-Nicolson time steppings are adopted
- several optimal order error estimates are obtained

We chose such time steppings because of their simplicity, overall low regularity requirements, and the fact that they are unconditinoally stable, so that no restriction on the time step size must be made. We remark however that they still require a globally smooth solution, over time. To decrease such requirement, discontinuous Galerkin space-time methods can be adopted, see e.g. [53]. The reason for this is that certain time integrals therein are not discretized in time, whereas the classical implicit Euler/Crank-Nicolson evaluate such quantities pointwise. The implicit Euler method can be in fact seen as a space-time method, with quadrature in time. More smoothness in time is therefore required, to treat this numerical quadrature.

We can reach such smoothness for the state equations, by requiring smooth data, and certain compatibility relations among them (see e.g. chapter 2 of [49]). Smoothness of the data alone is not enough: a regular solution is obtained, but only away from the starting time, where a singularity can develop (see e.g. the discussion in [40]). The adjoint equations are however, in a certain sense, fixed by the particular cost functional we chose, and the state equation itself: unfortunately, for them, compatibility relations do not hold, in general.

In [40], they work 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 adjoint. This would be enough for a low order space-time method, but not for the chosen fully discrete schemes. To obtain more compatibility, i.e., to modify the data that enters the adjoint equations, since we cannot modify the PDE solved by the states u, v, we can only tweak the cost functional. This is what we will do, by 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 2.2.11 in our case), and some adjoint states appear. Then, one proceeds with discretizing states and adjoints, and obtains an optimality system on the discrete level, amenable to numerical solution
- 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:

$$\begin{tikzcd}
 & \text{continuous optimality system} \arrow[dr, "\text{discretization}"] & \\
\text{continuous problem} \arrow[ur, "\text{optimization}"] \arrow[dr, "\text{discretization}"'] & & \text{discrete optimality system} \\
 & \text{discrete problem} \arrow[ur, "\text{optimization}"'] &
\end{tikzcd}$$

Although not a trivial task, there are several benefits implied by realizing a commutative scheme, we refer to the introduction of [50] for a comparison between the two strategies, and a discussion of advantages and disadvantages of each. See also [32], in the context of parabolic optimal control.

We can show that optimization and discretization commute, when using the implicit Euler case. We strongly suspect that this conclusion can be extended also to Crank-Nicolson, thanks to the work of [32].

Now:

- in section 3.1, the continuous states and adjoints are discretized and the error in doing so, is quantified. We are taking an optimize-then-discretize approach, and obtain optimal order estimates, optimal with respect to the approximation properties of the finite element spaces and time stepping schemes
- in section 3.2, a discretize-then-optimize approach is adopted, just like in chapter 4. A result on the convergence of the discrete shape gradient, to the continuous one, is presented, in the case the time-stepping is done by the implicit Euler method
- in section 3.3, we only discretize in space and show that a better result than in section 3.2 is available. This is then applied to the case of implicit Euler to obtain a fully discrete result

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

3.1. Approximation of PDEs, optimize-then-discretize

Consider the state and adjoint equations as seen in problem 2.1.1 and proposition 2.2.11. Let us have a unified notation (just like in problem B.2.3.1).

Problem 3.1.1 (Unified notation for state and adjoint equations)
State equations:

$$\begin{cases} u_t - \Delta u = 0 & \text{in } U \times (0,T) \\ u = u_D & \text{on } \Gamma_D \times (0,T) \\ \partial_\nu u = u_N & \text{on } \Gamma_N \times (0,T) \\ u(0) = 0 \end{cases}$$

Adjoint equations:

$$\begin{cases} -a_t - \Delta a = \eta(v-w) & \text{in } U \times (0,T) \\ a = 0 & \text{on } \Gamma_D \times (0,T) \\ \partial_\nu a = 0 & \text{on } \Gamma_N \times (0,T) \\ a(T) = 0 \end{cases}$$

We intend that u can be v, in which case a is p, or u is w and then a is q, so that the Dirichlet and Neumann boundaries are coherent between state and adjoint equation. Note that we added a temporal weighting function η which we will later specify.

We have dropped, for simplicity, all the references to the domain transformation. Let us discuss the presence of the temporal weight η. This is a function $\eta : [0,T] \to \mathbb{R}$ which in the above problem, we wrote equal for both adjoint states. This is a slight abuse of notation, in fact, for p and q we should be writing η and $-\eta$.

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:

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

This modification is reasonable for a reasonable η and its 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 problem, and viceversa. In fact, $J_\eta(\tau) = 0 \implies \eta \left\| v_\tau - w_\tau \right\|^2_{H_\tau} = 0 \implies v_\tau = w_\tau$. This equality holds on all $I = [0,T]$ by the time continuity of the states.

Modifying the final-time behaviour of the energy might have detrimental effects if the boundary data exhibts strong variations close to final time, which is physically implausible, given the physical nature of the partial differential equation. In fact, it is known that solutions to the heat equation tend to a steady state for long times, and we are only measuring the value of one such solution on the external boundary of U: we thus expect that in practice, this boundary data will not exhibit oscillatory behaviour for large times, and that the introduction of η will not cause issues.

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. If one chose an optimize-then-discretize approach this would be satisfactory (at least with regards to the numerical approximation of states and adjoints). However we will conduct experiments in a discretize-then-optimize setting, so that the upcoming results are only partially satisfactory.

The spatial discretization is done on a polygonal approxumation of U. We explicitly account for this, see the introductory discussion in appendix D. Note, the next assumption is formulated as if U, U_h were given, i.e. they are 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), U_h is polygonal/polyhedrak and ∂U_h interpolates ∂U. The mesh family of U_h must be (shape) regular and quasi-uniform (for such definitions, see [13])

2. $u_D \in H^1(I, H^2(\Gamma_D)) \cap H^{1/\theta+1}(I, H^{3/2}(\Gamma_D))$, $u_N \in H^2(I, L^2(\Gamma_N)) \cap H^{1/\theta}(I, H^2(\Gamma_D))$

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 the mesh of U_h, and δt one of the K uniform intervals $[t^k, t^{k+1}]$, $k = 0, ..., K-1$, into which I is subdivided.

Problem 3.1.3 (Numerical discretization of problem 3.1.1)
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:

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

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

$$u_h^0 = 0$$

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. We refrain from writing it fully, since we won't be using it in the implementation. 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 remind 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 it 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.

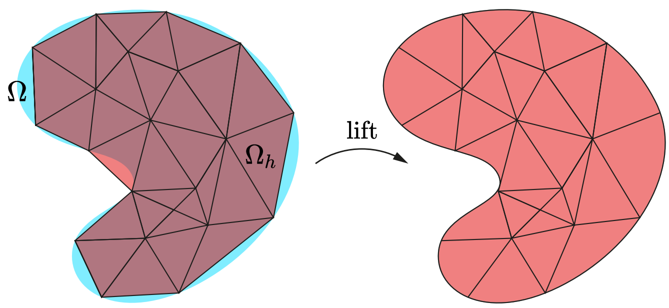

Figure 3.1.: Lifting action

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

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

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

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

and

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

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

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

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 $H^1_{0,D}(U)$ (i.e. it is 0 on the Dirichlet boundary), and $\lesssim$ means $\leq C$, with $C \geq 0$ independent of h and δt.

Note, writing $H^1_{0,D}$ is flexible because the Dirichlet boundary varies between v, w. In fact, 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 v. We do not track the dependency on the domain U.

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.2.3.2: we need to ensure that $u \in H^1(I, H^2(U))$. To do so we turn to theorem B.2.3.6, which we apply with $k = 1$. Hypothesis 1 to 3 suffice.

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" $\delta_h^k(0)$ are all 0 (see assumption D.3.1 for the notation) by hypothesis 3.

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 $\delta_h^k(0)$, $k = 0, ..., 1/\theta$, 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.2.3.6 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.2.3.2 is also easily verified.

Assumptions for spatial semidiscretization of a: to fulfill assumption D.2.6 we see by the triangle inequality that $\left\|\eta(u - u_h^l)\right\|_{L^2(U)} \lesssim C_u h^2$ 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 $\left\|u - u_h^l\right\|_{L^2(U)} \lesssim C_u h^2$ 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 also $\eta'(T) = 0$ in the case $\theta = 1/2$. We also have $u_h \in H^{1/\theta}(I, S_h^1)$ 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 $D(a)^2 \lesssim \delta t \sum_{k=0}^{K-1} \left\|\theta(u_h(t^{k+1}) - u_h^{k+1}) + (1-\theta)(u_h(t^k) - u_h^k)\right\|_{L^2(U_h)}^2$. This $O(\delta t^{2/\theta})$ by proposition D.3.3 and the above reasonings ($D = D(u) = 0$, $C = C(u)$ is bounded uniformly).

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

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

3.2. Approximation of shape gradient, discretize-then-optimize with implicit Euler

In the 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 with the fully discretized shape gradient.

A future line of research could be to extend such conclusions to the case of the Crank-Nicolson method, 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 [32], at least to show commutativity of optimization and discretization. But for now, we assume $\theta = 1$ throughout.

We begin by defining the discretized 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 $U_{r,h}$.

Problem 3.2.1 (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 $\Gamma_{m,h}$ and with small enough $W^{1,\infty}$ norm, so as to keep $U_{r,h}$ bounded Lipschitz and preserve the mesh quality, we solve:

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

where v_h^k, w_h^k are defined in problem 3.1.3, and their dependence on τ_h is not highlited in the notation.

At this level, for simplicity, but also for the sake of generality, we work with again with arbitrary vector fields in place of radial fields.

Proposition 3.2.2 (Discrete shape gradient)
The discrete shape gradient of problem 3.2.1 is:

$$\begin{aligned}
&J'_{h,\delta t}(\tau_h)[\delta\theta_h] = \\
&\delta t \sum_{k=1}^{K} \left(\frac{w_h^k - w_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h \circ \tau_h^{-1}) q_h^{k-1} \right)_{L^2(\tau_h(U_{r,h}))} + \delta t \sum_{k=1}^{K} (A'(\delta\theta_h \circ \tau_h^{-1}) \nabla w_h^k, \nabla q_h^{k-1})_{L^2(\tau_h(U_{r,h}))} + \\
&\delta t \sum_{k=1}^{K} \left(\frac{v_h^k - v_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h \circ \tau_h^{-1}) p_h^{k-1} \right)_{L^2(\tau_h(U_{r,h}))} + \delta t \sum_{k=1}^{K} (A'(\delta\theta_h \circ \tau_h^{-1}) \nabla v_h^k, \nabla p_h^{k-1})_{L^2(\tau_h(U_{r,h}))} + \\
&\frac{\delta t}{2} \sum_{k=1}^{K} \int_{\tau_h(U_{r,h})} \eta(t^k) |v_h^k - w_h^k|^2 \mathrm{div}(\delta\theta_h \circ \tau_h^{-1})
\end{aligned}$$

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

Problem 3.2.3

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

and

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

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

Sketch of proof.

We give a sketch of a proof, only to justify the time indices that appear in the expressions of the adjoint equations. For a rigorous proof one could adopt the same techniques employed in the continuous case. For simplicity we decide here to make use of the method proposed in and [12], section 4 (or more generally, [48]), to which we refer, for additional details: it is worth noting that such method can be fully justified, and that we numerically verified the correctness of such derivation.

To this end, we form a discretized Lagrangian just like in proposition 2.2.8, were integrals are replaced by Riemann sums (evaluated at the end of the time sub-intervals), and derivatives by difference quotients.

Since we have $v_h^0 = w_h^0 = 0$ we can slighlty simplify the procedure to obtain the discretized adjoints (that are exact on a discrete level): we only need to differentiate such Lagrangian by v_h^k, w_h^k, $k = 1, ..., K$.

In doing so, we obtain the following scheme, for e.g. p_h^k:

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

where we test by $v_h \in S^1_{h,0}$. For now, the time indices are only suggestive notation. However, note that by applying implicit Euler to the time reversed p, this is exactly the problem D.3.2 applied to the equation of p, modulo a time shift in the right hand side: we thus obtain an implicit method, with an "explicit" right hand side $\eta(t^k)(v_h^k - w_h^k)$.

Therefore p_h^k is an approximation of $p(t^k)$, and we will later quantify this assertion.

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 3.2.4 (τ and τ_h).
Throughout the rest of the section, we won't try to take into account the fact that the reference domains U_r and and $U_{r,h}$ are changing under the actions of τ and τ_h. It means that the estimates are τ, τ_h dependent. 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. 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. [42], where similar estimates to the ones we are up to derive, and in which H^2 regularity is asked on non-convex polygonal domains.

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

Proposition 3.2.5 (Error estimates for adjoint states)
The adjoints satisfy the same asymptotic, optimal order error estimates of proposition 3.1.4, under the same assumptions (with $\theta = 1$).

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 $\delta t \sum_{k=1}^K \left\|\eta(t^{k-1})u_h(t^{k-1}) - \eta(t^k)u_h^k\right\|^2_{L^2(U_h)}$, 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), $U_h = \tau_h(U_{r,h})$.

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:

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

There holds $2 \le \|\eta'\|^2_\infty \delta t^3 \sum_{k=1}^K \left\|u_h(t^k)\right\|^2_{L^2(U_h)}$. 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 $\|\pi u_h\|_{L^2(I,L^2(U_h))} \lesssim \delta t \|u_h'\|_{L^2(I,L^2(U_h))}$. This yields:

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

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

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

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

$\square$

Observation 3.2.6 (Optimization and discretization commute).
Optimization and discretization commute, in the case of $\theta = 1$. In fact, we could have started from the continuous states and adjoint (see problem 2.1.1 and proposition 2.2.11), applied the scheme of problem 3.1.3 to the states and the perturbed implicit Euler method of proposition 3.2.2 for the adjoints (which is a "legitimate" scheme, as we have just shown in proposition 3.2.5) to obtain exactly the same discrete quantities (states and adjoints).
With a diagram:

$$\begin{tikzcd}
 & \text{proposition 2.2.11} \arrow[dr, "\text{discretization}"] & \\
\text{problem 2.2.3} \arrow[ur, "\text{optimization}"] \arrow[dr, "\text{discretization}"'] & & \text{proposition 3.2.2} \\
 & \text{problem 3.2.1} \arrow[ur, "\text{optimization}"'] &
\end{tikzcd}$$

Before studying how well the discrete gradient approximates the continuous gradient, we need some additional error bounds for the state discretization. This is not strictly necessary: we do so to relax the smoothness requirements on the deformation field $\delta\theta$ in the upcoming arguments. This however entails assuming stronger compatibility relations for the state equations. From the physical point of view, this is not an issue: the state equations, unlike the adjoint ones, coming from a physical process, should naturally satisfy such compatibility.

The following proposition is proven in this section, applied to our concrete (state) equations. The proof also applies to the general case, of course, under suitable assumptions.

Proposition 3.2.7 (Another bound on the state discretization)
There holds, under assumption 3.1.2, the following error estimates:

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

Proof.
We again apply a separation into semidiscretization in space, and then full discretization, and adopt the notation u to represent either one of the two state variables.

Estimating Q_h^k in the L^2 norm

Going to the proof of proposition D.3.3, let us bound Q_h^k in the stronger L^2 norm. There holds (also see [57], page 388):

$$Q_h^k = -\frac{1}{\delta t}\int_{I_k} (s - t^k) u_h''(s) ds$$

From here, $\left\|Q_h^k\right\|^2_{L^2(U_h)} \leq \delta t \left\|u_h''\right\|^2_{L^2(I_k, L^2(U_h))}$, by an application of the Cauchy-Schwarz inequality.

Therefore, $\delta t \sum_{k=0}^{K-1} \left\|Q_h^k\right\|^2_{L^2(U_h)} \leq \delta t^2 \left\|u_h''\right\|^2_{L^2(I,L^2(U_h))}$. The latter norm can be bounded uniformly on h, thanks to assumption 3.1.2 and the reasoning of proposition B.1.8. Note, we need here the stronger compatibility condition that $\delta_h'(0)$ is bounded in H^1, see proposition D.3.3 for the notation. In the current concrete case, $\delta_h'(0) = 0$ and this is thus not an issue.

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 $\dfrac{e_h^{k+1} - e_h^k}{\delta t}$ to obtain:

$$\left(\frac{e_h^{k+1} - e_h^k}{\delta t}, \frac{e_h^{k+1} - e_h^k}{\delta t}\right)_{L^2(U_h)} + a_h\left(e_h^{k+1}, \frac{e_h^{k+1} - e_h^k}{\delta t}\right) = \left(Q_h^k, \frac{e_h^{k+1} - e_h^k}{\delta t}\right)_{L^2(U_h)}$$

Hence, employing Young and Cauchy-Schwarz inequalities, we find:

$$\left\|\frac{e_h^{k+1} - e_h^k}{\delta t}\right\|^2_{L^2(U_h)} + \frac{1}{2\delta t}\left(\left\|\nabla e_h^{k+1}\right\|^2_{L^2(U_h)} - \left\|\nabla e_h^k\right\|^2_{L^2(U_h)}\right) \leq \left\|Q_h^k\right\|_{L^2(U_h)} \left\|\frac{e_h^{k+1} - e_h^k}{\delta t}\right\|_{L^2(U_h)}$$

Passing to summations, because $e_h^0 = 0$ and by the Cauchy-Schwarz inequality:

$$\sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{L^2(U_h)}} \leq \sqrt{\delta t \sum_{k=0}^{K-1} \|Q_h^k\|^2_{L^2(U_h)}} \lesssim \delta t$$

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.1.2, and using proposition D.1.3 itself:

$$\delta t \sum_{k=0}^{K-1} \left\| \frac{u(t^{k+1}) - u(t^k)}{\delta t} - \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|^2_{L^2(U)} \lesssim \delta t \sum_{k=0}^{K-1} \left\| \frac{e(t^{k+1}) - e(t^k)}{\delta t} \right\|^2_{L^2(U)} + \delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{L^2(U_h)}$$

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 [43], we can reason as follows:

$$\delta t \sum_{k=0}^{K-1} \left\| \frac{e(t^{k+1}) - e(t^k)}{\delta t} \right\|^2_{L^2(U)} = \delta t \sum_{k=0}^{K-1} \left\| \frac{1}{\delta t} \int_{I_k} e' \right\|^2_{L^2(U)} \lesssim \|e'\|^2_{L^2(I, L^2(U))} \lesssim h^2$$

by corollary D.2.17 and assumption 3.1.2. □

Theorem 3.2.8 (Fully discrete estimate for shape gradients, implicit Euler case)
Let U be fixed and U_h as in assumption 3.1.2. The same assumption must hold. Let $\delta\theta \in W^{1,\infty}(U)$ and $\delta\theta_h$ be a vector valued finite element function of $S_h^1 = S_h^1(U_h)$. There exists a constant γ that depends on U, the shape regularity and quasi-uniformity of the meshes, independent of $h, \delta t$, such that, for $h, \delta t$ small enough, we have:

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

where 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 $dJ_{h,\delta t}(U_h)[\delta\theta] := dJ_{h,\delta t}(\tau_h)[\delta\theta_h \circ \tau]$, with $U_h = \tau_h(U_{r,h})$ and a suitable τ_h that(linearly) interpolates τ on the spatial discretization nodes.

Proof.

Forewarning

As we have already mentioned in observation 3.2.4, we consider U, U_h to be frozen in our estimate, and we assume U_h to be interpolating U, as in assumption 3.1.2. For simplicity, we are also considering $\delta\theta$ and $\delta\theta_h$ to be defined on the moving domain. We again recover the notation u, a to indicate a state and its correspondent adjoint (so, $u = v \iff a = p$ or $u = w \iff a = q$). Therefore, the quantities to be compared become, thanks to proposition 2.2.11 and proposition 3.2.2:

$$\partial := \delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \int_I (u_t, \operatorname{div}(\delta\theta) a)_{L^2(U)}$$

$$\nabla := \delta t \sum_{k=1}^{K} (A'(\delta\theta_h) \nabla u_h^k, \nabla a_h^{k-1})_{L^2(U_h)} - \int_I (A'(\delta\theta) \nabla u, \nabla a)_{L^2(U)}$$

$$\mathrm{J} := \frac{\delta t}{2} \sum_{k=1}^{K} \int_{U_h} \eta(t^k) |v_h^k - w_h^k|^2 \operatorname{div}(\delta\theta_h) - \frac{1}{2} \int_I \int_U \eta |v - w|^2 \operatorname{div}(\delta\theta)$$

Derivatives: rewriting

Denote again by $\pi a = a(t^k)$ on (t^k, t^{k+1}). Then:

$$\partial = \underbrace{- \int_I (u_t, \operatorname{div}(\delta\theta)(a - \pi a))_{L^2(U)}}_{1} + \underbrace{\delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \int_I (u_t, \operatorname{div}(\delta\theta) \pi a)_{L^2(U)}}_{\mathrm{R1}}$$

Now:

$$\text{R1} = \delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \delta t \sum_{k=1}^{K} \left(\frac{u(t^k) - u(t^{k-1})}{\delta t}, \operatorname{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)} =$$

$$\underbrace{-\delta t \sum_{k=1}^{K} \left(\frac{u(t^k) - u(t^{k-1})}{\delta t} - \frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \operatorname{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)}}_{2} +$$

$$\underbrace{\delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \delta t \sum_{k=1}^{K} \left(\frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \operatorname{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)}}_{\text{R2}}$$

Lastly:

$$\text{R2} = \underbrace{\delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \operatorname{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \delta t \sum_{k=1}^{K} \left(\frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \operatorname{div}(\delta\theta_h^l) a_h^{k-1,l} \right)_{L^2(U)}}_{3} +$$

$$\underbrace{-\delta t \sum_{k=1}^{K} \left(\frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, (\operatorname{div}(\delta\theta) - \operatorname{div}(\delta\theta_h^l)) a_h^{k-1,l} \right)_{L^2(U)}}_{4} + \underbrace{-\delta t \sum_{k=1}^{K} \left(\frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \operatorname{div}(\delta\theta) \left(a(t^{k-1}) - a_h^{k-1,l} \right) \right)_{L^2(U)}}_{5}$$

Derivatives: estimation

We start with 1, 2, 5.

We have, by the Cauchy-Schwarz inequality and lemma A.2.7:

$$\left| 1 \right| \leq \delta t \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \left\| u_t \right\|_{L^2(I, L^2(U))} \left\| a' \right\|_{L^2(I, L^2(U))} \lesssim \delta t \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)}$$

Then, using again the Cauchy-Schwarz inequality:

$$\left| 2 \right| \leq \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| a(t^k) \right\|_{L^2(U)}^2} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{u(t^{k+1}) - u(t^k)}{\delta t} - \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|_{L^2(U)}^2}$$

Employing proposition 3.2.7 at first, and lemma A.2.7 afterwards:

$$\left| 2 \right| \lesssim (h + \delta t) \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \sqrt{\sum_{k=0}^{K-1} \int_{I_k} \left\| a(t^k) \right\|_{L^2(U)}^2} \lesssim (h + \delta t) \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \left\| a' \right\|_{L^2(I, L^2(U))} \lesssim (h + \delta t) \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)}$$

Note, this is where we used proposition 3.2.7. One could alternatively assume higher differentiability for θ and proceed with proposition 3.1.4.

Then:

$$\left| 5 \right| \leq \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|_{L^2(U)}^2} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| a(t^k) - a_h^{k,l} \right\|_{L^2(U)}^2}$$

Thanks to proposition 3.2.5 we can write:

$$\left| 5 \right| \lesssim (h^2 + \delta t) \left\| \operatorname{div}(\delta\theta) \right\|_{L^\infty(U)} \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{u_h^{k+1,l} - u_h^{k,l}}{\delta t} \right\|_{L^2(U)}^2}$$

Using proposition 3.2.7 and the last step of its proof:

$$\left|5\right| \lesssim (h^2 + \delta t) \left\|\mathrm{div}(\delta\theta)\right\|_{L^\infty(U)}$$

And with similar reasonings:

$$\left|4\right| \lesssim \left\|\mathrm{div}(\delta\theta) - \mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U)}$$

Member 3 can be bound with the help of proposition D.1.5.

Gradients: rewriting

We have:

$$\begin{gathered}
\delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla u_h^k, \nabla a_h^{k-1})_{L^2(U_h)} - \int_I (A'(\delta\theta)\nabla u, \nabla a)_{L^2(U)} = \\
\underbrace{\delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla u_h^k, \nabla a_h^{k-1})_{L^2(U_h)} - \int_I (A'(\delta\theta)\nabla \tilde{\pi} u, \nabla \pi a)_{L^2(U)}}_{\text{R3}} + \\
\underbrace{-\int_I (A'(\delta\theta)\nabla u, \nabla(a - \pi a))_{L^2(U)}}_{6} \underbrace{- \int_I (A'(\delta\theta)\nabla(u - \tilde{\pi} u), \nabla \pi a)_{L^2(U)}}_{7}
\end{gathered}$$

Continuing the splitting:

$$\begin{gathered}
\text{R3} = \delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla u_h^k, \nabla a_h^{k-1})_{L^2(U_h)} - \delta t \sum_{k=1}^{K} (A'(\delta\theta)\nabla u(t^k), \nabla a(t^{k-1}))_{L^2(U)} = \\
\underbrace{\delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla u_h^k, \nabla a_h^{k-1})_{L^2(U_h)} - \delta t \sum_{k=1}^{K} (A'(\delta\theta_h^l)\nabla u_h^{k,l}, \nabla a_h^{k-1,l})_{L^2(U)}}_{8} + \underbrace{- \delta t \sum_{k=1}^{K} ((A'(\delta\theta) - A'(\delta\theta_h^l))\nabla u_h^{k,l}, \nabla a_h^{k-1,l})_{L^2(U)}}_{9} + \\
\underbrace{- \delta t \sum_{k=1}^{K} (A'(\delta\theta)\nabla(u(t^k) - u_h^{k,l}), \nabla a(t^{k-1}))_{L^2(U)}}_{10} + \underbrace{- \delta t \sum_{k=1}^{K} (A'(\delta\theta)\nabla u_h^{k,l}, \nabla(a(t^{k-1}) - a_h^{k-1,l}))_{L^2(U)}}_{11}
\end{gathered}$$

Gradients: estimation

The terms 10, 11 can be estimated in a common way. We only need to make sure that $\delta t \sum_{k=1}^{K} \left\|\nabla u_h^{k,l}\right\|_{L^2(U)}^2$ is bounded uniformly (true by proposition 3.1.4, lemma A.2.7 and the smoothness of u, ensured by assumption 3.1.2), and also that $\delta t \sum_{k=1}^{K} \left\|\nabla a(t^{k-1})\right\|_{L^2(U)}^2$ is uniformly bounded (true by lemma A.2.7 and the smoothness of a, ensured by assumption 3.1.2). Then an application of the Cauchy-Schwarz inequality, proposition 3.2.5 and proposition 3.1.4 yield:

$$\left|10\right|, \left|11\right| \lesssim (h + \delta t) \left\|A'(\delta\theta)\right\|_{L^\infty(U)}$$

Similarly:

$$\left|9\right| \lesssim (h + \delta t) \left\|A'(\delta\theta_h^l) - A'(\delta\theta)\right\|_{L^\infty(U)}$$

and the term 8 follows directly from proposition D.1.5.

Cost functions: estimation

We are missing a bound on:

$$\text{J} := \frac{\delta t}{2}\sum_{k=1}^{K}\int_{U_h}\eta(t^k)|v_h^k - w_h^k|^2\mathrm{div}(\delta\theta_h) - \frac{1}{2}\int_I\int_U \eta|v-w|^2\mathrm{div}(\delta\theta) =$$

$$\underbrace{\frac{\delta t}{2}\sum_{k=1}^{K}\int_{U_h}\eta(t^k)|v_h^k - w_h^k|^2\mathrm{div}(\delta\theta_h) - \frac{1}{2}\int_I\int_U \eta|v-w|^2\mathrm{div}(\delta\theta_h^l)}_{\text{R4}} + \underbrace{-\frac{1}{2}\int_I\int_U \eta|v-w|^2(\mathrm{div}(\delta\theta) - \mathrm{div}(\delta\theta_h^l))}_{12}$$

We find:

$$\left|12\right| \lesssim \left\|\mathrm{div}(\delta\theta) - \mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U)}$$

whereas:

$$\text{R4} = \underbrace{\frac{\delta t}{2}\sum_{k=1}^{K}\int_{U_h}\eta(t^k)|v_h^k - w_h^k|^2\mathrm{div}(\delta\theta_h) - \frac{\delta t}{2}\sum_{k=1}^{K}\int_{U}\eta(t^k)|v_h^{k,l} - w_h^{k,l}|^2\mathrm{div}(\delta\theta_h^l)}_{13} +$$

$$\underbrace{\frac{\delta t}{2}\sum_{k=1}^{K}\int_{U}\eta(t^k)(|v_h^{k,l} - w_h^{k,l}|^2 - |v(t^k) - w(t^k)|^2)\mathrm{div}(\delta\theta_h^l)}_{14} + \underbrace{\frac{1}{2}\int_I\int_U \tilde{\pi}\eta(|\tilde{\pi}v - \tilde{\pi}w|^2 - |v-w|^2)\mathrm{div}(\delta\theta_h^l)}_{15} + \underbrace{\frac{1}{2}\int_I\int_U (\tilde{\pi}\eta - \eta)|v-w|^2\mathrm{div}(\delta\theta_h^l)}_{16}$$

For 16 we can use the fact that that $\|\eta - \tilde{\pi}\eta\|_\infty \leq \delta t\,\|\eta'\|_\infty$ to ensure that:

$$\left|16\right| \lesssim \delta t\left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}$$

Similarly, also by applying the Cauchy-Schwarz' inequality and lemma A.2.7:

$$\left|15\right| \lesssim \left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}(\|v - \tilde{\pi}v\|_{L^2(I,L^2(U))} + \|w - \tilde{\pi}w\|_{L^2(I,L^2(U))}) \lesssim \delta t\left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}$$

The Cauchy-Schwarz' inequality also yields:

$$\left|14\right| \lesssim \left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}(E_v + E_w)(S_v + S_w)$$

where $E_u = \sqrt{\delta t\sum_{k=1}^{K}\left\|u(t^k) - u_h^{k,l}\right\|_{L^2(U)}^2}$ and $S_u = \sqrt{\delta t\sum_{k=1}^{K}\left\|u(t^k) + u_h^{k,l}\right\|_{L^2(U)}^2}$.
Through proposition 3.1.4 we find $E_u \lesssim \delta t + h^2$, whereas proposition 3.1.4 combined with lemma A.2.7 yield $S_u \lesssim 1$, so that:

$$\left|14\right| \lesssim (\delta t + h^2)\left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}$$

Similarly, and reasoning as in proposition D.1.5, we can also see that:

$$\left|13\right| \lesssim h\left\|\mathrm{div}(\delta\theta_h^l)\right\|_{L^\infty(U_h)}$$

This concludes the proof. □

Upon choosing $\delta\theta = \delta\theta_h^l$ we easily obtain the following corollary.

Corollary 3.2.9
With the same hypothesis and notation of theorem 3.2.8:

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

With this, similar estimates to those in [42] were derived, in a slightly different context: in a time-dependent setting, and a precise handling of the geometry error. However, in [42], order 2 estimates (in space) are obtained instead: this is because the deformation field $\delta\theta$ is assumed to have an additional order 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. It is however a strong hint for the realization of such phenomenon, which is indeed observable in practice (see again the experiments in [42]). In the next section we obtain similar superconvergence estimates, in our setting.

3.3. Approximation of shape gradient, superconvergence for spatial semidiscretization

We now show that for smooth displacement fields $\delta\theta$ that vanish in a neighbourhood of the fixed boundary, a superconvergence result for the shape gradient is available, in the spirit of [42]. Such "compact support" assumption is not very strong in our setting: admissible displacements must already be zero at the fixed boundary, so as to yield a transformation that preserves Γ_f.

This result, in turn, is shown initially only for the spatial semidiscretization, which however suggests that such a result may be available also in the fully discrete case. This is also confirmed by the experiments in 4.2, in both cases. We are able to give theoretical justification for the implicit Euler scheme.

The difference with the estimates of [42] lies in the fact that we are explicitly taking into account the geometry discrepancy $U \neq U_h$ (in the special case that U_h interpolates U), apart from the time dependent setting we are in.

Such estimates, as noted in [42], don't seem to be so easily obtainable for displacements $\delta\theta \in W^{1,\infty}$ only.

Let us briefly briefly introduce the semidiscretized shape optimization problem, and its shape gradient.

Proposition 3.3.1 (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 define $u_h : I \to S_h^1$ as:

$$\begin{aligned}
\left(u_h', v_h\right)_{L^2(U_h)} + (\nabla u_h, \nabla v_h)_{L^2(U_h)} = (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}, \quad &\text{for a.e. } t \in I \\
u_h|_{\Sigma_{D_h}} = g_{D,h}& \\
u_h(0) = 0&
\end{aligned}$$

and $v_h \in S^1_{h,0,D_h}$. 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 is:

$$\begin{aligned}
-\left(a_h', v_h\right)_{L^2(U_h)} + (\nabla a_h, \nabla v_h)_{L^2(U_h)} = (-1)^{[u_h = v_h]}\eta(v_h - w_h), \quad &\text{for a.e. } t \in I \\
a_h|_{\Sigma_{D_h}} = 0& \\
a_h(T) = 0&
\end{aligned}$$

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

$$\begin{aligned}
&dJ_h(\tau_h)[\delta\theta_h] = \\
&\int_I (w_h' \operatorname{div}(\delta\theta_h \circ \tau_h^{-1}), q_h)_{L^2(\tau_h(U_{r,h}))} + \int_I (A'(\delta\theta_h \circ \tau_h^{-1})\nabla v_h, \nabla p_h)_{L^2(\tau_h(U_{r,h}))} + \\
&\int_I (v_h' \operatorname{div}(\delta\theta_h \circ \tau_h^{-1}), p_h)_{L^2(\tau_h(U_{r,h}))} + \int_I (A'(\delta\theta_h \circ \tau_h^{-1})\nabla w_h, \nabla q_h)_{L^2(\tau_h(U_{r,h}))} + \\
&\frac{1}{2}\int_I \int_{\tau(U_{r,h})} |v_h - w_h|^2 \operatorname{div}(\delta\theta_h \circ \tau_h^{-1})
\end{aligned}$$

Proof.
We skip it, it can be done similarly to proposition 2.2.11 or proposition 3.2.2. □

Theorem 3.3.2 (Superconvergence result for shape gradients, spatially semidiscrete case)
Let U be fixed and U_h as in assumption 3.1.2. Let assumption 3.1.2 itself hold, $\delta\theta \in W^{2,\infty}(U)$, 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:

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

where the notation for the shape gradients is analogous to that in theorem 3.2.8.

Proof.

The proof is similar to that of theorem 3.2.8: we compare "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. We indicate $\delta\theta^{-l} =: \delta\theta_h$. For the expression of the semidiscretized shape gradient we make use of proposition 3.3.1.

Derivatives

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

We have:

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

We apply corollary D.2.17 to 1, a thing which we can do, as assumption 3.1.2 and by the reasonings of proposition 3.1.4, to obtain:

$$\left|1\right| \lesssim h^2 \|\mathrm{div}\delta\theta\|_{L^\infty(U)}$$

It is crucial here that θ has two weak derivatives, so that $a\theta$ is a test function, as required by corollary D.2.17.

On the other hand, employing theorem D.2.10, proposition D.1.3 and suitable energy estimates to u_h' (which are avaliable by assumption D.3.1), we come as well to:

$$\left|2\right| \lesssim h^2 \|\mathrm{div}\delta\theta\|_{L^\infty(U)}$$

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

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

Gradients

We perform a suitable splitting:

$$\int_I (A'(\delta\theta)\nabla u, \nabla a)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u_h, \nabla a_h)_{L^2(U_h)} =$$
$$\underbrace{\int_I (A'(\delta\theta)\nabla u, \nabla a)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u^{-l}, \nabla a^{-l})_{L^2(U_h)}}_{4} +$$
$$\underbrace{\int_I (A'(\delta\theta)\nabla(u_h^l - u), \nabla a_h^l)_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla(u_h - u^{-l}), \nabla a_h)_{L^2(U_h)}}_{5} +$$
$$\underbrace{\int_I (A'(\delta\theta)\nabla u, \nabla(a_h^l - a))_{L^2(U)} - \int_I (A'(\delta\theta_h)\nabla u^{-l}, \nabla(a_h - a^{-l}))_{L^2(U_h)}}_{6} +$$
$$-\underbrace{\int_I (A'(\delta\theta)\nabla(u_h^l - u), \nabla(a_h^l - a))_{L^2(U)}}_{7} + -\underbrace{\int_I (A'(\delta\theta)\nabla u, \nabla(a_h^l - a))_{L^2(U)}}_{8} + -\underbrace{\int_I (A'(\delta\theta)\nabla(u_h^l - u), \nabla a)_{L^2(U)}}_{9}$$

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

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

having used theorem D.2.10 in the last step. The same theorem D.2.10 is sufficient to conclude the bound $\left|7\right| \lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$. 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 $D\delta\theta$ and the fact that $u, u_h^l = 0$ on the moving boundary Γ_m, we obtain:

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

where we used again theorem D.2.10.

Cost function

There holds:

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

The first term is $\lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$ thanks to the Cauchy-Schwarz inequality and theorem D.2.10, the second one because of proposition D.1.5. This concludes the proof. □

As a corollary, we can derive the same result as in theorem 3.2.8, but with a better order of convergence in space.

Corollary 3.3.3 (Fully discrete superconvergence result)
With the same assumptions and notation of theorem 3.3.2 and in the discretize-then-optimize framework of section 3.2, we can conclude:

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

Sketch of a proof.

The proof applies the same techniques as in theorem 3.3.2, for what concerns the error committed by a time discretization. The overall argument is overall more transparent: it amounts to "inserting dJ_h between dJ and $dJ_{h,\delta t}$". Two pieces must then be estimated, and the first is exactly $O(h^2)$ by theorem 3.2.8. 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 $O(\delta t)$ by the same arguments as in theorem 3.2.8. Let us recover the unified notation of problem 3.1.1. Then:

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

and:

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

Finally:

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

Each of the pieces above is $O(\delta t)$, so that the conclusion follows. $\square$

4. Implementation

We now turn to discuss our implementation and to 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 B.2.1.2
- in section 4.2 some numerical experiments are reported, and the results are discussed and analyzed. We also verify the error estimates for the shape gradients

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 heavy use of the FEniCS package ([51]). 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 [34], [24] and [54]). That is, we only needed to code the "forward model" (cost functional and partial differential equations), and the 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 comparison with proposition 3.2.2 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 ([35]) was used for the meshing.

The shape identification problem problem 2.1.2 lends itself very well to debugging and numerical experiments, as one can build analytical solutions and then analyize whether that is recovered by the optimization process. One can for instance artificially create the "optimal" inclusion Ω_e and come up with e.g. 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

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: after a uniform refinement, not all discrete boundary nodes need to be again on the smooth boundary. One would need to correct for this, and to do so, one would need to know a parametrization of the entire boundary. We avoided this, as we tried to use the least possible knowledge of the smooth boundary.

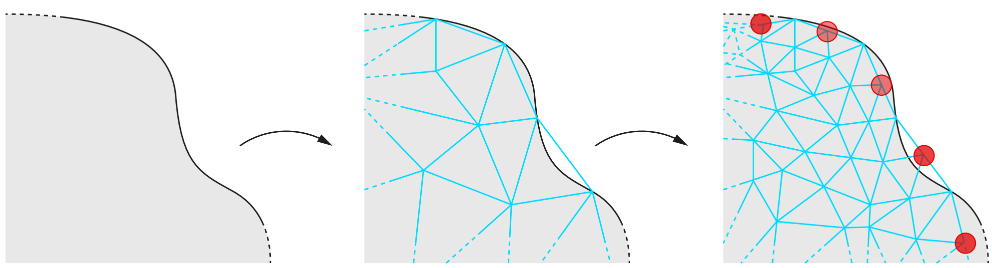

Figure 4.1.: Problems with uniform refinements

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 $D \setminus \overline{B_\epsilon(0)} =: U_r$, 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 (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 would 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 custom block in dolfin-adjoint.

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. The discrete Neumann trace need not to have an easy boundary expression, plus, we found the doing otherwise to be more complicated from a code point of view, at least with the tools at our disposal.

Using the same discretization parameters to generate the synthetic data, and then perform shape optimization, will result in committing an "inverse crime" (see [67]). To avoid this, there are 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 [40], 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 finite elements, for simplicity, but also computational efficiency. The framework of appendix D can be however potentially adapted to accommodate isoparametric elements, see the works of e.g. [26], [28], [27]. Isoparametric elements elements are necessary, when adopting higher order basis functions, in order to preserve optimal accuracy (see section 4.4 of [60] 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 felt it to be not flexible enough with the transfering of functions between non conforming meshes, something we needed to at several places throughout our code.

This in constrast to [40], where the authors employ order 2 isoparametric elements (in the context of the boundary element method).

The motivation for this is that the analysis of [42], which we partially repeated in our setting, suggests that the volume form of the shape gradient is more accurate a boundary form.

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 justificationa 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 [29], a work centered around a very similar shape optimization problem to ours, in an attempt to alleviate some spurious artifacts we observed, 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:

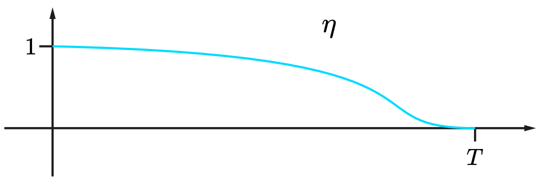

Figure 4.2.: The temporal weight η

4.2. Experiments

All the experiments are run on a laptop's 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 have $T = 2$ throughout, and the reference mesh looks as follows. Note that in the following plots, the "exact" domain 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 become 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 three 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.

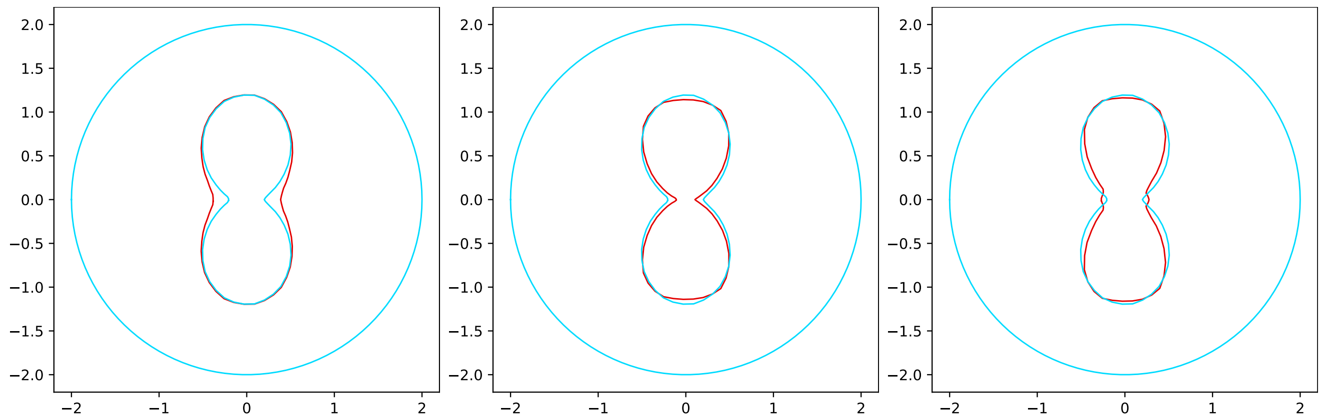

Figure 4.3.: Exact and simulated inclusion (in red) for the runs with g_2, g_3 adn g_4, in order from left to right

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

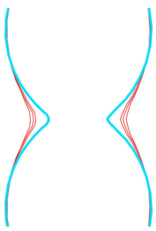

Figure 4.4.: From the outside to the inside: run with g_6, g_5, g_1 and exact solution in blue

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

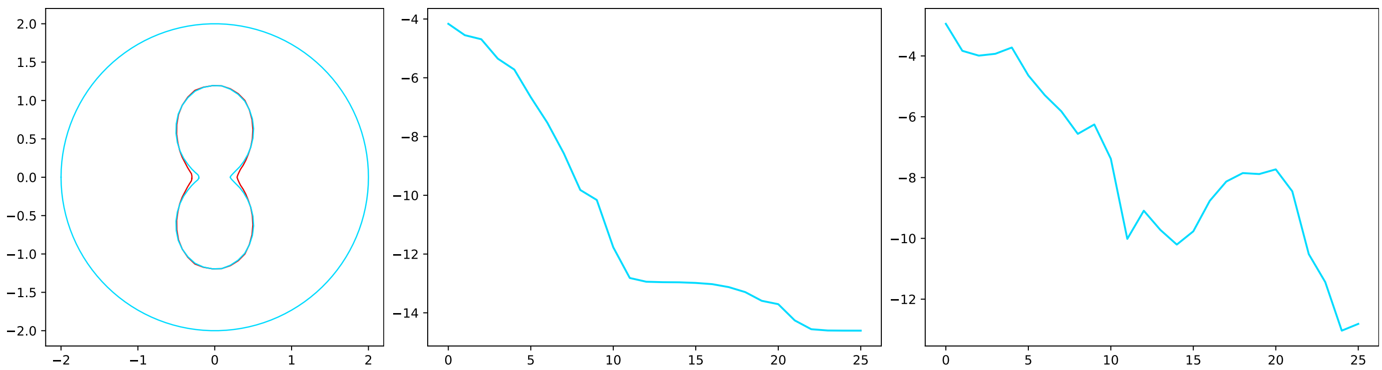

Figure 4.5.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 25 iterations

The effect of η

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 $a = 0$.

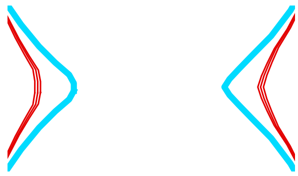

Figure 4.6.: From outside to inside: run with g_1 and $a = 0$, $a = 0.05$, $a = 0.005$ and exact solution in blue

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. Doing so we obtain smoother 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.

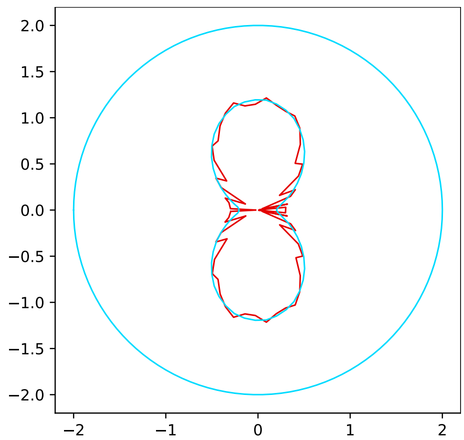

Figure 4.7.: Reconstruction for the run g_1 and the L^2 inner product

Ill-posedness

Degeneration of the boundary

It has already been noted in [40] 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 [29] in an "elliptic" version of problem 2.1.2, but we expect their conclusions to be applicable 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. [44], 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:

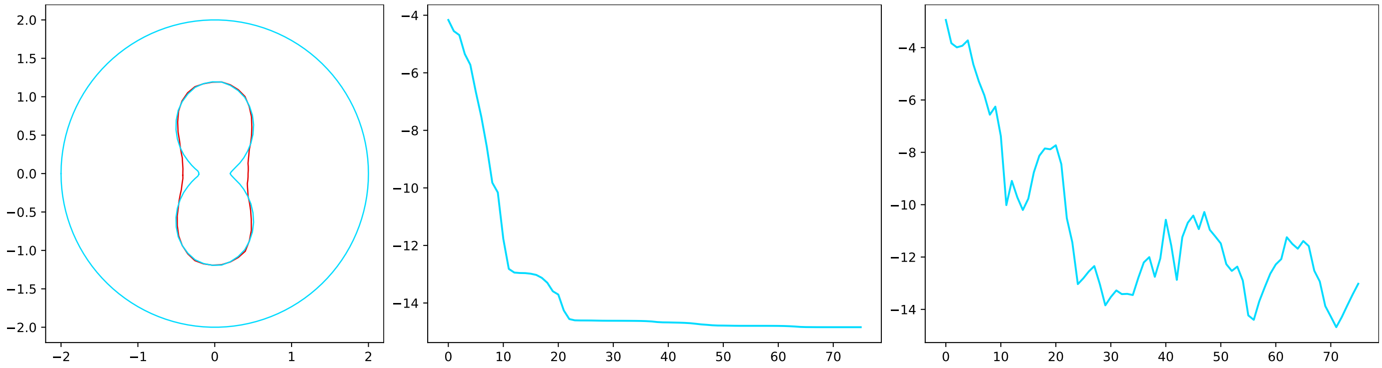

Figure 4.8.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 75 iterations

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 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 show again reconstruction, cost function and gradient history.

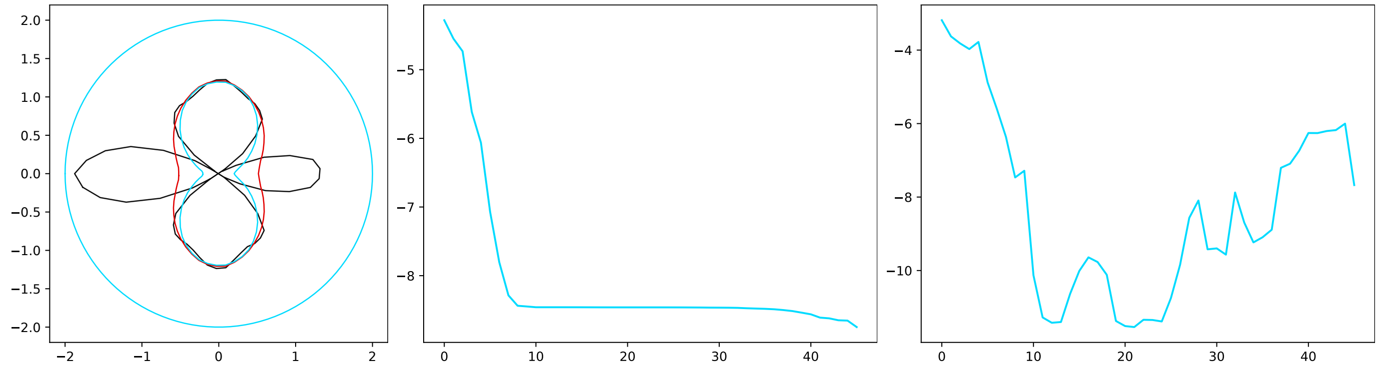

Figure 4.9.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run. The black boundary corresponds to 45 iterations, the blue one to 25. The presence of the lateral lobes in the black reconstruction indicates a negative radial function.

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 as in the above runs, but it starts to present spurious oscillations very late (only after iteration 80, in the case of the g_1 run). The discrepancy between exact data, and data avalailable during optimization, is randomly distributed and of zero mean in the second approach, whereas we noted that it presents a "trend" given by the chosen PDEs discretization algorithm in the first one. This seems to be key to the degeneration behaviour that we observed.

We did most of the experiments with different discretizations between inversion and synthesis, because this approach highlited better 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, hence another reason to proceed as we did.

Second order information

The shape optimization problem is ill-posed, which is reflected in an ill-conditioned Hessian, at the optimal domain. This can cause undesired oscillations when employing 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 [29] (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.

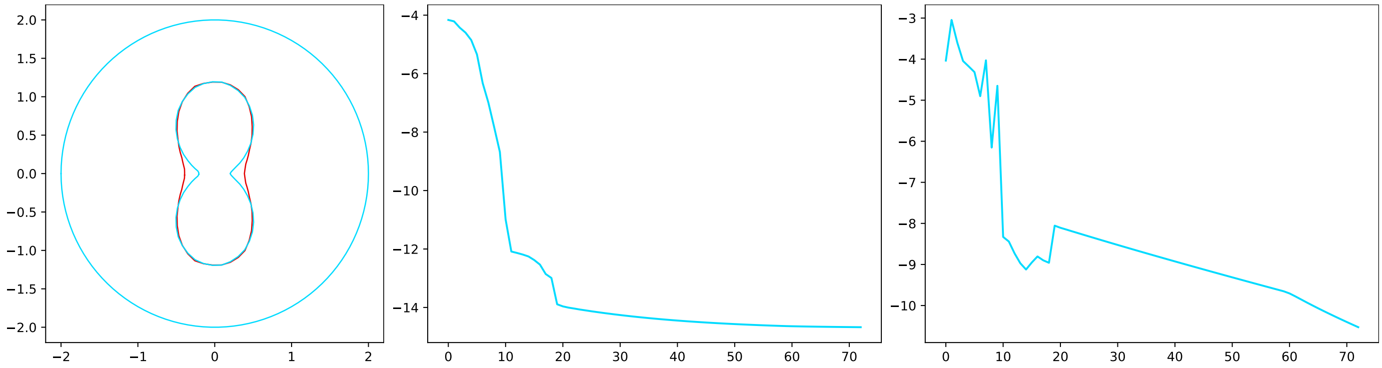

Figure 4.10.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run, and the regularized Newton method from [29]. The reconstructions after 20 and 70 shape are visually indistinguishable.

<u>Sea urchin</u>

Lastly, we show the reconstruction of a 2D version of the more complicated "sea urchin" inclusion of [40]. The discretization configuration is the standard one. The reconstruction ran for 30 iterations. This time, for completeness, we also applied 1% noise to the data.

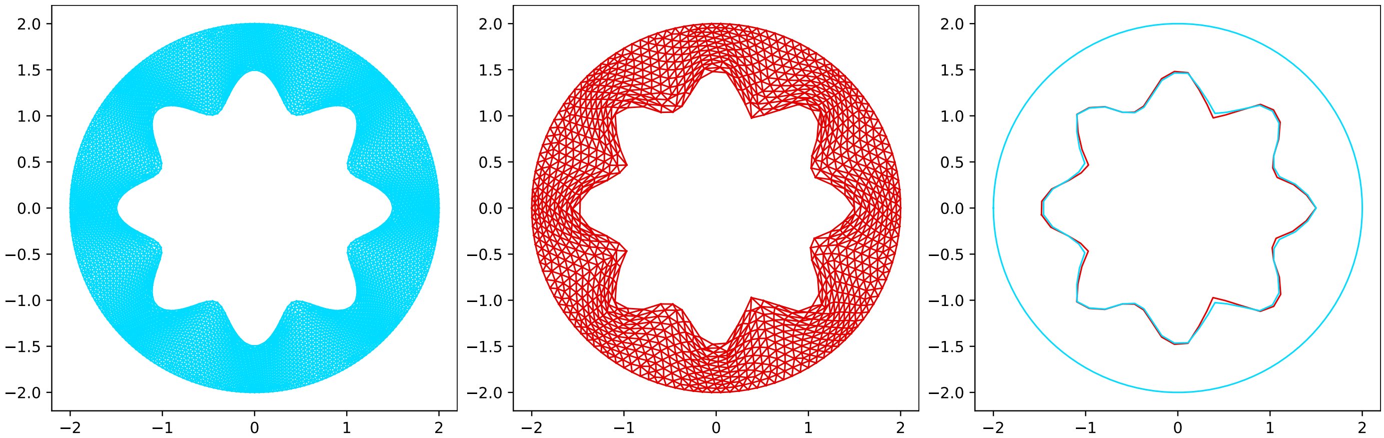

Figure 4.11.: "Exact" domain, reconstruction, and comparison between reconstruction and the exact domain, interpolated to the optimization finite element space.

4.2.2. Estimates for the shape gradients

We go on to present some numerical evidence of the estimates shown in section 3.2 and section 3.3. 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 mesh: the rationale is to have the resulting displacement field (a finite element vector field on the mesh of size h) approximating a vector field that is in $W^{1,\infty}$ but not $W^{2,\infty}$. Doing so, we 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:

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

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 $\dfrac{\log Q_h - \log Q_{2h}}{\log h - \log 2h}$ 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 computational reasons, we made one less refinement in the implicit Euler case.

Note that we register an infinite order of convergence when the refinement brings us from $2h_f$ to h_f, and that the order of convergence value in the refinement before this, might be higher 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 and section 3.3. In particular, we note the following facts:

- the above tables suggest a superconvergence effect, for the implicit Euler's method, even with "rough" displacement vector fields, compare with corollary 3.2.9 and corollary 3.3.3

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

- although we haven't given a proof of the convergence behaviour in the case of the Crank-Nicolson method, 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

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, 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.

Numerical experiments support such conclusions, and even suggest that the bounds that we proved for the implicit Euler method, might be obtainable with 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 [32] suggests
- from here, fully discrete estimates analogous to those for implicit Euler, should be derivable for the Crank-Nicolson method
- the error estimates for the shape gradients derived assuming a specific for 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 τ, τ_h (where $U = \tau(U_r), U_h = \tau(U_{r,h})$) in these estimates

Appendices

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:

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

Proof.
This follows from [47], 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. □

Proposition A.1.2 (Characterization of $W^{1,\infty}$)
Let Ω be a bounded Lipschitz domain, or $\mathbb{R}^n$. Then $W^{1,\infty}(\Omega) = C^{0,1} \cap L^\infty(\Omega)$.
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 the case Ω is bounded Lipschitz, then Ω is an extension domain for $W^{1,\infty}(\Omega)$ (see [47], 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 [47], 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. □

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 [46]).

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 [46]) 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, $\int_T Tf = \lim_n T\int_I f_n = T\lim_n \int_I f_n = T\int_I f$. □

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 $k \geq 0$, $f \in H^k(I, X) \implies Tf \in H^k(I, Y)$, with weak derivatives $\partial_{t^i} Tf = T\partial_{t^i} f$, $0 \leq i \leq k$.
The map $f \mapsto Tf$, $H^k(I, X) \to H^k(I, Y)$ 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 [46] at page 26, thanks to theorem 6 at page 146 of [33], a mean value theorem for vector valued function. $\square$

We also need a time dependent trace lemma, which we provide under non-optimal regularity assumptions, but for the sake of making some arguments easier and more transparent.

Definition A.2.5 (Time dependent trace)
Let Ω be a bounded Lipschitz domain. For $k \geq 0$ we define $\mathrm{tr} : H^k(I, H^1(\Omega)) \to H^k(I, H^{1/2}(\partial\Omega))$ 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, $E(g)(t) := E(g(t))$ (for E a right inverse of the static trace)
3. tr and E, in the case of $k \in \mathbb{N}_0$, coincide (in the time a.e. sense) for the case $l \geq k$
4. for $k \geq 1$, $\mathrm{tr}u(0) = 0 \iff u(0) = 0$ (in the sense of continuous representatives)

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 [52]). The first three points are consequences of this fact and of proposition A.2.1.

The fourth property follows by the definition of tr, E and the fact that $H^l \subseteq H^k$, for $k \leq l$.

Let now $k \geq 1$. We know that $H^1, H^{1/2}$ are separable and Banach (the latter is separable because the continuos image of H^1 separable, and Banach (see [38], page 20). Therefore, by [30], theorem 2 of page 286, we obtain the embeddings $H^k(I, H^1) \hookrightarrow C([0,T], H^1)$ and the same goes for $H^k(I, H^{1/2})$, and we conclude by continuity in time of u and $\mathrm{tr}u$.

$\square$

Lemma A.2.7 (Piecewise constant approximation)
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 $\pi u \in L^2(I,X)$ the function $\pi u(t) = u(t^k)$, for $t \in (t^k, t^{k+1})$.
Then, $\|u - \pi u\|_{L^2(I,X)} \leq C\delta t \|u'\|_{L^2(I,X)}$, for $C = 1/\sqrt{2}$, and the same holds for $\tilde{\pi} u(t) = u(t^{k+1})$ for $t \in (t^k, t^{k+1})$.

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

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

B. Parabolic equations

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 [64] at page 147. This embedding is $H \ni f \mapsto (f, \cdot)_H$. We thus obtain a Gelfand triple, and we have $W(I, V) \subseteq C(I, H)$.
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 energy 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 [37] 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)
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:

$$\|u\|^2_{C([0;T],H)} + \alpha \|u\|^2_{L^2(I,V)} \leq C \exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1} \|f\|^2_{L^2(I,V^*)}) \tag{B.1.9}$$
$$C \left\|u'\right\|_{L^2(I,V^*)} \leq \|A\|_{L(V,V^*)} \alpha^{-1/2} \sqrt{\exp(2\lambda T)} \|u_0\|_H + \tag{B.1.10}$$
$$\left(\|A\|_{L(V,V^*)} \alpha^{-1} \sqrt{\exp(2\lambda T)} + 1\right) \|f\|_{L^2(I,V^*)} \tag{B.1.11}$$

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

$$C \left\|u'\right\|^2_{L^2(I,H)} \leq (1 + (1 + C_0)\alpha^{-1}) \|f_2\|^2_{H^1(I,V^*)} + \tag{B.1.12}$$
$$(1 + \|A\|_{L(V,V^*)}) \|u_0\|_V^2 + C_0 \|u_0\|_H^2 + \tag{B.1.13}$$
$$\|f_1\|^2_{L^2(I,H)} + C_0\alpha^{-1} \|f_1\|^2_{L^2(I,V^*)} \tag{B.1.14}$$

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.
<u>No regularity</u>
From page 21 of [37] we obtain that $\|u\|^2_{C([0;T],H)} + \alpha \|u\|^2_{L^2(I,V)} \leq \exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1} \|f\|^2_{L^2(I,V^*)})$, 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:

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

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

More regularity

We tie back to page 25 of [37]. In particular:

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

Then:

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

whereas, with integration by parts:

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

Also:

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

This brings us to:

$$\frac{1}{2} \int_0^t \|u_n'\|^2_H + \frac{\alpha}{4} \|u_n(t)\|^2_V - \frac{\lambda}{2} \|u_n(t)\|^2_H \leq \tag{B.1.15}$$

$$\frac{1}{2} \|f_2'\|^2_{L^2(I,V^*)} + \frac{1}{2} \|u_n\|^2_{L^2(I,V)} + \tag{B.1.16}$$

$$+ \frac{8+\alpha}{2\alpha} \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1 + \|A\|}{2} \|u_{n0}\|^2_V + \tag{B.1.17}$$

$$+ \frac{1}{2} \|f_1\|^2_{L^2(I,H)} \tag{B.1.18}$$

and thus, because norms are lower semicontinuous and because we have weak convergence of the time derivative, and V-strong convergence of the initial data (see again [37] for this):

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

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

$$\operatorname{limsup}_n \left(\frac{\lambda}{2} \|u_n\|^2_{C([0,T],H)} + \frac{1}{2} \|u_n\|^2_{L^2(I,V)} \right) \leq C_0(\|u_0\|^2_H + \alpha^{-1} \|f_1\|^2_{L^2(I,V^*)} + \alpha^{-1} \|f_2\|^2_{L^2(I,V^*)}) \tag{B.1.19}$$

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

Therefore:

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

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:

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

□

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

Proposition B.1.20 (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 [68], theorem 27.2, page 406.

□

B.2. Application to inhomogeneous parabolic problems

B.2.1. Inhomogeneous Dirichlet problem

We make the following assumption.

Assumption B.2.1.1 (Assumptions for problem B.2.1.2)
We assume $\Omega \subset\subset D$ to be bounded Lipschitz domains, so that $U := D \setminus \Omega$ is 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 [52]). For such a choice we also have $H^1_0 = H^1 \cap \ker \mathrm{tr}$, see [47], page 595, theorem 18.7.
Moreover, we select $f \in H^1(I, H^{1/2}(\Gamma_f))$, $f(0) = 0$.

Note that, given a bounded extension operator $E : H^{1/2}(\partial U) \to H^1(U)$, we obtain by corollary A.2.2 that $Ef \in H^1(I, H^1(U))$. We have defined $\mathrm{tr}u(t) := tr(u(t))$ and analogously $Eu(t) := E(u(t))$ (see proposition A.2.6).
Call $H = L^2(U)$, $V = \{v \in H^1(U), \mathrm{tr}u = 0 \text{ on } \Gamma_m\} =: H^1_{0,m}$. 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 problem under consideration is the following. For $U = D \setminus \Omega$ we have:

Problem B.2.1.2 (Inhomogeneous heat equation, Dirichlet conditions)

$$u_t - \Delta u = 0 \text{ in } (0,T) \times U \tag{B.2.1.3}$$
$$u(\Sigma_f) = f \tag{B.2.1.4}$$
$$u(\Sigma_m) = 0 \tag{B.2.1.5}$$
$$u(0) = 0 \tag{B.2.1.6}$$

By this we mean:

$$u \in W(I, H^1_{0,m}) \tag{B.2.1.7}$$
$$u_t|_{H^{-1}} + Au = 0 \text{ in } H^{-1} \text{ and for a.e. } t \in (0,T) \tag{B.2.1.8}$$
$$\mathrm{tr}u = f \text{ on } \Sigma_f \tag{B.2.1.9}$$
$$u(0) = 0 \tag{B.2.1.10}$$

Theorem B.2.1.11 (Well posedness and regularity for problem B.2.1.2)
Given assumption B.2.1.1, the solution u to problem B.2.1.2 is unique with $u_t \in L^2(I, H)$.
The problem is equivalent to:

Problem B.2.1.12 (Equivalent formulation with extension)

$$\delta \in W(I, H_0^1) \tag{B.2.1.13}$$

$$\delta' + A\delta = -((\bar{u}', \cdot)_H + A\bar{u}) \text{ in } H^{-1} \text{ and for a.e. } t \in (0,T) \tag{B.2.1.14}$$

$$\delta(0) = 0 \tag{B.2.1.15}$$

with $\bar{u}$ any given $\bar{u} \in H^1(I, H^1_{0,m}(U))$ such that $\mathrm{tr}\bar{u} = f$ on Σ_f, and with $\bar{u}(0) = 0$. This means that u solves problem B.2.1.2, then $u - \bar{u}$ solves problem B.2.1.12, and if $\delta(\bar{u})$ solves problem B.2.1.12, then $\bar{u} + \delta(\bar{u})$ solves problem B.2.1.2.
Furthermore:

$$\|u\|^2_{C([0;T],H)} + \|u\|^2_{L^2(I,H)} + \|\nabla u\|^2_{L^2(I,H)} + \|u'\|^2_{L^2(I,H)} \leq C(T)\,\|\bar{u}\|^2_{H^1(I,V)} \tag{B.2.1.16}$$

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

Proof.

Extension of the boundary data

Let $\bar{u} \in H^1(I, H^1_{0,m}(U))$ be such that $\mathrm{tr}\bar{u} = f$ on Σ_f, and with $\bar{u}(0) = 0$. We can choose for instance $E\tilde{f}$, see proposition A.2.6, where $\tilde{f} = 0$ on Σ_m, $\tilde{f} = f$ on Σ_f. $\tilde{f} \in H^1(I, H^{1/2}(\partial U))$, because Γ_f and Γ_m have positive distance (see the definition of the norm in [38], page 20).

Reformulation (first part)

We consider the problem:

$$\delta \in W(I, H_0^1) \tag{B.2.1.17}$$

$$\delta' + A\delta = -(f_1 + f_2) \text{ in } H^{-1} \text{ and for a.e. } t \in (0,T) \tag{B.2.1.18}$$

$$\delta(0) = 0 \tag{B.2.1.19}$$

Here, $f_1 := u_t \in L^2(I,H)$. Moreover, $A \in L(V, H^{-1})$, so, by corollary A.2.2, $f_2 := A\bar{u} \in H^1(I, H^{-1})$.

Existence

By proposition B.1.8 we get a solution of the above problem with $\delta' \in L^2(I,H)$, which is easily seen to satisfy problem B.2.1.2.

Uniqueness

For two solutions u_1, u_2 of *problem B*.2.1.2 we can form $d := u_1 - u_2 \in W(I, H_0^1)$. Clearly, $d(0) = 0$. Moreover, $d' - Ad = 0$. By uniqueness stated in theorem B.1.5 we obtain $d = 0$ in $L^2(I,H)$, so that the solution is unique and doesn't depend on the choice of the extension of the Dirichlet datum.

Reformulation (part 2)

Therefore $u = \bar{u} + \delta$ above is the unique solution of problem B.2.1.2. So, given any $\bar{u} \in H^1(I, H^1_{0,m}(U))$ such that $\mathrm{tr}\bar{u} = f$ on Σ_f, and with $\bar{u}(0) = 0$, we can construct δ as above and get $u = \bar{u} + \delta$ solving problem B.2.1.2.

Viceversa, let u solve problem B.2.1.2. Call $\delta = u - \bar{u}$. Then, as seen above, $\delta \in W(I, H_0^1)$ and it is readily seen that δ solves problem B.2.1.12.

Regularity

Let $u = \bar{u} + \delta$ be the unique solution, as before, of problem B.2.1.2. But $u' = \bar{u}' + \delta'$, proving the additional time smoothness claim.

Stability

Let $\bar{u} \in H^1(I, H^1_{0,m}(U))$ such that $\mathrm{tr}\bar{u} = f$ on Σ_f, and with $\bar{u}(0) = 0$. Then $u = \bar{u} + \delta$. The desired estimate follows by such splitting and upon applying proposition B.1.8 to δ. Note that we norm H_0^1 with the full H^1 norm, and that we can choose $\alpha = \lambda = 1$. □

B.2.2. Inhomogeneous Neumann-Dirichlet problem

We make the following assumption.

Assumption B.2.2.1 (Assumptions for problem B.2.1.2)
We keep assumption B.2.1.1 (apart from the Dirichlet datum). We consired $g \in H^1(I, L^2(\Gamma_f))$, $g(0) = 0$.

Again, call $H = L^2(U)$, $V = \{v \in H^1(U), \mathrm{tr}u = 0 \text{ on } \Gamma_m\} =: H^1_{0,m}$. H, V induce a Gelfand triple as seen before.
The problem under consideration is:

Problem B.2.2.2 (Inhomogeneous heat equation, Neumann conditions)

$$u_t - \Delta u = 0 \text{ in } (0,T) \times U \tag{B.2.2.3}$$
$$\partial_\nu u(\Sigma_f) = g \tag{B.2.2.4}$$
$$u(\Sigma_m) = 0 \tag{B.2.2.5}$$
$$u(0) = 0 \tag{B.2.2.6}$$

By this we mean:

$$u \in W(I, H^1_{0,m}) \tag{B.2.2.7}$$
$$u_t + Au = G \text{ in } V^* \text{ and for a.e. } t \in (0,T) \tag{B.2.2.8}$$
$$u(0) = 0 \tag{B.2.2.9}$$

where $\langle G(t), v\rangle_{V^*,V} := \int_{\Gamma_f} g(t)\mathrm{tr}v d\sigma$, σ the 1-codimensional Hausdorff measure, and A was introduced before in $L(V, H^{-1})$.

Note, by corollary A.2.2, $G \in H^1(I, V^*)$. Moreover, $\langle Av, v\rangle_{V^*,V} + 1 \cdot \|v\|_H = 1 \cdot \|V\|$, so that we can immediately conclude:

Theorem B.2.2.10 (Well posedness and regularity for problem B.2.2.2)
Given assumption B.2.2.1, the solution u to problem B.2.2.2 is unique with $u_t \in L^2(I, H)$.
Furthermore:

$$\|u\|^2_{C([0;T],H)} + \|u\|^2_{L^2(I,H)} + \|\nabla u\|^2_{L^2(I,H)} + \left\|u'\right\|^2_{L^2(I,H)} \leq C(T)\, \|g\|^2_{H^1(I,L^2(\Gamma_f))} \tag{B.2.2.11}$$

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

Proof.
It is an application of theorem B.1.5, proposition B.1.8 and proposition B.1.8. □

B.2.3. Space-time regularity for a more general problem

Here, we build on the results of the last subsections, and prove higher spatial and time regularity, under suitable smoothness assumptions.
The overall problem, comprehensive of both problem B.2.1.2 and problem B.2.2.2, is:

Problem B.2.3.1 (Inhomogeneous heat equation, general case)

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

Calling $V := H^1_{0,m}(U)$ (see assumption B.2.2.1), and $H = L^2(U)$, we mean:

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

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 [49], 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 assuming more regularity on the data, it is possible to obtain higher regularity of the solution in a fairly easy way.

Assumption B.2.3.2 (Basic assumption for problem B.2.3.1)

1. $u_0 \in H^1(U)$
2. $\Omega \subset\subset D$ are bounded Lipschitz domains

3. $A : H^1 \to (H^1)^*$, $(Au)v = \int_U \nabla u \nabla v$

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

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

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

Assumption B.2.3.3 (Time regularity assumption for problem B.2.3.1)
Let $k \geq 1$, consider any splitting $u = \bar{u} + \delta$, where, similarly to problem B.2.1.12, $\bar{u}$ extends the Dirichlet data.
We ask, aside from assumption B.2.3.2:

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.1.20, for the equation satisfied by δ
5. $g_j(\delta) \in H$

Assumption B.2.3.4 (Additional time regularity assumptions)
Apart from assumption B.2.3.2 and assumption B.2.3.3, 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.2.3.5 (Spatial regularity assumptions)
Let assumption B.2.3.2 for $k = 0$, and also assumption B.2.3.3 and assumption B.2.3.4 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.2.3.6 (Regularity results for problem B.2.3.1)
Under assumption B.2.3.2:

- there exists a unique $u \in W(I, H^1(U))$ solution to problem B.2.3.1
- for such u there holds $u' \in L^2(I, L^2(U))$ with:

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

Under assumption B.2.3.3 have that $u \in H^k(I, V) \cap (H^{k+1}(I, V) + H^{k+1}(I, V^*))$.
Under assumption B.2.3.4, $u^{k+1} \in H^1(I, H)$, or $u \in H^{(k+1)}(I, H)$, and, for $1 \leq j \leq k$:

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

Finally, if assumption B.2.3.5 holds, then $u \in H^k(I, H^2(U)) \cap H^{k+1}(I, H)$.

Proof.

Well-posedness, stability

Existence and uniqueness follow with similar arguments as in the previous subsections. In particular, $u = G_D + \delta$, where $G_D = \bar{u}$ is (for a.e. t), an extension of g_D. Using the results of trace theory we know, in particular, that $G_D \in H^1(U)$ with $\|G_D\|_{H^1} \leq C(U)\,\|g_D\|_{H^{1/2}(U)}$.
$\delta \in W(I, V) \cap H^1(I, H)$ is the solution to:

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

Note that $G_D(0)$ makes sense, being $g_D \in C([0,T], H^{1/2}(\Gamma_D))$ and $g_D \mapsto G_D$ is linear bounded, so that we can apply corollary A.2.2. We can therefore deduce the estimate:

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

Regularity: time smoothness

So, proposition B.1.20 ensures then that $\delta \in H^k(I,V)$, $\delta^{(k+1)} \in L^2(I,V^*)$. Because we $G_D \in H^{k+1}(I,H^1(U))$ by our assumptions and corollary A.2.2 we obtain that $u = G_D + \delta$ 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.1.20 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 $F^{(k)} = (f^{(k)} - G_D^{(k+1)}, \cdot)_H + (g_N^{(k)}, \mathrm{tr}(\cdot))_{L^2(\Gamma_N)}$ 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 $g_k \in V$.

With analogous reasoning to theorem B.2.1.11 we conclude that $u \in H^{(k+1)}(I,H)$, and, for $1 \leq j \leq k$:

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

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 [38] let us conclude the proof. □

B.3. Reformulation of parabolic equations

We just saw that the two parabolic equations of interest can be recasted into the problem of finding $u \in W(I,V)$, $u(0) = 0$, $u_t + Au = f$ for a.e. t in V^*, with notation from preceding sections.

In particular, $f \in L^2(I,V^*)$ and so is Au (because $A \in L(V,V^*)$, and by corollary A.2.2).

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

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

We can view $L^2(I,V^*) \cong L^2(I,V)^*$. Hence $\langle E(u), v\rangle_{L^2(I,V)^*,L^2(I,V)} = \int_I \langle E(u)(t), v(t)\rangle_{V^*,V} dt$ (see [41], theorem 1.31 at page 39). We are now ready to restrict both state and adjoint space, in view of the proof of proposition 2.2.11.

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 $\|v\|_Q^2 = \|v\|^2_{L^2(I,V)} + \|v_t\|^2_{L^2(I,H)}$.

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: $\int_I (v_t, w)_H = -\int_I (w_t, v)_H + (v(T), w(T))_H - (v(0), w(0))_H$
- 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 [30], 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 [41], 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 [64].

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 V is bounded by the full H^1 norm, as we declared already. Therefore, 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. □

We can therefore restrict the testing space.

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

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

We have also seen that with smoothness assumption on data (assumption B.2.1.1 and assumption B.2.2.1) we obtain that the solutions of problem B.2.1.2, problem B.2.2.2 have $Q_0(I, V)$ smoothness.

We can therefore formulate the two partial differential equations directly on $Q_0(I, V)$ as follows.

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

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.2.1.1, assumption B.2.2.1. Thanks to proposition B.3.5, by the regularity ensured by theorem B.2.1.11, theorem B.2.2.10, and thanks to proposition B.3.3, we get:

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

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

Conversely, a solution $w \in Q_0(I, H^1_{0,m}), \bar{u} + v_0 \in Q_0(I, H^1_{0,m}), v_0 \in Q_0(I, H^1_0)$ to the above problem satisfies $w \in W_0(I, H^1_{0,m}), \bar{u} + v_0 \in W_0(I, H^1_{0,m}), v_0 \in W_0(I, H^1_0)$, see proposition B.3.3, and the proof of theorem B.2.1.11 . And by proposition B.3.3 at first, and then by proposition B.3.4 we obtain back:

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

Therefore:

Proposition B.3.5 (Equivalent formulation)
Under assumption B.2.1.1, assumption B.2.2.1, problem B.2.1.2, problem B.2.2.2 can be equivalently formulated as:

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

Existence, uniqueness and stability proved already in theorem B.2.1.11, theorem B.2.2.10 carry over to this new formulation.

C. Domains transformations

C.1. Transforming domains

Throughout, D is a bounded Lipschitz domain. We define as in [59] the following spaces of transformations:

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

- $\mathcal{V}^k = \{\tau \in \mathcal{M}, \tau - \mathrm{Id} \in W^{k,\infty}(\mathbb{R}^n, \mathbb{R}^n)\}$, $k \geq 1$
- $\mathcal{T}^k = \{\tau \in \mathcal{V}^k$ 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 [59], lemme 2.1 at page II-6, lemme 4.2, pag. IV-7.

□

We go on to define the space of admissible transformations.

Definition C.1.3 (Admissible transformations)
We define $\Theta := \{\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ with $\theta = 0$ 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.
<u>Perturbation of identity</u>
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 [59], 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.
<u>Perturbation, not of identity</u>
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. □

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 $\|\tau - \mathrm{Id}\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \le C(U)$, 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. □

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 $f \in L^p(\tau(U))$:
$$\|f\|_{L^p(\tau(Q))} \le \left(\|\det D\tau\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \|f \circ \tau\|_{L^p(Q)}$$
2. $f \in W^{1,p}(\tau(U)) \iff f \circ \tau \in W^{1,p}(U)$ and there holds, for $f \in W^{1,p}(\tau(U))$:
$$Df \circ \tau = (Df)^{-t} D(f \circ \tau)$$
$$\|Df\|_{L^p(\tau(Q);\mathbb{R}^n)} \le \left(\|\det D\tau\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \left\|(D\tau)^{-1}\right\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})} \|D(f \circ \tau)\|_{L^p(Q;\mathbb{R}^n)}$$
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 $H^1_{0,m}(U)$ and $H^1_{0,m}(\tau(U))$ ($H^1_{0,m}$ is defined in appendix B.2.1 as $\{u \in H^1, u(\Gamma_m) = 0)$

Proof.
We need to prove only the last points, for the other are proved in [59], pages IV.4, IV.5, IV.6.
Static strace
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:
$$\mathrm{tr}_D f \leftarrow_{L^2(\partial D)} \mathrm{tr}(f_n) = f_n|_{\partial D} = (f_n \circ \tau)|_{\partial D} = \mathrm{tr}(f_n \circ \tau) \to_{L^2(\partial D)} \mathrm{tr}_D(f \circ \tau)$$
Moving trace
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: $\mathrm{tr}_{\tau(U)} f|_{\partial D} = \mathrm{tr}_D \bar{f} = \{$ 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 $H^1_0(\tau(U))$ (theorem 18.7 at page 595 of [47])). □

C.3. Transforming Bochner spaces

Proposition C.3.1 (Isomorphism between Q spaces)
Let $\tau \in \mathcal{T}$. Then:

$$\circ\tau : Q(I, V_\tau) \to Q(I, V)$$

is a linear isomorphism, and so is:

$$\circ\tau : Q_0(I, V_\tau) \to Q_0(I, V)$$

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 $\circ\tau^{-1}$. □

C.4. Transforming partial differential equations

We consider again the two parabolic equations of interest, namely, problem B.2.1.2 and problem B.2.2.2. We are working under the assumption:

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 $H^1_{0,m}(\tau(U)) = \mathtt{W}_\tau, H^1_{0,m}(U) = \mathtt{W}, H^1_0(U) = \mathtt{V}$ 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
- $w^\tau_t \circ \tau = (w^\tau \circ \tau)_t$ 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:

$$\begin{aligned} w^\tau \in Q_0(I, \mathtt{W}_\tau), v^\tau_0 \in Q_0(I, \mathtt{V}_\tau) \\ \int_I ((w^\tau \circ \tau)_t, q|\det(D\tau)|)_H + (A_\tau \nabla(w^\tau \circ \tau), \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W}) \\ \int_I ((v^\tau_0 \circ \tau)_t, p|\det(D\tau)|)_H + (A_\tau \nabla(v^\tau_0 \circ \tau), \nabla p)_H = \\ -\int_I ((\bar{u} \circ \tau)', p|\det(D\tau)|)_H + (A_\tau \nabla(\bar{u} \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V}) \end{aligned}$$

and by proposition C.3.1, we also get $w^\tau \circ \tau \in Q_0(I, \mathtt{W}), v^\tau_0 \circ \tau \in Q_0(I, \mathtt{V})$. Here $A_\tau = |\det(D\tau)| D\tau^{-1}(D\tau)^{-t}$.

On the other hand, consider:

$$\begin{aligned} w \in Q_0(I, \mathtt{W}), v_0 \in Q_0(I, \mathtt{V}) \\ \int_I (w_t, q|\det(D\tau)|)_H + (A_\tau \nabla w, \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W}) \\ \int_I (v_{0t}, p|\det(D\tau)|)_H + (A_\tau \nabla v_0, \nabla p)_H = \\ -\int_I ((\bar{u} \circ \tau)', p|\det(D\tau)|)_H + (A_\tau \nabla(\bar{u} \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V}) \end{aligned}$$

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:

$$
\begin{aligned}
w \circ \tau^{-1} \in Q_0(I, \mathtt{W}_\tau), v_0 \circ \tau^{-1} \in Q_0(I, \mathtt{V}_\tau) \\
\int_I ((w \circ \tau^{-1})_t, q^\tau)_{H_\tau} + (\nabla(w \circ \tau^{-1}), \nabla q^\tau)_{H_\tau} = \int_I (g, \mathrm{tr}_{\tau(U)} q^\tau)_{L^2(\Gamma_f)}, \quad \forall q^\tau \in Q^0(I, \mathtt{W}_\tau) \\
\int_I ((v_0 \circ \tau^{-1})_t, p^\tau)_{H_\tau} + (\nabla(v_0 \circ \tau^{-1}), \nabla p^\tau)_{H_\tau} = -\int_I (\bar{u}', p^\tau)_{H_\tau} + (\nabla \bar{u}, \nabla p^\tau)_{H_\tau}, \quad \forall p^\tau \in Q^0(I, \mathtt{V}_\tau)
\end{aligned}
$$

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.2.1.1, assumption B.2.2.1, assumption C.4.1 hold.
Consider the following problems, where $\tau \in \mathcal{T}$.

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

$$
\begin{aligned}
w^\tau \in Q_0(I, \mathtt{W}_\tau), v_0^\tau \in Q_0(I, \mathtt{V}_\tau) \\
\int_I (w_t^\tau, q^\tau)_{H_\tau} + (\nabla w^\tau, \nabla q^\tau)_{H_\tau} = \int_I (g, \mathrm{tr}_{\tau(U)} q^\tau)_{L^2(\Gamma_f)}, \quad \forall q^\tau \in Q^0(I, \mathtt{W}_\tau) \\
\int_I (v_{0t}^\tau, p^\tau)_{H_\tau} + (\nabla v_0^\tau, \nabla p^\tau)_{H_\tau} = -\int_I (\bar{u}', p^\tau)_{H_\tau} + (\nabla \bar{u}, \nabla p^\tau)_{H_\tau}, \quad \forall p^\tau \in Q^0(I, \mathtt{V}_\tau)
\end{aligned}
$$

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

$$
\begin{aligned}
w \in Q_0(I, \mathtt{W}), v_0 \in Q_0(I, \mathtt{V}) \\
\int_I (w_t, q|\det(D\tau)|)_H + (A_\tau \nabla w, \nabla q)_H = \int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W}) \\
\int_I (v_{0t}, p|\det(D\tau)|)_H + (A_\tau \nabla v_0, \nabla p)_H = \\
-\int_I ((\bar{u} \circ \tau)', p|\det(D\tau)|)_H + (A_\tau \nabla(\bar{u} \circ \tau), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V})
\end{aligned}
$$

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. Finite element method on smooth domains

Handling smooth geometries in finite element analysis is not a trivial task. On one hand, finite element discretization is naturally done on polygonal/polyhedral domains, whereas the solution smoothness 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 [63]): an example of this in a setting close to ours, is contained in [42].

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 [69]. 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 [63]: 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 the approach that was the least intrusive 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 ([35]), and powerful finite element libraries can be directly used to simulate the partial differential equations, we used Fenics ([51]).

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 require "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 virtually all 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 [28], [27], [10] and [26].

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 quasi-uniform mesh. There exists, for h small enough, $G_h : \overline{\Omega_h} \to \overline{\Omega}$ satisfying:

- $G_h|_T = \mathrm{Id}$ 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 [28])
- G_h is bi-Lipschitz, with $\|\mathrm{Id} - G_h\|_{W^{1,\infty}(\Omega_h)} \lesssim h$, 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 [28] for the first two points, which follow from the definition of G_h. See also Lemma 8.16 of [27].

The last one is contained in Lemma 8.12, [27]. We give more detail for the third and fourth point, which are not addressed in [27], [28].

G_h 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 [27] shows that $\|\mathrm{Id} - G_h\|_{W^{1,\infty}(\Omega_h)} \lesssim h$. 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 $\mathrm{Lip}(\mathrm{Id} - G_h) \lesssim \|\mathrm{Id} - G_h\|_{W^{1,\infty}(\Omega_h)}$.

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

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 [66]) 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 [27] (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. [39], chapter 1) yields that G_h extends to a C^1 diffeomorphism around K, so that the smoothness of ∂K follows. □

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 $u_h^l := u_h \circ G_h^{-1}$. We also need the mesh to be quasi-uniform (see proposition 4.7 of [28]).
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. $\|v_h\|_{L^2(\partial\Omega_h)} \sim \left\|v_h^l\right\|_{L^2(\partial\Omega)}$
  2. $\|v_h\|_{L^2(\Omega_h)} \sim \left\|v_h^l\right\|_{L^2(\Omega)}$
  3. $\|\nabla v_h\|_{L^2(\Omega_h)} \sim \left\|\nabla v_h^l\right\|_{L^2(\Omega)}$
- 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 [47].

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 [28], see e.g proposition 4.9 and 4.13. □

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 [28]. □

Proposition D.1.5 (Approximation of linear and bilinear forms)
Let $v_h, w_h \in S_h^1$, $v, w \in H^2(\Omega)$, $\delta\theta_h \in (S_h^1)^d$ (d is the dimension of Ω), $\delta\theta \in W^{1,\infty}(\Omega;\mathbb{R}^d)$, $\delta_h\theta \in W^{1,\infty}(\Omega_h;\mathbb{R}^d)$. 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 [26], and in particular, for the second point, Lemma 5.6 of [45]. Only the last three points are not already present in the literature, but the follow with very similar arguments as the others. See for instance, section 6 of [28]: 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, [28], as suggested in Lemma 6.4 of [28], 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 [25]), 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.2.3.1, 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.2.3.2.

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 [62] in e.g. theorem 1.2. To deal with the polygonal/polyhedral domain approximation we adapt some arguments contained in [27], 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:

$$a_h(R_h z, v_h) = a(z, v_h^l), v_h \in S^1_{h,0,D_h}$$
$$R_h z = \Pi_h z \text{ on } \partial\Omega_h$$

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 $S^1_{h,0,D_h}$ by proposition D.1.6 and the Lax-Milgram lemma yield existence, uniqueness follows as in theorem B.2.1.11

Now, for the stability: by uniform coercivity and the definition of R_h: $\|R_h z\|^2_{H^1(\Omega_h)} \lesssim a_h(R_h z, R_h z) = a_h(\delta_h, R_h z) + a_h(\Pi_h z, R_h z)$, 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 [27], 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:

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

and:

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

The first term is bounded as in the proof of lemma 3.8 of [27], 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. □

Assumption D.2.4 (Smoothness requirement on continuous solution)
We assume that $u \in H^1(I, H^2(\Omega))$.

Note, for the parabolic problems arising from shape optimization (problem 2.1.1), theorem B.2.3.6 suffices.

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

Problem D.2.5 (Spatially semidiscrete approximation of problem D.2.1)
We look for $u_h \in H^1(I, S_h^1)$ satisfying:

$$(\partial_t u_h, v_h)_{L^2(\Omega_h)} + a_h(u_h, v_h) = (f_h, v_h)_{L^2(\Omega_h)} + (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}, v_h \in S^1_{h,0,D_h}, \text{ for a.e. } t \in I$$

$$u_h = g_{D,h} \text{ for a.e. } t, \text{ on } \Gamma_{D_h}$$

$$u_h(0) = u_{0h}$$

We are making the following assumptions on the data:

Assumption D.2.6 (Assumptions for the spatial semidiscretization)

- assumption D.1.1
- $g_N \in L^2(I, H^2(\Omega))$, so that $g_{N,h} := \Pi_h g_N \in L^2(I, S_h^1(\Gamma_{N_h}))$
- $g_D \in H^1(I, H^2(\Gamma_D))$, so that, with reference to proposition A.2.6, we have $G_D := Eg_D \in H^1(I, H^2(\Omega))$ and therefore (see corollary A.2.2), there holds $G_{D,h} := \Pi_h G_D \in H^1(I, S_h^1)$ and $g_{D,h} := G_{D,h}|_{\Gamma_{D_h}} \in H^1(I, S_h^1(\Gamma_{D_h}))$ (note, $g_{D,h} = \Pi_h g_D$)
- $f \in L^2(I, L^2(\Omega))$ and $f_h \in L^2(I, S_h^1)$, with error bound $\|f - f_h^l\|_{L^2(\Omega_h)} \lesssim C_f h^2$, for a.e. t, C_f independent of h and belonging to $L^2(I)$.
- $u_0 \in H^2(\Omega)$, with the compatibility condition $u_0 = g_D(0)$ on Γ_D, and $u_{0h} := \Pi_h u_0$

(note that these assumptions can be relaxed for proving the well posedness of the scheme, and other choices of the discrete data might be possible. They become important when proving error bounds, so that we assume them right away. In particular, one could choose $f_h = \Pi_h f$, for $f \in L^2(U, H^2(\Omega))$ and obtain the same results).

Proposition D.2.7 (Well posedness of problem D.2.5)
There exists a unique solution to problem D.2.5, and this satisfies the stability estimate, holding for small enough h:

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

We remember that $\lesssim$ stands for $\leq C$, $C \geq 0$ independent of h and t.

Proof.
Existence and uniqueness
A function $\delta_h \in H^1(I, S^1_{h,0,D_h})$ can be written as $\delta_h = \sum_j d_{hj}(t) v_{hj}$, for the usual finite element basis $\{v_{hj}\}_j$ of $S^1_{h,0,D_h}$. 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 $S^1_{h,0,D_h}$. 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 [56], 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 energy estimates. Stability
Following [37], page 20, 21, we can prove energy 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 $H^2(\Omega) \to S_h^1$ 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:

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

□

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

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

where $A^2 := \|u\|^2_{H^1(I,H^2(\Omega))} + \|g_D\|^2_{H^1(I,H^2(\Gamma_D))} + \|u_0\|^2_{H^2(\Omega)} + \int_0^T C_f^2 + \int_0^T \|f_h\|^2_{H^1(\Omega_h)} + \int_0^T \|g_N\|^2_{H^2(\Gamma_N)}$.
For this to hold, assumption D.2.4, assumption D.2.6 and assumption B.2.3.2 must be fulfilled.

Proof.
Also here, we adapt the argument from [27], in particular, those of pages 1727, 1728, 1729, which are modifications of standard techniques that can be traced in e.g. [62], 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 $\theta_h := R_h u - u_h$. Is 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 $v_h \in S^1_{h,0,D_h}$:

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

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

$$\begin{aligned}(\partial_t \theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h) = (\partial_t R_h u, v_h)_{L^2(\Omega_h)} - (\partial_t R_c u, v_h^l)_{L^2(\Omega)} \quad &\text{(D.2.11)} \\ -(\partial_t \rho, v_h^l)_{L^2(\Omega)} \quad &\text{(D.2.12)} \\ +(f, v_h^l)_{L^2(\Omega)} - (f_h, v_h)_{L^2(\Omega_h)} \quad &\text{(D.2.13)} \\ +(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})} \quad &\text{(D.2.14)}\end{aligned}$$

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:

$$\begin{aligned}|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \leq \\ |(g_N - g_{N,h}^l, v_h^l)_{L^2(\Gamma_N)}| + |(g_{N,h}^l, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}|\end{aligned}$$

By proposition D.1.5 and trace theorems there holds:

$$
\begin{aligned}
&|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \lesssim \\
&\left\| g_N - g_{N,h}^l \right\|_{L^2(\Gamma_N)} \left\| v_h^l \right\|_{H^1(\Omega)} + h^2 \left\| g_{N,h} \right\|_{L^2(\Gamma_{N_h})} \left\| v_h \right\|_{H^1(\Omega_h)}
\end{aligned}
$$

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:

$$
\begin{aligned}
&|(f, v_h^l)_{L^2(\Omega)} - (f_h, v_h)_{L^2(\Omega_h)}| \lesssim \\
&\left\| f - f_h^l \right\|_{L^2(\Omega)} \left\| v_h \right\|_{H^1(\Omega_h)} + h^2 \left\| f_h \right\|_{H^1(\Omega_h)} \left\| v_h \right\|_{H^1(\Omega_h)} \lesssim (C_f + \left\| f_h \right\|_{H^1(\Omega_h)}) h^2 \left\| v_h \right\|_{H^1(\Omega_h)}
\end{aligned}
$$

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: energy 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 [37]), 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 apply also 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:

$$
\begin{aligned}
&\left\| e(t) \right\|_{L^2(\Omega)}^2 + h^2 \int_0^T \left\| e \right\|_{H^1(\Omega)}^2 \lesssim \\
&h^4 \left\| u(t) \right\|_{H^2(\Omega)}^2 + h^4 \left\| g_D(t) \right\|_{L^2(\Gamma_D)}^2 + h^2 h^2 \int_0^T \left\| u \right\|_{H^2(\Omega)}^2 + h^4 \int_0^T Q^2 + \left\| \theta_h^l(0) \right\|_{L^2(\Omega)}^2
\end{aligned}
$$

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.2.3.2, 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 $B := \left\| u \right\|_{H^1(I, H^2(\Omega))}^2 + \left\| g_D \right\|_{H^1(I, H^2(\Gamma_D))}^2 + \int_0^T C_f^2 + \left\| f_h \right\|_{L^2(I, L^2(\Omega_h))}^2 + \left\| g_N \right\|_{H^1(H^2(\Gamma_N))}^2 + \left\| u_0 \right\|_{H^2(\Omega)}^2$.

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 $\partial_t \theta_h \in L^2(I, S^1_{h,0,D_h})$. This is possible also by the reasonings in [41], (1.61), page 42. Integrate from 0 to t to obtain:

$$
\begin{aligned}
\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} + \frac{1}{2}\left(a_h(\theta_h(t), \theta_h(t)) - a_h(\theta_h(0), \theta_h(0))\right) = \int_0^t (\partial_t R_h u, \partial_t \theta_h)_{L^2(\Omega_h)} - \int_0^t (\partial_t R_c u, \partial_t \theta_h^l)_{L^2(\Omega)} \\
- \int_0^t (\partial_t \rho, \partial_t \theta_h^l)_{L^2(\Omega)} \\
+ \int_0^t (f, \partial_t \theta_h^l)_{L^2(\Omega)} - \int_0^t (f_h, \partial_t \theta_h)_{L^2(\Omega_h)} \\
+ \int_0^t (g_N, \partial_t \theta_h^l)_{L^2(\Gamma_N)} - \int_0^t (g_{N,h}, \partial_t \theta_h)_{L^2(\Gamma_{N_h})}
\end{aligned}
$$

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:

$$
\begin{aligned}
\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} + \frac{1}{2}\|\theta_h(t)\|^2_{H^1(\Omega_h)} \leq \frac{1}{2}\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \frac{1}{2}\|\theta_h(0)\|^2_{H^1(\Omega_h)} \\
+ Ch^2 \int_0^t \|\partial_t u\|^2_{H^2(\Omega)} + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} \\
+ Ch^2 \int_0^t \left(\|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}\right)^2 + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} \\
+ Ch^2 \int_0^t C_f^2 + Ch^2 \int_0^t \|f_h\|^2_{L^2(\Omega_h)} + \frac{1}{6}\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} \\
+ Ch^2 \int_0^t \|\partial_t g_N\|^2_{H^2(\Gamma_N)} + \int_0^t \|\theta_h\|^2_{H^1(\Omega_h)} \\
+ Ch^2 \|g_N(t)\|^2_{H^2(\Gamma_N)} + \frac{1}{4}\|\theta_h(t)\|^2_{H^1(\Omega_h)} \\
+ Ch^2 \|g_N(0)\|^2_{H^2(\Gamma_N)} + \frac{1}{2}\|\theta_h(0)\|^2_{H^1(\Omega_h)}
\end{aligned}
$$

where C is independent of h and t. We re-arrange, and apply eq. (D.2.16) to the term $\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \int_0^t \|\theta_h\|^2_{H^1(\Omega_h)}$.
Calling $q = \int_0^T \left[\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)} + C_f^2 + \|f_h\|^2_{L^2(\Omega_h)} + Q^2 + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t g_N\|^2_{H^2(\Gamma_N)}\right]$, and upon using proposition D.1.3, proposition D.2.3 and proposition D.1.4:

$$
\int_0^T \left\|\partial_t \theta_h^l\right\|^2_{L^2(\Omega)} + \left\|\theta_h(t)^l\right\|^2_{H^1(\Omega)} \lesssim \|\theta_h(0)\|^2_{H^1(\Omega_h)} + h^4 q \lesssim h^2 \|u_0\|^2_{H^2(\Omega)} + h^4 q
$$

Conclusion
There holds

$$
\begin{aligned}
\|e(t)\|^2_{H^1(\Omega)} + \int_0^T \|\partial_t e\|^2_{L^2(\Omega)} \leq \\
\int_0^T \|\partial_t \rho\|^2_{L^2(\Omega)} + h^2\|\rho(t)\|^2_{H^1(\Omega)} + \int_0^T \left\|\partial_t \theta_h^l\right\|^2_{L^2(\Omega)} + \left\|\theta_h^l(t)\right\|^2_{H^1(\Omega)} \leq \{ \text{ above, and proposition D.2.3 } \} \leq \\
h^2 \int_0^T \left(\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}\right) + h^2\|u(t)\|^2_{H^2(\Omega)} + h^2\|u_0\|^2_{H^2(\Omega)} + h^4 q
\end{aligned}
$$

□

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.2.3.2 we have, for all $w \in L^2(I, H^1_{0,D}(\Omega))$:

$$\left|\int_I (\partial_t(u-u_h^l), w)_{L^2(\Omega)}\right| \lesssim h^2 A \left\|w\right\|_{L^2(I,H^1(\Omega))}$$

Proof.
We introduce the L^2 projection $\pi_h : L^2(\Omega) \to S^1_{h,0,D_h}$, given by:

$$(\pi_h w, v_h)_{L^2(\Omega_h)} = (w, v_h^l)_{L^2(\Omega)}, \quad \forall v_h \in S^1_{h,0,D_h}$$

The definition is remimniscent of that of the Ritz projection. We will prove well-posedness and H^k stability of such projection, i.e. $\left\|\pi_h w\right\|_{H^k(\Omega_h)} \lesssim \left\|w\right\|_{H^k(\Omega)}$, for $k = 0, 1$. First, let us show how this projection helps in the estimate.
<u>Conclusion</u>
For $w \in H^1_{0,D}(\Omega)$ we estimate $(\partial_t(\theta_h^l), w)_{L^2(\Omega)} = (w, (\partial_t\theta_h^l))_{L^2(\Omega)} = (\pi_h w, \partial_t\theta_h)_{L^2(\Omega_h)}$. We have also used that lifting and differentiating with respect to time commute, by proposition D.1.3 and corollary A.2.2. We can now apply eq. (D.2.11):

$$\begin{aligned}(\partial_t(\theta_h^l), w)_{L^2(\Omega)} = a_h(\theta_h, \pi_h w) - E_h(\pi_h w) \lesssim \{\text{ eq. (D.2.15) }\} \lesssim \\ \left\|\theta_h\right\|_{H^1(\Omega_h)} \left\|\pi_h w\right\|_{H^1(\Omega_h)} + h^2(\left\|\pi_h w\right\|_{H^1(\Omega_h)} C_f + \left\|f_h\right\|_{H^1(\Omega_h)} + \left\|g_N\right\|_{H^2(\Gamma_N)} + \left\|\partial_t u\right\|_{H^2(\Omega)} + \left\|\partial_t g_D\right\|_{H^2(\Gamma_D)}) \lesssim \\ \left\|\theta_h\right\|_{H^1(\Omega_h)} \left\|w\right\|_{H^1(\Omega)} + h^2 \left\|w\right\|_{H^1(\Omega)} (C_f + \left\|f_h\right\|_{H^1(\Omega_h)} + \left\|g_N\right\|_{H^2(\Gamma_N)} + \left\|\partial_t u\right\|_{H^2(\Omega)} + \left\|\partial_t g_D\right\|_{H^2(\Gamma_D)})\end{aligned}$$

where in the last step we used the supposed stability of π_h. Integrating in time and using the Cauchy-Schwarz inequality:

$$\begin{aligned}\left|\int_I (\partial_t(\theta_h^l), w)_{L^2(\Omega)}\right|^2 \lesssim \\ \left(\int_I \left\|\theta_h\right\|^2_{H^1(\Omega_h)} + h^4 \int_I (C_f^2 + \left\|f_h\right\|^2_{H^1(\Omega_h)} + \left\|g_N\right\|^2_{H^2(\Gamma_N)} + \left\|\partial_t u\right\|^2_{H^2(\Omega)} + \left\|\partial_t g_D\right\|^2_{H^2(\Gamma_D)})\right) \int_I \left\|w\right\|^2_{H^1(\Omega)} \lesssim \{\text{ eq. (D.2.16) }\} \lesssim \\ h^4 \left(\int_I Q^2 + \left\|u_0\right\|^2_{H^2(\Omega)} + \int_I (C_f^2 + \left\|f_h\right\|^2_{H^1(\Omega_h)} + \left\|g_N\right\|^2_{H^2(\Gamma_N)} + \left\|\partial_t u\right\|^2_{H^2(\Omega)} + \left\|\partial_t g_D\right\|^2_{H^2(\Gamma_D)})\right) \left\|w\right\|^2_{L^2(I,H^1(\Omega))}\end{aligned}$$

We can also estimate:

$$\begin{aligned}\left|\int_I (\rho_t, w)_{L^2(\Omega)}\right| \lesssim \{\text{ as in the proof of theorem D.2.10 }\} \lesssim \\ \int_I h^2(\left\|\partial_t w\right\|_{H^2(\Omega)} + \left\|\partial_t g_D\right\|_{H^2(\Gamma_D)}) \left\|w\right\|_{H^1(\Omega_h)} \lesssim \{\text{ Cauchy-Schwarz }\} \lesssim \\ h^2 \sqrt{\left\|\partial_t u\right\|^2_{H^2(\Omega)} + \left\|\partial_t g_D\right\|^2_{H^2(\Gamma_D)}} \left\|w\right\|_{L^2(I,H^1(\Omega))}\end{aligned}$$

and by the usual splitting $e = \rho + \theta_h^l$ we can conclude.
<u>L^2 projection: well-posedness</u>
From the definition of π_h we obtain:

$$(\pi_h w, v_h)_{L^2(\Omega_h)} = (w, v_h^l)_{L^2(\Omega)} = (w^{-l}\xi, v_h)_{L^2(\Omega_h)}$$

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.
<u>L^2 projection: stability</u>
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 $(\pi_h w - \pi_h^* w^{-l}, v_h)_{L^2(\Omega_h)} = (w, v_h^l)_{L^2(\Omega)} - (w^{-l}, v_h)_{L^2(\Omega_h)}$. An application of proposition D.1.5 and of proposition D.1.3 yields:

$$\left\|\pi_h w - \pi_h^* w^{-l}\right\|^2_{L^2(\Omega_h)} \lesssim h \left\|w\right\|_{L^2(\Omega)} \left\|\pi_h w - \pi_h^* w^{-l}\right\|_{L^2(\Omega_h)}$$

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: $|\pi_h w - \pi^* w^{-l}|_{H^1(\Omega_h)} \lesssim h^{-1} \left\|\pi_h w - \pi^* w^{-l}\right\|_{L^2(\Omega_h)} \lesssim \left\|w\right\|_{L^2(\Omega)}$.
For the second term, consider a suitable $w_h \in S^1_{h,0,D_h}$. We have: $|\pi_h^* w^{-l}|_{H^1(\Omega_h)} \leq |\pi_h^*(w^{-l} - w_h)|_{H^1(\Omega_h)} + |\pi_h^* w_h|_{H^1(\Omega_h)} \lesssim h^{-1} \left\|\pi_h^*(w^{-l} - w_h)\right\|_{L^2(\Omega_h)} + \left\|w_h\right\|_{H^1(\Omega_h)}$, 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 [27], 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 [27], 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:

- $\left\|w - w_h^l\right\|_{L^2(\Omega)} \lesssim h\,\|w\|_{H^1(\Omega)}$
- $|w - w_h^l|_{H^1(\Omega)} \lesssim \|w\|_{H^1(\Omega)}$

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.

□

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:

- $g_N \in H^{1/\theta}(I, H^2(\Gamma_N))$
- $g_D \in H^{1/\theta+1}(I, H^{3/2}(\Gamma_D))$
- $f_h \in H^{1/\theta}(I, S^1_h)$
- $\left\|\delta_h(0)^{(1/\theta)}\right\|_{L^2(\Omega_h)}$ is bounded uniformly for small h

We consider f_h^k to be a suitable approximation of $f_h(t^k)$, i.e. $f_h^k \simeq f_h(t^k)$.

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 $u_h \in H^{1/\theta+1}(I, S^1_h)$ and, for $1 \leq n \leq K$:

$$\delta t \sum_{k=0}^{n-1} \left\|\frac{e_h^{k+1} - e_h^k}{\delta t}\right\|^2_{(H^1_{0,D_h}(\Omega_h))^*} + \|e_h^n\|^2_{L^2(\Omega_h)} + \delta t \sum_{k=0}^{n-1} \left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|^2_{H^1(\Omega_h)} \lesssim D^2 + (\delta t)^{2/\theta} C^2$$

where $C^2 := \int_I \left\|f_h^{(1/\theta)}\right\|^2_{-1,h} + \int_I \left\|g_N^{(1/\theta)}\right\|^2_{H^2(\Gamma_N)} + \int_I \left\|g_D^{(1/\theta+1)}\right\|^2_{H^{3/2}(\Gamma_D)} + \left\|\delta_h(0)^{(1/\theta)}\right\|^2_{L^2(\Omega_h)}$, $D_n^2 := \delta t \sum_{k=0}^{n-1} \left\|\theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|^2_{L^2(\Omega_h)}$. See the proof of proposition D.2.7 for the definition and properties of δ_h.

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 [57], 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 $Q_h^k := \dfrac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} - \theta \partial_t u_h(t^{k+1}) - (1-\theta)\partial_t u_h(t^k)$. The proof now consists in deriving discrete energy estimates for eq. (D.3.4), exactly how it is done in [57]. We only remark a few facts that will be referenced in other proofs.

Estimating Q_h^k

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 [57]:

$$\delta t \sum_{k=0}^{n-1} \left\|Q_h^k\right\|_{-1,h}^2 \lesssim \delta t^4 \int_I \left\|u_h'''\right\|_{-1,h}^2$$

Differentiating problem D.2.5 twice we obtain:

$$\left\|u_h'''(t)\right\|_{-1,h} \leq \left\|f_h''\right\|_{-1,h} + \left\|g_{N,h}''\right\|_{L^2(\Gamma_{N_h})} + \left\|u_h''\right\|_{H^1(\Omega_h)}$$

By energy 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, $\left\|g_{N,h}''\right\|_{L^2(\Gamma_{N_h})} \lesssim \left\|\Pi_c g_N''\right\|_{L^2(\Gamma_N)} \leq (1+h^2)\left\|g_N''\right\|_{H^2(\Gamma_N)}$, 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.

Estimates for the difference quotient

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 $v \in H_{0,D}^1(\Omega)$, so that $v^{-l} \in H_{0,D_h}^1(\Omega_h)$ (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. $\square$

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:

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

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

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

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 $H^1_{0,D}(\Omega)$.

Proof.
<u>L^2 norm</u>
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:

$$\begin{aligned} &\left\| u(t^k) - (u_h^k)^l \right\|_{L^2(\Omega)} \lesssim \\ &\left\| u(t^k) - u_h^l(t^k) \right\|_{L^2(\Omega)} + \left\| u_h(t^k) - u_h^k \right\|_{L^2(\Omega)} \lesssim \\ &Ah^2 + \sqrt{\delta t \sum_{k=0}^{n-1} \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)}^2} + C(\delta t)^{1/\theta} \end{aligned}$$

<u>H^1 norm</u>
Using proposition D.3.3 and proposition D.1.3:

$$\begin{aligned} &\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h^{k+1})^l) + (1-\theta)(u(t^k) - u_h^k)^l) \right\|_{H^1(\Omega)}^2 \lesssim \\ &\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h(t^{k+1})^l) + (1-\theta)(u(t^k) - u_h(t^k)^l) \right\|_{H^1(\Omega)}^2 + \delta t \sum_{k=0}^{K-1} \left\| \theta e_h^{k+1} + (1-\theta) e_h^k \right\|_{H^1(\Omega)}^2 \end{aligned}$$

By employing corollary D.2.17:

$$\begin{aligned} &\delta t \sum_{k=0}^{K-1} \left\| \theta(u(t^{k+1}) - u_h(t^{k+1})^l) + (1-\theta)(u(t^k) - u_h(t^k)^l) \right\|_{H^1(\Omega)}^2 \leq \\ &2\delta t \sum_{k=0}^{K} \left\| u(t^k) - u_h(t^k)^l \right\|_{H^1(\Omega)}^2 \lesssim \\ &2\delta t K h^2 B^2 \end{aligned}$$

<u>Estimate for the derivative</u>
Let $w \in L^2(I, H^1_{0,D}(\Omega))$ be piecewise constant in time, with values w_k on $[t^k, t^{k+1}]$. We can then write:

$$\begin{aligned} &\int_I (\partial_t u, w)_{L^2(\Omega)} - \delta t \sum_{k=0}^{K-1} \left(\frac{(u_h^{k+1})^l - (u_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)} = \\ &\int_I (\partial_t (u - u_h^l), w)_{L^2(\Omega)} + \delta t \sum_{k=0}^{K-1} \left(\frac{(e_h^{k+1})^l - (e_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)} \end{aligned}$$

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:

$$h \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)}^2} \leq \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k \right\|_{L^2(\Omega_h)}^2} + (\delta t)^{1/\theta} C$$

$\square$

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