Technical University of Munich

Department of Mathematics

[Thesis Title]

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.

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Acknowledgements

[text of acknowledgements]

German Abstract

[abstract text]

English Abstract

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Contents

1. Introduction

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

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 $I = (0, T)$, $\Sigma_f = I \times \Gamma_f$, $\Sigma_m = I \times \Gamma_m$.

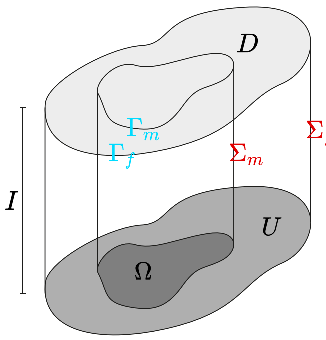

Figure 2.1.: Space-time cylinder with labels

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. [37]).

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 [15], [14]).

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.

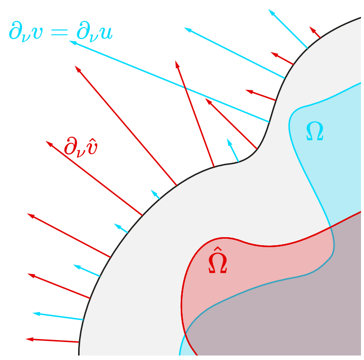

Figure 2.2.: Discrepancy between the Neumann data corresponding to the correct domain Ω, and a guess of it, $\hat{\Omega}$

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 [37] 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. no source: very important We are not concerned with the problem of existence of Ω, likewise this aspect is not addressed in the aforementioned work [37]. Some advances in this direction are done in the case where Ω is allowed to evolve with time, this is addressed in [11].

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.1.6.
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.1.9. 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 corollary A.1.4), 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, $H = L^2, \mathtt{V} = H_0^1, \mathtt{W} = H_{0,m}^1 = \{v \in H^1, v(\Gamma_m) = 0\}$ (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 [37], the heat equations for the adjoint states (see proposition 2.2.11) will have compatibility between initial condition and boundary conditions. This 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.1.8, 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.1.8 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 [56], but a valid alternative, at least formally, is the method of Cea, see [13]. 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 proposition 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 [56] 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.

The first point is immediate.

Proof of 2

All the pieces are linear in ψ. We only check the boundedness of the various differentials. For simplicity, call $|\det(D\tau_k)| = d$, and note that $\|qd\|_{H_\tau} \leq C(d)\,\|q\|_{H_\tau}$.

And now, for instance:

$$\int_I (w_t, \delta q|\det(D\tau_k)|)_{H_\tau} = \int_I (w_t, \delta q d)_{H_\tau} \leq$$
$$C(d) \int_I \|w_t\|_{H_\tau} \|\delta q\|_{H_\tau} \leq C(d) \|w_t\|_{L^2(I,H_\tau)} \|\delta q\|_{L^2(I,H_\tau)} \leq$$
$$C(d) \|w\|_{Q(I,\mathtt{W}_\tau)} \|\delta q\|_{Q(I,\mathtt{W}_\tau)} \leq C(d) \|w\|_{Q(I,\mathtt{W}_\tau)} (\|\delta q\|_{Q(I,\mathtt{W}_\tau)} + \|\delta p\|_{Q(I,\mathtt{W}_\tau)}) =$$
$$C(d) \|w\|_{Q(I,\mathtt{W}_\tau)} \|\delta\psi\|_F$$

Or also:

$$\int_I (g, \mathrm{tr}_U \delta q)_{L^2(\Gamma_f)} \leq \int_I \|g\|_{L^2(\Gamma_f)} \|\delta q\|_{\mathtt{W}_\tau} \leq \|g\|_{H^1(I,L^2(\Gamma_f))} \|\delta\psi\|_F$$

and:

$$\int_I (A_{\tau_k} \nabla \bar{u}_\tau, \nabla \delta p)_{H_\tau} \leq C \|A_{\tau_k}\|_{L^\infty(D;\mathbb{R}^{n\times n})} \int_I \|\nabla \bar{u}_\tau\|_{L^2(I,H_\tau)} \|\nabla \delta p\|_{L^2(I,H_\tau)} \leq$$
$$C(\tau) \|\delta\psi\|_F \|\bar{u}\|_{H^1(I,\mathtt{W}_\tau)}$$

<u>Proof of 3</u>

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.

<u>Proof of 4</u>

Every piece but b is linear or constant in the state ϕ. We only need to prove that $[0,1] \ni s \mapsto b(k, su^k + (1-s)u^0)$ is $AC[0,1]$. But by the structure of the cost function J, transported on $\tau(U_r)$, we see that the latter is a quadratic polynomial in s, hence, absolutely continuous.

<u>Proof of 5</u>

For the pieces with the gradients, it follows as above, by in case employing the simmetry of A_{τ_k}.

Now, for instance the linear form $\delta v_0 \mapsto \int_I (\delta v_{0t}, p|\det(D\tau_k)|)_{H_\tau}$ is also bounded by $C(d) \|\delta v_0\|_{Q(I,\mathtt{V}_\tau)} \|\delta q\|_{Q(I,\mathtt{W}_\tau)}$ just like before.

What remains to check is the Fréchet differentiability of b.

To do so, perturb ϕ by $\delta\phi$ and expanding the square:

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

Now, $\int_I \int_{\tau(U_r)} |\delta v_0 - \delta w|^2 |\det(D\tau_k)| \leq C(\tau_k) \|\delta v_0 - \delta w\|^2_{L^2(I,H_\tau)} \leq C(\tau_k) \|\phi\|^2_E$, so that this term is of higher term.

And $\int_I \int_{\tau(U_r)} (v_0 + \bar{u}_\tau - w)(\delta v_0 - \delta w) |\det(D\tau_k)|$ is linear and bounded by reasonings similar to the former ones.

<u>Proof of 6</u>

By the last point:

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

so that:

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

which is a degree 1 polynomial in s, hence, $L^1(0,1)$.

<u>Proof of 7</u>

Rewriting the formula above and integrating in s, we come to:

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

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:

$$
\begin{aligned}
&\int_0^1 d_\phi G(k, su^k+(1-s)u^0,\psi)[\delta\phi]ds= \\
&\int_I \left(\frac{v_0^k-w^k}{2}\circ\tau_k^{-1}+\frac{v_0^0-w^0}{2}\circ\tau_k^{-1}+\bar{u}_\tau\circ\tau_k^{-1}, \delta v_0\circ\tau_k^{-1}-\delta w\circ\tau_k^{-1}\right)_{H_{\tau_k\circ\tau}} + \\
&\int_I ((\delta w\circ\tau_k^{-1})_t, q\circ\tau_k^{-1})_{H_{\tau_k\circ\tau}} + (\nabla(\delta w\circ\tau_k^{-1}), \nabla(q\circ\tau_k^{-1}))_{H_{\tau_k\circ\tau}} + \\
&\int_I ((\delta v_0\circ\tau_k^{-1})_t, p\circ\tau_k^{-1})_{H_{\tau_k\circ\tau}} + (\nabla\delta(v_0\circ\tau_k^{-1}), \nabla(p\circ\tau_k^{-1}))_{H_{\tau_k\circ\tau}}
\end{aligned}
$$

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 of $\mathtt{W}$), 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 $\delta W, \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau})$, $\delta V_0 \in Q_0(I, \mathtt{V}_{\tau_k \circ \tau})$.

By testing first with $\delta W = 0$ and then with $\delta V_0 = 0$ we can equivalently look for:

$$(Q^k, P^k) \in Q^0(I, \mathtt{W}_{\tau_k \circ \tau}) \times Q^0(I, \mathtt{V}_{\tau_k \circ \tau}) \text{ with}$$
$$\int_I (\delta W_t, Q^k)_{H_{\tau_k \circ \tau}} + (\nabla \delta W, \nabla Q^k)_{H_{\tau_k \circ \tau}} =$$
$$\int_I \left(\frac{v_0^k + w^k - v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1}, \delta W \right)_{H_{\tau_k \circ \tau}}$$
$$\int_I (\delta V_{0t}, P^k)_{H_{\tau_k \circ \tau}} + (\nabla \delta V_0, \nabla P^k)_{H_{\tau_k \circ \tau}} =$$
$$-\int_I \left(\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1}, \delta V_0 \right)_{H_{\tau_k \circ \tau}}$$

An application of integration by parts in time (see proposition B.3.3) yields the problem:

$$(Q^k, P^k) \in W^0(I, \mathtt{W}_{\tau_k \circ \tau}) \times W^0(I, \mathtt{V}_{\tau_k \circ \tau}) \text{ with}$$
$$-\int_I (Q_t^k, \delta W)_{H_{\tau_k \circ \tau}} + (\nabla \delta W, \nabla Q^k)_{H_{\tau_k \circ \tau}} =$$
$$\int_I \left(\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1}, \delta W \right)_{H_{\tau_k \circ \tau}}$$
$$-\int_I (P_t^k, \delta V_0)_{H_{\tau_k \circ \tau}} + (\nabla \delta V_0, \nabla P^k)_{H_{\tau_k \circ \tau}} =$$
$$-\int_I \left(\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} + \bar{u}_\tau \circ \tau_k^{-1}, \delta V_0 \right)_{H_{\tau_k \circ \tau}}$$

But these are the weak formulations (cfr. theorem C.4.2, problem B.2.1.12, problem B.2.2.2) of the problems:

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

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.

$\square$

We now turn to the verification of Gateaux differentiability of J, applying the techniques proposed in [56].

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.

We have $G(k, u^k, \pi^k) - G(k, u^0, \pi^k) = \int_0^1 d_\phi G(k, su^k + (1-s)u^0, \pi^k)[u^k - u^0] ds = 0$ because $u^k - u^0 \in E$, and by absolute contintinuity and integrability of derivative as seen in proposition 2.2.8.

Moreover, calling $g_k = G(k, u^k, 0) - G(0, u^0, 0)$, we have:

- $g_0 = 0$
- $g_k = J((\mathrm{Id} + \delta\theta_k \circ \tau^{-1}) \circ \tau) - J(\tau)$, thanks again to a change of variables
- $g_k = G(k, u^k, \pi^k) - G(0, u^0, \pi^k)$ thanks to $\pi^k \in F$ and the state equations (note, this is possible because k, u^k appear, and $0, u^0$ appear, so that the indices don't mix)

And now, $J(\tau + \delta\theta_k) - J(\tau) = J((\mathrm{Id} + \delta\theta_k \circ \tau^{-1}) \circ \tau) - J(\tau) = g_k = G(k, u^k, \pi^k) - G(0, u^0, \pi^k) = G(k, u^k, \pi^k) - G(k, u^0, \pi^k) + G(k, u^0, \pi^k) - G(0, u^0, \pi^k) = G(k, u^0, \pi^k) - G(0, u^0, \pi^k)$.

$\square$

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:

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

where p^τ, q^τ solve:

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

and where $A'(\delta\theta) = -D\delta\theta - (D\delta\theta)^t + \mathrm{div}(\delta\theta) I$.

Proof.

The shape derivative is linear and bounded

Linearity is immediate. For the boundedness:

$$
\begin{aligned}
&|J'(\tau)[\delta\theta]| \leq \\
&\left\|\operatorname{div}(\delta\theta\circ\tau^{-1})\right\|_{L^\infty(\tau(U_r))}\left(\int_I (\|q_t^\tau\|_{H_\tau}\|q^\tau\|_{H_\tau}+\|v_t^\tau\|_{H_\tau}\|p^\tau\|_{H_\tau})+\frac{1}{2}\|v^\tau-w^\tau\|^2_{L^2(I,H_\tau)}\right)+ \\
&\left(\sum_{ij}\left\|(A'(\delta\theta\circ\tau^{-1})_{ij}\right\|_{L^\infty(\tau(U_r))}\right)\left(\int_I \|\nabla v^\tau\|_{H_\tau}\|\nabla p^\tau\|_{H_\tau}+\int_I \|\nabla w^\tau\|_{H_\tau}\|\nabla q^\tau\|_{H_\tau}\right)
\end{aligned}
$$

and then, for C independent of $\delta\theta$:

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

where in the last step we applied point i) of lemme 2.2, [54]. This shows the boundedness.

Conclusion

Assume $p^k \rightharpoonup p^0$ in $Q(I,\mathtt{V}_\tau)$ and $q^k \rightharpoonup q^0$ in $Q(I,\mathtt{W}_\tau)$.

Now, using that $u^0=(w^\tau,v_0^\tau)$:

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

Grouping some terms 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, [54]. 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 [44]. Their Fréchet derivatives are $\mathrm{div}(\beta)$ 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, whose derivatives at 0, in direction $\delta\theta \in \Theta$ are exactly:

- $\mathrm{div}(\delta\theta \circ \tau^{-1})$
- $A'(\delta\theta \circ \tau^{-1})$

These maps are:

- $\delta\theta_k \mapsto |\det(D\tau_k)|$
- $\delta\theta_k \mapsto A_{\tau_k}$

Therefore:

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

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:

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

Thanks to the assumed weak convergence, $a_k \to J'(\tau)[\delta\theta]$.

So, we still have to show that:

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

goes to zero. This is true because again we can write:

$$\begin{aligned}
|o_k| \leq& \\
\left\| o_k^1 t_k^{-1} \right\|_{L^\infty(\tau(U_r))} \left(\int_I (\|v_t^\tau\|_{H^\tau} \left\|p^k\right\|_{H_\tau} + \|v_t^\tau\|_{H_\tau} \left\|p^k\right\|_{H_\tau}) + \frac{1}{2}\|v^\tau - w^\tau\|^2_{L^2(I,H_\tau)} \right) +& \\
\left(\sum_{ij} \left\| ((t_k^{-1} o_k^2)_{ij} \right\|_{L^\infty(\tau(U_r))} \right) \left(\int_I \|\nabla v^\tau\|_{H_\tau} \left\|\nabla p^k\right\|_{H_\tau} + \int_I \|\nabla w^\tau\|_{H_\tau} \left\|\nabla q^k\right\|_{H_\tau} \right)&
\end{aligned}$$

which goes to 0, thanks to the boundedness of the averaged adjoint states, which stems from their weak convergence.

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.

Weak convergence of states

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 showing a bound, uniform in k.

To do this, recall that $V_0^k := v_0^k \circ \tau_k^{-1}$ and $W^k := w^k \circ \tau_k^{-1}$ satisfy, as seen in theorem C.4.2:

$$\begin{aligned}
&W^k \in Q_0(I, \mathtt{W}_{\tau_k \circ \tau}), V_0^k \in Q_0(I, \mathtt{V}_{\tau_k \circ \tau})\\
\int_I (W_t^k, Q)_{H_{\tau_k \circ \tau}} + (\nabla W^k, \nabla Q)_{H_{\tau_k \circ \tau}} &= \int_I (g, \mathrm{tr}_{\tau_k \circ \tau(U)} Q)_{L^2(\Gamma_f)}, \quad \forall Q \in Q^0(I, \mathtt{W}_{\tau_k \circ \tau})\\
\int_I (V_{0t}^k, P)_{H_{\tau_k \circ \tau}} + (\nabla V_0^k, \nabla P)_{H_{\tau_k \circ \tau}} &= -\int_I (U_k', P)_{H_{\tau_k \circ \tau}} + (U^k, \nabla P)_{H_{\tau_k \circ \tau}}, \quad \forall P \in Q^0(I, \mathtt{V}_{\tau_k \circ \tau})
\end{aligned}$$

where $U^k := \bar{u} \circ \tau_k^{-1}$, where we used that pullbacks and time derivatives commute, see proposition C.3.1.

Thanks to theorem B.2.1.11 and theorem B.2.2.10 we obtain the stability estimates:

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

where C is independent of k.

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

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

and the same goes 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, [54].

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 [54], we obtain that, for instance:

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

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 proposition B.3.3). The closedness follows from the fact that the embedding into continuous function is linear bounded, and evaluation at 0 is linear bounded from continuous functions.

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 analyize 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:

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

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:

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

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 [54].

In a similar fashion for the other pieces, and by passing to the limit:

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

By uniqueness, $v^? = v^0$.

Weak convergence of averages adjoint states

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. To do so, remember that $P^k := p^k \circ \tau_k^{-1}$ and $Q^k := q^k \circ \tau_k^{-1}$ solve:

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

and

$$\begin{aligned}-P_t^k - \Delta P^k &= -\frac{v_0^k - w^k + v_0^0 - w^0}{2} \circ \tau_k^{-1} - \bar{u}_\tau \circ \tau_k^{-1} \\ P^k(T) &= 0 \\ P^k &= 0 \text{ on } \Sigma_m \sqcup \Sigma_f\end{aligned}$$

By proposition B.1.14, we will obtain a bound in Q of the tranported averaged adjoints 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 [54] 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.

But what we want is a bound on q^k, p^k in the $Q(I, \mathtt{W}_\tau)$ and $Q(I, \mathtt{V}_\tau)$ sense. This can be accomplished in exactly the same way as before.

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).
Fréchet differentiability could be proved 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

You can add a generalization to a different star shaped reparametrization, if need be

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

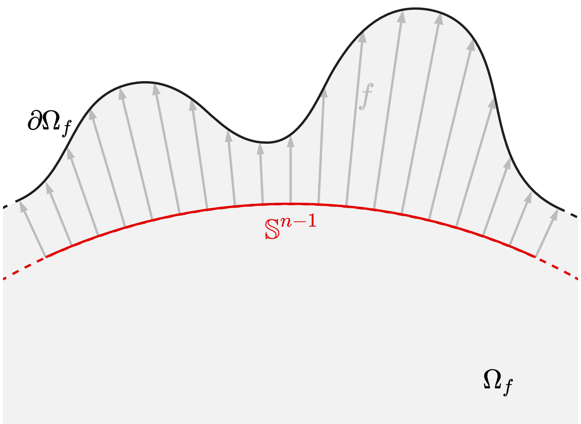

Figure 2.3.: Illustration of radial displacement

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 [12], and lemma 5 at page 151 also of [12], a fact that was not discussed in [20]. Note that the definition of Lipschitz domain of [12] is completely equivalent to that of [2] (and at least implies that of [48], [35], [43], [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 [51].

$\square$

We now define maps relating a radial function to its correspondent a star-shaped domain. We choose $0 < \epsilon < f_D \in W^{1,\infty}(\mathbb{S}^{n-1})$, to parametrize the non moving part of the optimization domain. The reference domain 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 $\overline{D} \setminus \Omega_f \to \overline{D} \setminus B_\epsilon$

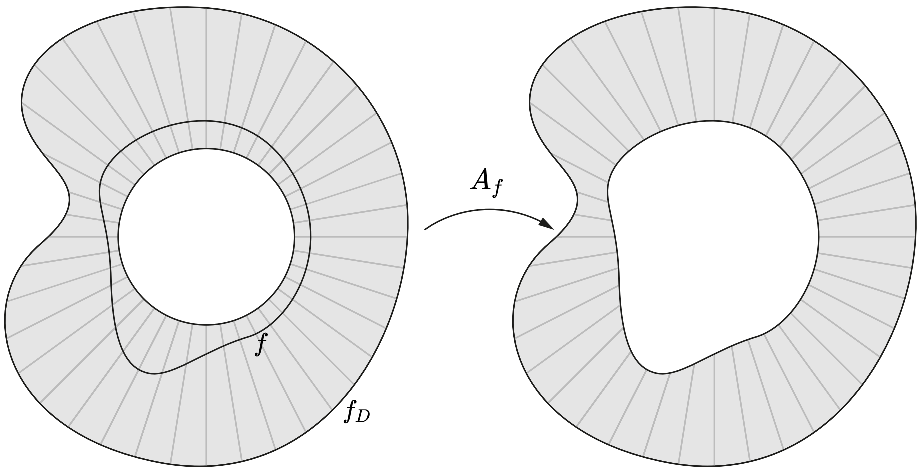

Figure 2.4.: Illustration of the action of A_f

Proof.

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

They also satisfy a bi-Lipschitz condition.

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

Proof.

The second part of the proposition is contained in [20] 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 [20]) 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}.

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 [60] 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 $A \supseteq \overline{B_\epsilon}$. 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 limits

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

But this is:

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

Now, we derive the expression of a displacement field V_h, to connect this difference quotient to the already computed shape derivative, see also [20]. 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 $h \mapsto V_j$ 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 [20]) $DH_f(x) = f(\hat{x})I + \hat{x} \otimes D_T f(\hat{x})$, 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 (local sense).

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 $\phi(x) = 0$.

ϕ is a C^1 diffeomorphism, so $D\phi_n(x) \neq 0$, and we can assume $D\phi_n(x)$ to be proportional to $-e_n$ by a rotation of the axis.

Thus $\partial_n\phi_n(z) < 0$ in some $B(x) \subseteq A$. $B(x)$ is chosen small that ϕ is Lipschitz on $B(x)$.

Apply the implicit function theorem to obtain V', I open with $x \in V' \times I \subseteq B(x)$ and a function $\eta : V' \to I$ that is C^o and Lipschtiz, with $\phi_n(z', z_n) = 0 \iff z_n = \eta(z')$, for $z \in V' \times I$.

V' is open around x', so let's restrict it to a square centered at x'. Relabel η as the restriction to this new V' and restrict I to be the connected component of G hosting $\eta(V')$, which is now an interval, as continuous image of a connected set. Because $x_n \in I$, and by continuity, V' can be shrunk such that $\eta(V') \subset\subset J \subset\subset I$ for some open interval J.

All these shrinkings don't change the character of being the implicit function, i.e. η still satisfies $\phi_n(z', z_n) = 0 \iff z_n = \eta(z')$, for $z \in V' \times I$, and also, $x \in V' \times I \subseteq B(x)$ and $\eta : V' \to I$ is still C^o and Lipschitz.

Now, the choice of $B(x)$ makes $z_n \mapsto \phi(z', z_n)$ strictly decreasing, for $(z', z_n) \in B(x)$. So, for $z \in V' \times I$, we have $\phi_n(z', z_n) = \phi_n(z) > 0 = \phi_n(z', \eta(z')) \iff z_n < \eta(z')$ (by basic properties of strictly decreasing functions).

But also, $\phi_n(z) > 0 \iff \phi(z) \in B \cap \mathbb{R}^n_+ \iff z \in \phi^{-1}(\mathbb{R}^n_+ \cap B) = A \cap \Omega$.

Therefore, $z \in V' \times I, z_n < \eta_n(z) \iff z \in V' \times I, \phi_n(z) > 0 \iff z \in A \cap \Omega \cap (V' \times I) = (V' \times I) \cap \Omega$.

Summing up we have the following:

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

<u>Conclusion</u>

Let a radial function $f > 0$ be of class C^o. 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 [12], which yields, modulo an application of the Lebesgue number lemma, a C^o and Lipschitz domain in the style of [35].

<u>Remarks about the usage of the implicit function theorem</u>

Examining the proofs of the inverse and implicit function theorems as given e.g. at pages 310, 311 of [33], we see that solving $f = 0$ for f Lipschitz and C^o, yields a Lipschitz and C^o implicit function.

□

2.4. Hilbertian regularization framework

todo

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 remark that such time stepping schemes require a globally smooth solution, over time. To decrease such requirement, discontinuous Galerkin space-time methods can be adopted, see e.g. [49]. 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 [45]). 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 [37]). 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 [37], 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 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 [46] for a comparison between the two strategies, and a discussion of advantages and disadvantages of each. See also [29], 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 [29].

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:

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

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, $J_\eta(\tau) = 0 \implies \eta \|v_\tau - w_\tau\|^2_{H_\tau} = 0 \implies v_\tau = w_\tau$. 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.2.2.2 (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.

Check $g_N(0) = 0$, wtf

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 also be quasi-uniform be precise
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 $g^k_{N,h}, g^k_{D,h}$ to be the Lagrange interpolant of $g_N(t^k), g^k_{D,h}$. For the state u we adopt:

$$\left(\frac{u_h^{k+1} - u_h^k}{\delta t}, v_h\right)_{L^2(\Omega_h)} + (\nabla(\theta u_h^{k+1} + (1-\theta)u_h^k), \nabla v_h)_{L^2(\Omega_h)} = (\theta g^{k+1}_{N,h} + (1-\theta) g^k_{N,h}, v_h)_{L^2(\Gamma_{N_h})}, \quad 1 \leq k \leq K$$
$$u_h^{k+1}|_{\Gamma_{D_h}} = g^{k+1}_{D,h}, \quad 1 \leq k \leq K$$
$$u_h^0 = 0$$

and $v_h \in S^1_{h,0,D_h}$. Here $\Gamma_{D_h}, \Gamma_{N_h}$ are the discrete counterparts of Γ_D, Γ_N, and $S^1_{h,0,D_h}$ 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.

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.1.4.

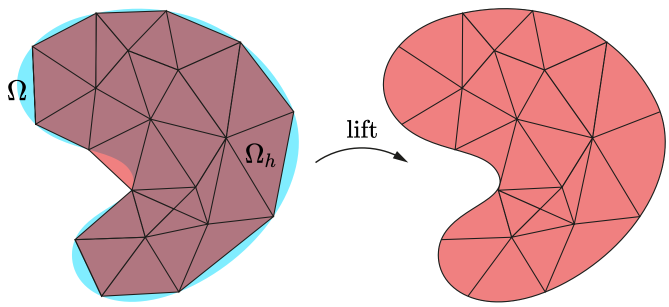

Figure 3.1.: Lifting action

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

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

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

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

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.2.2.11 (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. This is just a more detailed repetition of the proof of the more general result corollary D.2.2.12.

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.2.1.4 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.2.1.6

They are also satisfied by $1 - 3$.

Assumptions for full discretization of u: assumption D.2.2.1

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.2.2.1 for the notation) by hypothesis 3.

Bounding the constants A, B, C, D of u: theorem D.2.2.11

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.2.1.6 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.2.1.6 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.2.1.10 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.2.2.1 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.2.2.11, 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.2.2.3 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.2.2.7).

To bound $A(a)$ (equivalently $B(a)$), we need to check the boundedness of $\int_I C_{\eta(v-w)}^2 + \int_I \|\eta(v_h - w_h)\|_{H^1(U_h)}^2$. 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.2.1.6 and we see that, thanks to theorem D.2.1.10, it is dominated by $A(v) + A(w)$, which we have already estimated.

□

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 [29], 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 that are linear finite element vector fields that preserve the fixed boundary, we aim at solving:

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

where v_h^k, w_h^k are defined in problem 3.1.3, with $\theta = 1$, 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:

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

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

Problem 3.2.3

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

and

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

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 [10], section 4 (or more generally, [44]), 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 $v_h \in S_{h,0}^1$. 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.2.2.2 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 [10] 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. [39], 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 $\delta t \sum_{k=1}^K \left\|\eta(t^{k-1})u_h(t^{k-1}) - \eta(t^k)u_h^k\right\|_{L^2(U_h)}^2$, where u denotes the generic state corresponding state to the generic adjoint a (this is the same notation as in the proof of proposition 3.1.4), $U_h = \tau_h(U_{r,h})$.

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:

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

There holds $2 \leq \|\eta'\|^2_\infty \delta t^3 \sum_{k=1}^{K} \left\| u_h(t^k) \right\|^2_{L^2(U_h)}$. Call $\pi u_h := u_h(t^k)$ for $t \in (t^k, t^{k+1})$. By lemma A.2.1.1 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:

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

On the other hand, $1 \leq \|\eta\|^2_\infty \delta t \sum_{k=1}^{K} \left\| u_h(t^{k-1}) - u_h(t^k) \right\|^2_{L^2(U_h)}$, and with a similar reasoning as in the proof of lemma A.2.1.1, we conclude:

$$
1 \leq \|\eta\|^2_\infty \delta t \sum_{k=1}^{K} \delta t \int_{I_k} \|u_h'\|^2_{L^2(I_k, L^2(U_h))}
$$

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.2.1.17).

Note, it is clear from this estimate that a very steep η will yield higher discretization errors.

Finally, by proposition D.2.2.3 (which we can apply by assumption 3.1.2), we obtain $3 \lesssim (h^2 + \delta t) \|\eta\|^2_\infty$.

□

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:

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

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.2.2.3, let us bound Q_h^k in the stronger L^2 norm. There holds (also see [53], page 388):

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

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

Therefore, $\delta t \sum_{k=0}^{K-1} \left\|Q_h^k\right\|_{L^2(U_h)}^2 \leq \delta t^2 \left\|u_h''\right\|_{L^2(I, L^2(U_h))}^2$. The latter norm can be bounded uniformly on h, thanks to assumption 3.1.2 and the reasoning of theorem B.1.8. Note, we need here the stronger compatibility condition that $\delta_h'(0)$ is bounded in H^1, see proposition D.2.2.3 for the notation. In the current concrete case, $\delta_h'(0) = 0$ and this is thus not an issue.

Semidiscrete bound

Consider eq. (D.2.2.4), 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's and Cauchy-Schwarz' inequalities, we find:

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

Because $e_h^0 = 0$ we get:

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

This means that:

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

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.1.3, and using proposition D.1.4 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 [40], we can reason as follows:

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

by corollary D.2.1.17 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. Therefore, the quantities to be compared become, after simplifying the notation, and employing proposition 2.2.11 and proposition 3.2.2:

$$\delta t \sum_{k=1}^{K} \left(\frac{w_h^k - w_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h) q_h^{k-1} \right)_{L^2(U_h)} + \delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla w_h^k, \nabla q_h^{k-1})_{L^2(U_h)} +$$
$$\delta t \sum_{k=1}^{K} \left(\frac{v_h^k - v_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h) p_h^{k-1} \right)_{L^2(U_h)} + \delta t \sum_{k=1}^{K} (A'(\delta\theta_h)\nabla v_h^k, \nabla p_h^{k-1})_{L^2(U_h)} +$$
$$\frac{\delta t}{2} \sum_{k=1}^{K} \int_{U_h} \eta(t^k) |v_h^k - w_h^k|^2 \mathrm{div}(\delta\theta_h)$$

and

$$\int_I (w_t \mathrm{div}(\delta\theta), q)_{L^2(U)} + \int_I (A'(\delta\theta)\nabla v, \nabla p)_{L^2(U)} +$$
$$\int_I (v_t \mathrm{div}(\delta\theta), p)_{L^2(U)} + \int_I (A'(\delta\theta)\nabla w, \nabla q)_{L^2(U)} +$$
$$\frac{1}{2}\int_I \int_U \eta |v-w|^2 \mathrm{div}(\delta\theta)$$

To make a fair comparison we also need to have $\delta\theta$ and $\delta\theta_h$ to be somewhat related. We will discuss in the end some possible choices.

Splitting into pieces

We separately bound the five pieces, which, if we again recover the notation u, a to indicate a state and its correspondent adjoint (so, $u = v \iff a = p$ or $u = w \iff a = q$), means to find bounds just for the following three quantities:

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

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

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

Derivatives: rewriting

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

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

Now:

$$\mathrm{R1} = \delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \delta t \sum_{k=1}^{K} \left(\frac{u(t^k) - u(t^{k-1})}{\delta t}, \mathrm{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)} =$$
$$\underbrace{-\delta t \sum_{k=1}^{K} \left(\frac{u(t^k) - u(t^{k-1})}{\delta t} - \frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \mathrm{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)}}_{2} +$$
$$\underbrace{\delta t \sum_{k=1}^{K} \left(\frac{u_h^k - u_h^{k-1}}{\delta t}, \mathrm{div}(\delta\theta_h) a_h^{k-1} \right)_{L^2(U_h)} - \delta t \sum_{k=1}^{K} \left(\frac{u_h^{k,l} - u_h^{k-1,l}}{\delta t}, \mathrm{div}(\delta\theta) a(t^{k-1}) \right)_{L^2(U)}}_{\mathrm{R2}}$$

Lastly:

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

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

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

<u>Derivatives: estimation</u>

We start with 1, 2, 5.

We have, by the Cauchy-Schwarz inequality and lemma A.2.1.1:

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

Then, using again the Cauchy-Schwarz inequality:

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

Employing proposition 3.2.7 at first, and lemma A.2.1.1 afterwards:

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

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:

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

Thanks to proposition 3.2.5 we can write:

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

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.1.7.

Gradients: rewriting

We have:

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

Continuing the splitting:

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

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.2.1.1 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.2.1.1 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:

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

Similarly:

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

and the term 8 follows directly from proposition D.1.7.

Cost functions: estimation

We are missing a bound on:

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

We find:

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

whereas:

$$\begin{aligned}
\text{R4} = \underbrace{\frac{\delta t}{2}\sum_{k=1}^K \int_{U_h} \eta(t^k)|v_h^k - w_h^k|^2 \mathrm{div}(\delta\theta_h) - \frac{\delta t}{2}\sum_{k=1}^K \int_U \eta(t^k)|v_h^{k,l} - w_h^{k,l}|^2 \mathrm{div}(\delta\theta_h^l)}_{\text{13}} + \\
\underbrace{\frac{\delta t}{2}\sum_{k=1}^K \int_U \eta(t^k)(|v_h^{k,l} - w_h^{k,l}|^2 - |v(t^k) - w(t^k)|^2)\mathrm{div}(\delta\theta_h^l)}_{\text{14}} + \\
\underbrace{\frac{1}{2}\int_I\int_U \tilde{\pi}\eta(|\tilde{\pi}v - \tilde{\pi}w|^2 - |v-w|^2)\mathrm{div}(\delta\theta_h^l)}_{\text{15}} + \\
\underbrace{\frac{1}{2}\int_I\int_U (\tilde{\pi}\eta - \eta)|v-w|^2\mathrm{div}(\delta\theta_h^l)}_{\text{16}}
\end{aligned}$$

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

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

Similarly, also by applying the Cauchy-Schwarz' inequality and lemma A.2.1.1:

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

The Cauchy-Schwarz' inequality also yields:

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

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.2.1.1 yield $S_u \lesssim 1$, so that:

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

Similarly, and reasoning as in proposition D.1.7, we can also see that:

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

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 [39] were derived, in a slightly different context: in a time-dependent setting, and a precise handling of the geometry error. However, in [39], 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 [39]). 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 [39]. 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. We are able to give a positive answer for the implicit Euler scheme.

The difference with the estimates of [39] 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 [39], don't seem to be so easily obtainable for displacements $\delta\theta \in W^{1,\infty}$ only.

Introduce and derive semidiscrete shape gradient

Theorem 3.3.1 (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:

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

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.1.7, apart from the semidiscretization error estimates for the partial differential equations, to obtain an overall $O(h^2)$ term. We indicate $\delta\theta^{-l} =: \delta\theta_h$.

Derivatives

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

We have:

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

We apply corollary D.2.1.17 to 1, a thing which we can do, as assumption 3.1.2 and by the reasonings of proposition 3.1.4, to obtain:

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

It is crucial here that θ has two weak derivatives, so that $a\theta$ is a test function, as required by corollary D.2.1.17.

On the other hand, employing theorem D.2.1.10, proposition D.1.4 and suitable energy estimates to u_h' (which are avaliable by assumption D.2.2.1), we come as well to:

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

Employing proposition D.1.7, and proposition D.1.4, 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:

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

We refer directly to proposition D.1.7 to show that $|④| \lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$. We also obtain, by additionally invoking proposition D.1.4 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.2.1.10 in the last step. The same theorem D.2.1.10 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:

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

where we used again theorem D.2.1.10.

Cost function

There holds:

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

The first term is $\lesssim h^2 \|\delta\theta\|_{W^{1,\infty}(U)}$ thanks to the Cauchy-Schwarz inequality and theorem D.2.1.10, the second one because of proposition D.1.7. This concludes the proof.

$\square$

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 3.3.2 (Fully discrete superconvergence result)
With the same assumptions and notation of theorem 3.3.1 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 3.3.1, 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 3.1.1. Then:

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

and:

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

Finally:

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

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

$\square$

4. Implementation

We now turn to discussing our implementation and to verifying some of the results that were previosly 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 wrote our code in Python, making heavy use of the FEniCS package ([47]). 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 [31], [21] and [50]). 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 ([32]) 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.

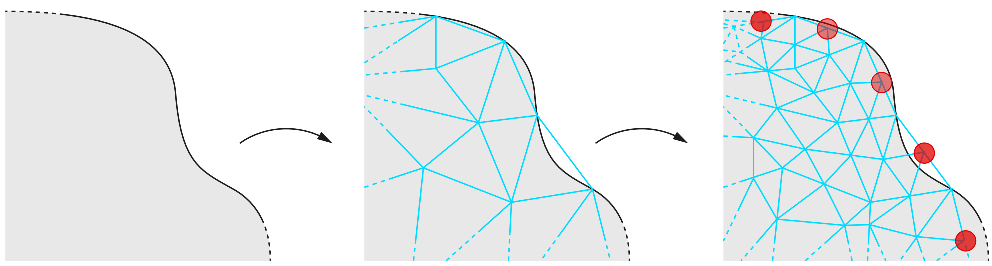

Figure 4.1.: Problems with uniform refinements

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 $B_{\tilde{h}}^1$. Our control, i.e. our optimization variable, will be a function $q_{\tilde{h}} \in B_{\tilde{h}}^1$, and we would be solving:

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

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:

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

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 [62]). 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 [37], 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. [23], [25], [24]. Isoparametric elements elements are necessary, when adopting higher order basis functions, in order to preserve optimal accuracy (see section 4.4 of [55] 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 [37], 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 [39], 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 4.2 for a justification.

We mostly experimented with an L-BFGS algorithm, and with a modified Newton's method. We implemented the latter following the observations contained in [26], a work centered around a very similar shape optimization problem to ours, in an attempt to alleviate some spurious artifacts we observed, and attributed to the ill-posedness of the shape identification problem. We will soon discuss these 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:

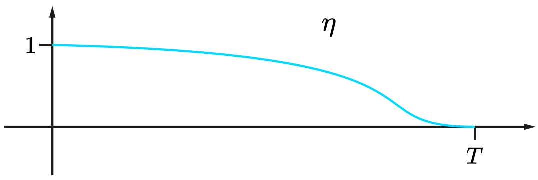

Figure 4.2.: The temporal weight η

Scalar product say something about this, please

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.

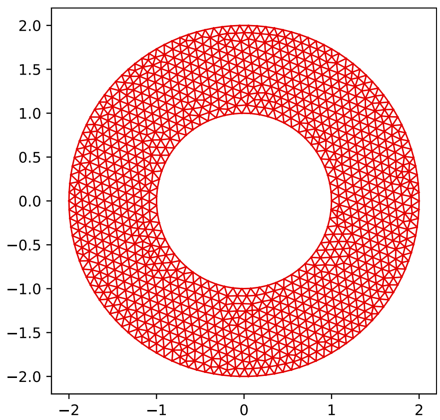

Figure 4.3.: Initial guess for the shape optimization process

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.

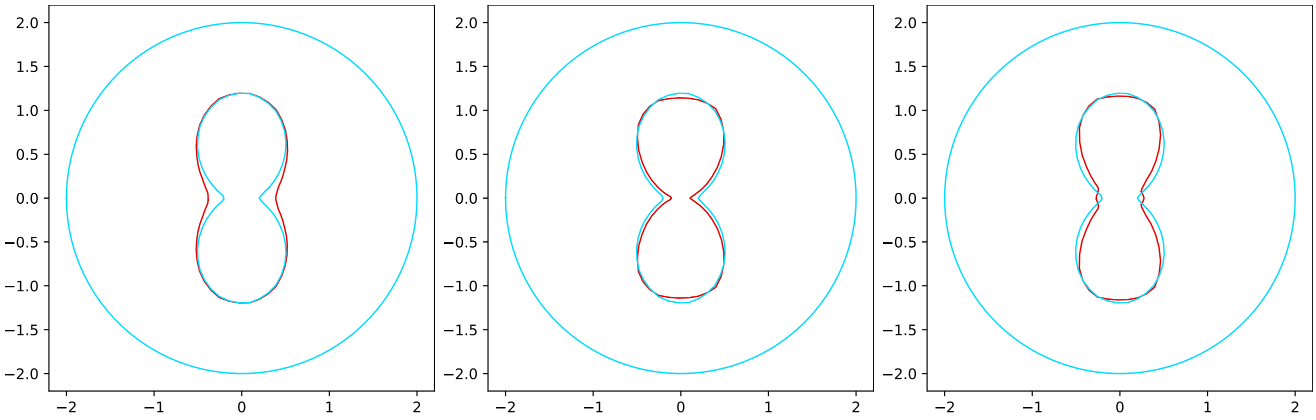

Figure 4.4.: Exact and simulated inclusion (in red) for the runs with g_2, g_3 adn g_4, in order from left to right

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:

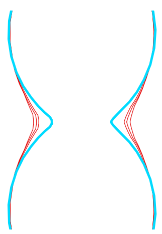

Figure 4.5.: From the outside to the inside: run with g_6, g_5, g_1 and exact solution in blue

For completeness, we report a picture of the final deformed mesh corresponding to the g_1 run:

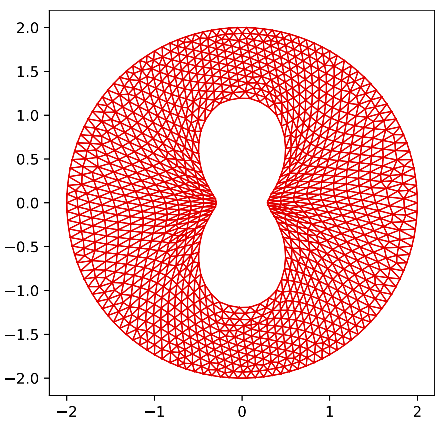

Figure 4.6.: Estimated domain in the g_1 run

and of the history of the cost function and the gradient l^∞ norm:

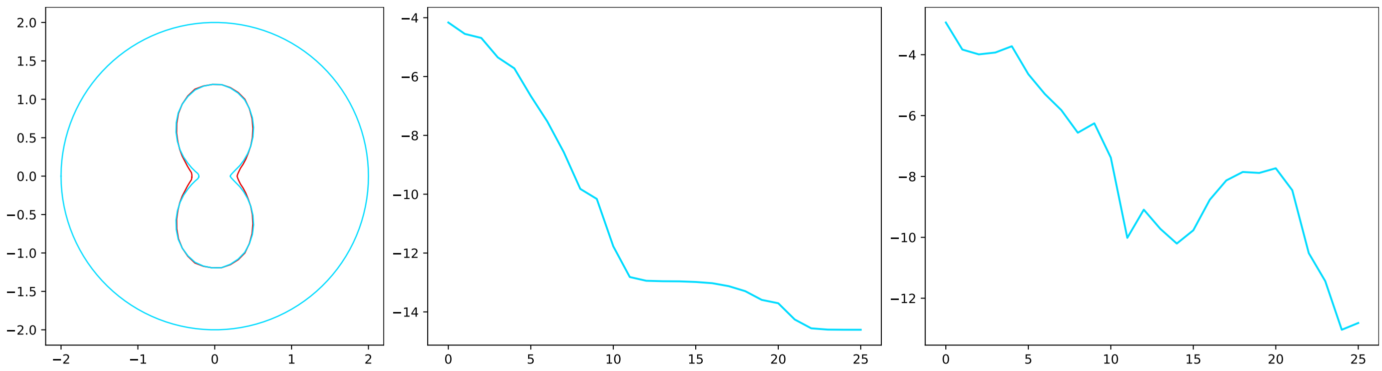

Figure 4.7.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 25 iterations

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 $a = 0$.

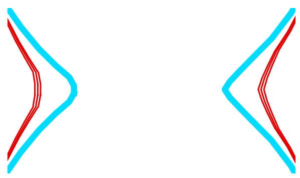

Figure 4.8.: From outside to inside: run with g_1 and $a = 0$, $a = 0.05$, $a = 0.005$ and exact solution in blue

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. 4.5: $a = 0$ 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.

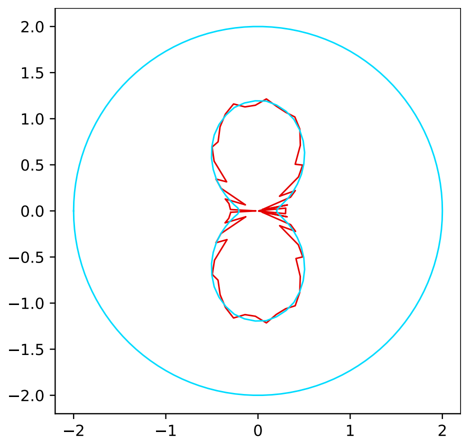

Figure 4.9.: Reconstruction for the run g_1 and the L^2 inner product

Ill-posedness

Degeneration of the boundary

It has already been noted in [37] 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 [26] 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. [**kirsch**], 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:

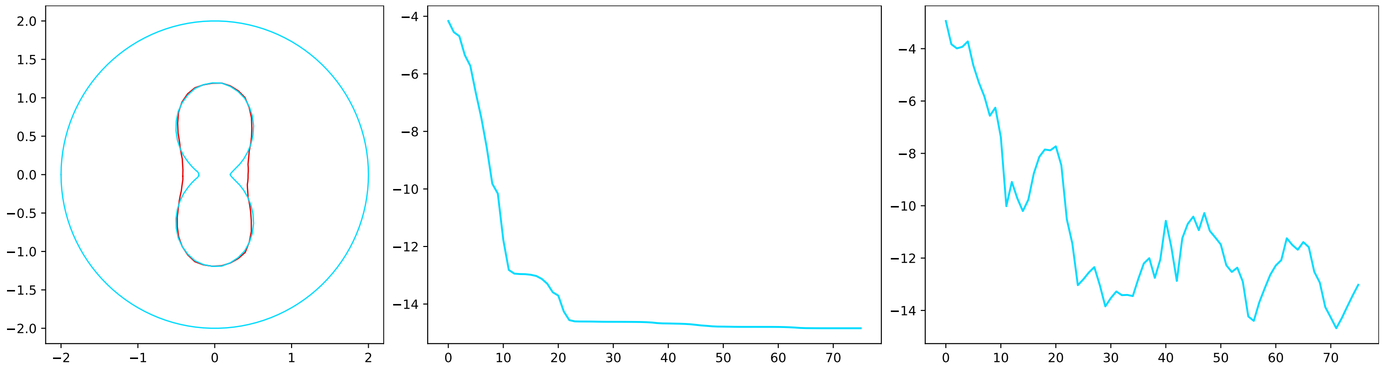

Figure 4.10.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run and 75 iterations

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.

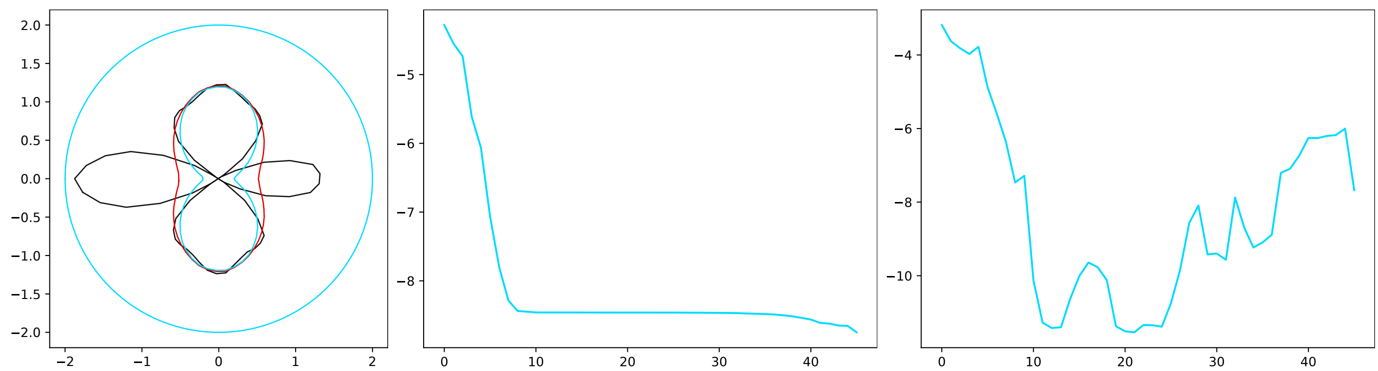

Figure 4.11.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run. The black boundary corresponds to 45 iterations, the blue one to 25. The presence of the lateral lobes in the black reconstruction indicates a negative radial function.

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 tend 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 [26] (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.

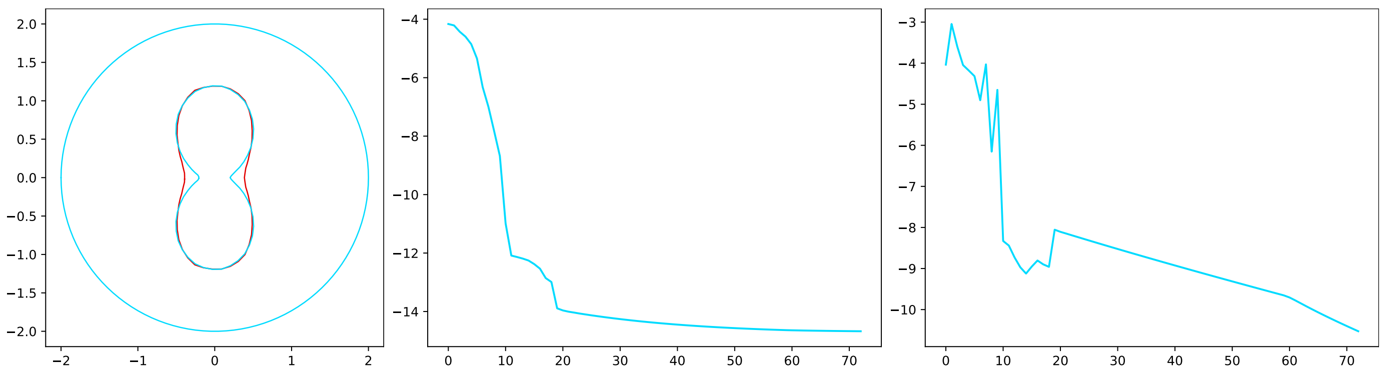

Figure 4.12.: Reconstruction, cost function (logarithm) and gradient history (logarithm) for the g_1 run, and the regularized Newton method from [26]. The reconstructions after 20 and 70 shape are visually indistinguishable.

<u>Sea urchin</u>

Lastly, we show the reconstruction of a 2D version of the more complicated "sea urchin" inclusion of [37]. 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.

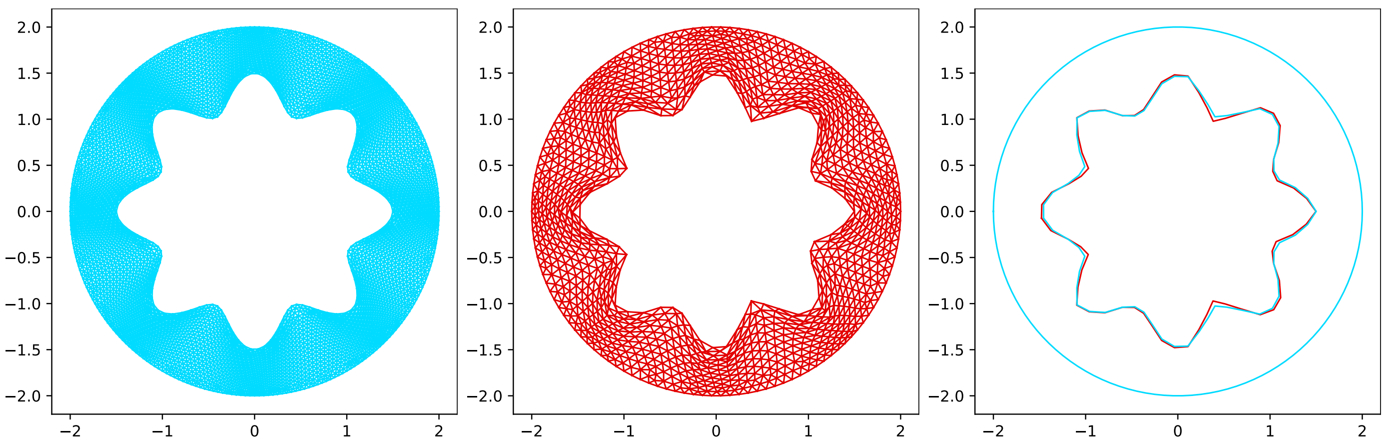

Figure 4.13.: "Exact" domain, reconstruction, and comparison between reconstruction and the exact domain, interpolated to the optimization finite element space.

regularization doesn't really work, mention Github, time of simulation mention in the theory that we are using H1 scalar products... cite allaire

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 $\delta t = h^{2\theta}$. 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 constant size $\tilde{h} = 0.5$. This mesh size stays fixed across all the runs. Note, this yields a very coarse mesh: the rationale is to have the resulting displacement field approximating a vector field that is in $W^{1,\infty}$ but not $W^{2,\infty}$. Doing so, we obtain 20 different displacement fields $\delta\theta^i_{h,\tilde{h}}$, with which we test the shape gradients.

Not being able to represent non-discretized shape gradients, we therefore content ourselves to analyzing the quantity:

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

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

5. Conclusion

Appendices

A. Functional spaces

A.1. Sobolev spaces

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

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

Proof.

This follows from [43], 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 developed here.

□

Lemma A.1.2
$f \in L^\infty(\Omega; \mathbb{R}^N) \iff f_i \in L^\infty$, and two equivalent norms are $\|f\|_a := \||f|\|_\infty$, $\|f\|_b := \max_i \|f_i\|_\infty$, for $|\cdot|$ any finite dimensional norm.

Proof.

We choose $|\cdot| = |\cdot|_1$.

Consider $f_n \in X_a = \{[f], f : \Omega \to \mathbb{R}^n \text{ measurable }, \|f\|_a\}$, Cauchy. Then every component is Cauchy in the scalar L^∞, so that $f_n^i \to f^i$ in L^∞. The limit f is in X_a because the functions $|f_i|$ are essentially bounded, and so is $|f|$.

Then $\|f_n - f\|_a \le \|f_n - f_m\|_a + \sum_i \left\|f_m^i - f^i\right\|_\infty$ for all n, m. Choose $m \ge n$ with $\left\|f_m^i - f^i\right\| \le 1/(Nn)$ and conclude X_a is Banach.

We know from [43], theorem B.88 at page 671, and page 669, we know that $X_b = \{[f], f : \Omega \to \mathbb{R}^n \text{ measurable }, \|f\|_b\}$ is Banach.

Moreover $X_a = X_b$ as sets, so that the thesis follows.

□

Proposition A.1.3 (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.

Extension

In the case Ω is bounded Lipschitz, then Ω is an extension domain for $W^{1,\infty}(\Omega)$, meaning that there is $E : W^{1,\infty}(\Omega) \to W^{1,\infty}(\mathbb{R}^n)$ linear bounded with $Eu = u$ a.e. on Ω (see [43], theorem 13.17 at page 425, 13.13 at page 424, and definition 9.57 at page 273).

The proof

Let $u \in W^{1,\infty}(\Omega)$. By [43], 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. [3]), we can extend $\bar{u}$ to a Lipschitz function e on $\mathbb{R}^n$.

Then, for a large enough cube Q containing Ω, $\displaystyle\int_\Omega \bar{u}\partial_i\phi = \int_Q e\partial_i\phi = -\int_Q \partial_i e\phi$, by Fubini's theorem and integration by parts for AC functions.

Because $e = \bar{u}$ on Ω, we conclude $\displaystyle\int_\Omega \bar{u}\partial_i\phi = -\int_\Omega \partial_i\bar{u}\phi$, 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.

□

Corollary A.1.4 ($W^{k,\infty} = C_B^{k,1}$)
For a bounded Lipschitz domain Ω, or for $\Omega = \mathbb{R}^n$, then $W^{k,\infty} = C_B^{k,1}$ ($C^{k,1}$ bounded functions with bounded classical derivatives up to order $k+1$).

Proof.

We have already proved the case $k = 1$. We prove, for instance, the case $k = 2$. Then, $u \in W^{k,2} \implies u, \partial_i u \in W^{k,1}$ ([43], 11.7 at page 321), so that by proposition A.1.3, we find bounded Lipschitz h, g_i with $u = h$ a.e., $\partial_i u = \partial_i h$ a.e., $g_i = \partial_i u$ a.e..

Therefore h is continuous, with continuous weak derivatives g_i, which implies that $h \in C^1(\Omega)$ (see here and here).

Now, $\partial_i h = g_i$ a.e., so everywhere, so that:

- h is bounded Lipschitz and C^1
- $\partial_i h$ are bounded Lipschitz

□

A.2. Bochner spaces

Here are some useful results about Bochner spaces.

Proposition A.2.1 (Bochner integral and bounded operators)
Let X, Y be separable Banach, let $T \in L(X, T)$ 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.

First of all, a clarification on the definition. What is really happening is that from the time equivalence class f, we select a g, and then $Tf(t) := T(g(t))$. Tf is then the equivalence class of $t \mapsto Tf(t)$. The definition is well posed, because $g_1(t) = g_2(t) \implies T(g_1(t)) = T(g_2(t))$.

Let f_n be simple, $f_n \to f$ a.e., with $\lim_n \int_I f_n = \int_I f$ and $\|f_n\|_X \le C\|f\|_X$ (see page 6, and corollary 2.7 at page 8 of [42]).

<u>Measurability</u>

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

<u>Integrability</u>

By the assumptions, $\|Tf_n\| \le \|T\|\,\|f_n\| \le C\|f\| \in L^1(I)$, so that by dominated convergence (corollary 2.6 of [42]) Tf is integrable too. 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, $\int_T Tf = \lim_n T\int_I f_n = T\lim_n \int_I f_n = T\int_I f$.

□

Proposition 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 $\|T\|$.

Proof.

The case $k = 0$ is proved above.

We prove now that $\partial_{t^i} Tf = T\partial_{t^i} f$ for $i = 1$. Note that $T\partial_t f \in L^2(I, Y)$, which qualifies as weak derivative.

In fact, for $\phi \in C_c^\infty(I)$, we have $\int_I \phi T\partial_i f = \int_I T(\phi\partial_t f) = T\int_I \phi\partial_t f = -T\int_I \phi' f = -\int_I \phi' Tf$.

Higher weak derivatives are treated analogously and the rest of the claims follow from the time stationarity of T and by $\|\partial_{t^i} Tf\| = \|T\partial_{t^i} f\| \leq \|T\| \|\partial_{t^i} f\|$.

□

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

Proof.

Assume there exists two such continuous representatives, so that we get a function $\delta : [0, T] \to X$ that is zero almost everywhere and continuous. Hence, $[0, T] \ni t \mapsto \|\delta(t)\|$ is continuous in $\mathbb{R}$ and zero a.e., so that it must be zero everywhere. □

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.

We rely on proposition 3.8 of [42] at page 26.

<u>Absolute continuity</u>

Consider $\epsilon > 0$. Divide $[a, b] \subset\subset (0, T)$ into a uniform partition t_i. By theorem 6 at page 146 of [30], we get that $\|\phi(t_i) - \phi(t_{i-1})\|_X \leq (t_i - t_{i-1}) \|\phi(\xi_i)\|_X \leq (b - a) \|\phi'\|_\infty /n$, and by choosing n small enough, we conclude that ϕ is (locally) absolutely continuous.

<u>Weak derivative</u>

Therefore, ϕ is locally AC, differentialble everywhere and ϕ' is bounded, so that $\phi \in H^1(I, X)$ and weak and classical derivatives coincide.

□

And now, introduce a time dependent version of the trace operator which is useful for our computations.

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
2. is linear bounded
3. admits a linear bounded right inverse, for instance, $E(g)(t) := E(g(t))$ (for E a right inverse of the static trace)
4. tr and E, in the case of $k \in \mathbb{N}_0$, coincide (in the time a.e. sense) for the case $l \geq k$
5. for $k \geq 1$, $\mathrm{tr}u(0) = 0 \iff u(0) = 0$ (in the sense of continuous representatives)
6. it coincides with the trace treated for instance in [45]

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 [48]).

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 [35], page 20). Therefore, by [27], 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 $H^k(I, H^{1/2})$. The embedding is U, the unique continuous representative of a certain time equivalence class (proposition A.2.3). We also introduce brackets to indicate equivalence classes in time, so, $u = [Uu]$.

We want to prove $(Uu)(0) = 0 \iff U(\mathrm{tr}u)(0) = 0$. But we have $[t \mapsto U(\mathrm{tr}u)(t)] = tru := [t \mapsto \mathrm{tr}((Uu)(t))]$. So, $U(\mathrm{tr}u)(t) = \mathrm{tr}((Uu)(t))$ for all $t \in [0,T]$ by continuity.

For the last point, let $k = 0$. We have:

1. $H^1(\Omega) \cap C^1(\overline{\Omega})$ is dense in $H^1(\Omega)$ (see [1], theorem 3.18 at page 54, where being Ω bounded Lipschitz is important)
2. functions $\sum_{i \leq m} \phi_i(t) f_i$ for $\phi_i \in C_c^\infty(I), f_i \in H^1(\Omega) \cap C^1(\overline{\Omega})$ are dense in $L^2(I, H^1)$ (see [38], page 39, lemma 1.9)

It follows by the third point that $C^1(\overline{\Omega \times I})$ is dense in $L^2(I, H^1)$, so that $u \mapsto u|_{I \times \partial\Omega}$ admits a unique extension by continuity to $L^2(I, H^1)$, so that this definition of trace coincides with the one from the literature in the case of the space $H^{1,0} := L^2(I, H^1)$ (see [45], theorem 4.1), we expand this argument below.

Proof of leftover facts

We call $C^k(\overline{\Omega}) := \{u \in C^k(\Omega)$ with $\partial_\alpha f$ extendable by continuity to $\overline{\Omega}\}$.

Consider $u(x,t) := \phi(t)v(x)$, for $\phi \in C^1([0,T]), v \in C^1(\overline{\Omega})$. Then, it has partial derivatives $u_t = \phi_t v, u_i = \phi u_i$. u and all its partial derivatives are continuous on $I \times \Omega$, meaning that $u \in C^1(\Omega \times I)$.

Moreover, $u, u_i, u_t \in C([0,T], C(\overline{\Omega}))$. We claim $C([0,T], C(\overline{\Omega})) = C(\overline{\Omega \times I})$. In fact, one direction is trivial, and so, let $f \in C([0,T], C(\overline{\Omega})) = C(\overline{\Omega})$. Fix $(t,x) \in \overline{\Omega \times I}$. Then, $|f(s,y) - f(t,x)| \leq |f(t,y) - f(t,x)| + |f(t,y) - f(s,y)| \leq |f(t,y) - f(t,x)| + \|f(t,\cdot) - f(s,\cdot)\|_\infty$. If now s is close to t, and y is close to x, then $|f(s,y) - f(t,x)|$ is small.

This shows $u, u_i, u_t \in C([0,T], C(\overline{\Omega})) \in C(\overline{\Omega \times I})$, i.e. $u \in C^1(\overline{Q \times I})$.

To conclude, let $u \in L^2(I, H^1)$. Approximate u by $u_k := \sum_{i \leq m_k} \phi_i^k(t) f_i^k$ as in point 2, and approximate f_i^k by suitable $g_i^k \in H^1(\Omega) \cap C^1(\overline{\Omega})$, to obtain $u_k := \sum_{i \leq m_k} \phi_i^k(t) g_i^k$

Then $\|u - w_k\|_{L^2(I,H^1)} \leq \|u_k - w_k\|_{L^2(I,H^1)} + \|u_k - u\|_{L^2(I,H^1)}$. We only need to estimate $\|u_k - w_k\|_{L^2(I,H^1)} \leq T \sum_{i \leq m_k} \left\|\phi_i^k\right\|_\infty \left\|f_i^k - g_i^k\right\|_{H^1}$.
By the first point, $\left\|f_i^k - g_i^k\right\|_{H^1}$ can be made as small as it is necessary to conclude.

Last remarks

Again with reference to [45], consider the anisotropic spaces $H^{r,s} := L^2(I, H^r) \cap H^s(I, L^2)$. We restrict to the case $r = 1$, $s \geq 0$.

Denote the traces tr_s defined in theorem 4.1, mapping $H^{1,s}(\Omega \times I) \to H^{1/2,s/2}(\partial\Omega \times I)$. For $\partial\Omega$ Lipschitz this theorem is still valid, as $1/2 \leq 1$, see the discussion above lemma 2.4 in [19]. As stated in [45], tr_s is an extension of $u \mapsto u|_{I\times\partial\Omega}$, defined on the dense suspace $C^\infty(\overline{Q \times I})$ of $H^{1,s}$ (that this space is dense can be proved as in lemma 2.22 of [19]). So, let $C^\infty(\overline{Q \times I}) \ni u_n \to_{H^{r,s}} u \in H^{1,s}$.

We have $\mathrm{tr}_s u_n = \mathrm{tr}_0 u_n$. Then, $u_n \to_{H^{1,s}} u$, $u_n \to_{H^{1,0}} u$, so that $\mathrm{tr}_s u_n \to_{H^{1/2,s/2}} \mathrm{tr}_s u$ (hence $\mathrm{tr}_0 u_n \to_{H^{1/2,0}} \mathrm{tr}_s u$) and $\mathrm{tr}_0 u_n \to_{H^{1/2,0}} \mathrm{tr}_\sigma u$.

Thus $\mathrm{tr}_0 u = \mathrm{tr}_s u$.

Using what we derived before, we can conclude the characterization of the traces in the anisotropic settign define

□

And now some sanity checks in the case of Gelfand triples.

Proposition A.2.7 (Sanity checks for Gelfand triples)
Consider the following Gelfand triples (the diagram commutes):

$$\begin{tikzcd}
V \arrow[dr, hook, "a"] & & & V^* \arrow[dd, "c^*"] \\
& H \arrow[r, "r"] & H^* \arrow[ur, hook, "a^*"] \arrow[dr, hook, "b^*"'] & \\
W \arrow[uu, hook, "c"] \arrow[ur, hook, "b"'] & & & W^*
\end{tikzcd}$$

Here $W \subseteq V \subseteq H$ are all separable Hilbert spaces, a, b, c the trivial injections, r the Riesz isomorphism of H. We denote by i_V the Gelfand triple embedding $V \hookrightarrow V^*$, so, $i_V = a^* r a$.
Then:

1. $H^1(I, V) \subseteq W(I, V)$ with continuous embedding. The $W(I, V)$ derivative of $u \in H^1(I, V)$ is $i_V u_t$.
2. for $u \in W(I, W)$ with $(i_W u)' \in L^2(I, H)$ (i.e. $(i_W u)_t = b^* r h$ for h in $L^2(I, H)$) we obtain $u \in W(I, V)$ (i.e. $cu \in W(I, V)$), with derivative $(i_V cu)' = a^* r h$, so that also $(i_V cu)' \in L^2(I, H)$. It also holds $(i_V cu)'|_W = (i_W u)'$. h is also the weak derivative $L^2(I, H)$ of bu.
3. let $u, v \in W(I, V)$ with $u - v \in W$. Then $u - v \in W(I, W)$ with derivative $(i_W(u - v))' = (i_V u)'|_W - (i_V v)'|_W$.

Proof.

We use several times that time integrals and bounded linear static operators commute, see proposition A.2.1. ϕ denotes $\phi \in C_c^\infty(I)$.

First point

We need to check that $a^* r a u \in H^1(I, V^*)$. This follows from proposition A.2.2, so that $(a^* r a u)_t = a^* r a u_t$.

Second point

At first we claim that h is a weak derivative of $bu \in L^2(I, H)$. In fact, $b^* r \int_I bu\phi' = \int_I (i_W u)\phi' = \{\ u \in W(I, W)\ \} = -\int_I (i_W u)'\phi = -\int_I b^* r h\phi = b^* r(-\int_I h\phi)$. By density (definition of Gelfand triple), b^* is injective, r is too, and thus $\int_I bu\phi' = -\int_I h\phi$, which shows that bu has weak derivative h, in the $H^1(I, H)$ sense.

And now $\int_I i_V cu\phi' = \int_I a^* r a c u\phi' = a^* r \int_I bu\phi' = \{$ by what we just proved $\} = -a^* r \int_I h\phi$, proving that $(i_V cu)' = a^* r h$.

Morevoer $(i_V cu)'|_W = c^* a^* r h = b^* r h = \{$ assumption $\} = (i_W u)'$.

Third point

We check the derivative. We have $\int_i i_W(u - v)\phi' = \{\ u - v \in W \subseteq V\ \} = \int_I b^* r a(u - v) = c^* \int_I (i_V u - i_V v)\phi' = -\int c^*((i_V u)' - (i_V v)')\phi$.

□

A.2.1. Some approximation properties

Lemma A.2.1.1 (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 $C = 1/\sqrt{2}$.
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 [59] 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 [34] 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. $\langle Au, v\rangle_{V^*,V} = \langle Av, u\rangle_{V^*,V}$).

Theorem B.1.8 (Regularity of time derivative)
Suppose assumption B.1.1 and assumption B.1.7. Then $u_t \in L^2(I, H)$ with the estimate:

$$\|u\|_{W(I,V)} + \|u\|_{C(I,H)} + \|u_t\|_{L^2(I,H)} \leq \tag{B.1.9}$$
$$c(\lambda, \alpha, \|A\|_{V^*}, T)(\|u_0\|_V + \|f_1\|_{L^2(I,H)} + \|f_2\|_{H^1(I,V^*)}) \tag{B.1.10}$$

That $u_t \in L^2(I, H)$ means precisely that there is $h \in L^2(I, H)$ with $a^* rh = (i_V u)'$, with the notation introduced in proposition A.2.7.

Proof.

We refer to page 26 of [34], theorem 28, and only prove the necessary modifications.

Product rule for A

We have

$$\int_0^t \langle Au_n, u_n'\rangle_{V^*,V} = \sum_{k,l\le n} \langle Aw_k^n, w_l^n\rangle_{V^*,V} \int_0^t g_k^n {g_l^n}' =$$

$$\sum_{k,l\le n} \langle Aw_k^n, w_l^n\rangle_{V^*,V} \left(-\int_0^t {g_k^n}' g_l^n + g_k^n(t) g_l^n(t) - g_k^n(0) g_l^n(0) \right)$$

By linearity at first and then symmetry we get:

$$= \langle Au_n, u_n\rangle_{V^*,V}(t) - \langle Au_n, u_n\rangle_{V^*,V}(0) - \int_0^t \langle Au_n', u_n\rangle_{V^*,V} =$$
$$= \langle Au_n, u_n\rangle_{V^*,V}(t) - \langle Au_n, u_n\rangle_{V^*,V}(0) - \int_0^t \langle Au_n, u_n'\rangle_{V^*,V}$$

so that:

$$\int_0^t \langle Au_n, u_n'\rangle_{V^*,V} = \frac{1}{2} \left(\langle Au_n, u_n\rangle_{V^*,V}(t) - \langle Au_n, u_n'\rangle_{V^*,V}(0) \right)$$

<u>Estimate for right hand side</u>

We have:

$$\int_0^t \langle f_2, u_n'\rangle_{V^*,V} = \sum_{k\le n} \int_0^t {g_k^n}' \langle f_2, w_k^n\rangle_{V^*,V}$$

By the smoothness of f_2 we have that $t \mapsto \langle f_2(t), w_k^n\rangle_{V^*,V}$ is $H^1(0,T)$, in particular $AC[0,t]$, so that we can integrate by parts:

$$= -\sum_{k\le n} \int_0^t g_k^n \langle f_2', w_k^n\rangle_{V^*,V} + \sum_{k\le n} g_k^n(t) \langle f_2(t), w_k^n\rangle_{V^*,V} - \sum_{k\le n} g_k^n(0) \langle f_2(0), w_k^n\rangle_{V^*,V} =$$
$$- \int_0^t \langle f_2', u_n\rangle_{V^*,V} + \langle f_2, u_n\rangle_{V^*,V}(t) - \langle f_2, u_n\rangle_{V^*,V}(0)$$

Here we have used proposition A.2.2 to take the derivative inside the bracket.

Note that by the smoothness of f_2, we can write, for instance, $\langle f_2, u_n\rangle_{V^*,V}(0) = \langle f_2(0), u_n\rangle_{V^*,V}$.

NB: here I need $f_2(0) \in V$ probably, but I'm not yet using the compatibility condition!.

Going to the absolute values:

$$\left| \int_0^t \langle f_2, u_n'\rangle_{V^*,V} \right| \le \int_0^T |\langle f_2', u_n\rangle_{V^*,V}| + \|f_2(t)\|_{V^*} \|u_n(t)\|_V + \|f_2(0)\|_{V^*} \|u_n(0)\|_V \le$$
$$\frac{1}{2} \|f_2'\|^2_{L^2(I,V^*)} + \frac{1}{2} \|u_n\|^2_{L^2(I,V)} + \frac{\alpha}{4} \|u_n(t)\|_V^2 +$$
$$+ \frac{4}{\alpha} \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1}{2} \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1}{2} \|u_{n0}\|_V^2$$

Now, u_n converges weakly in $L^2(I,V)$ by estimate (59) of [34] and thus $\frac{1}{2} \|u_n\|_{L^2(I,V)}$ is bounded. The term $\frac{\alpha}{4} \|u_n(t)\|_V$ can be pulled to the left hand side, u_{0n} is V convergent hence bounded. Therefore as in [34] we are able to conclude that u_n' is bounded in $L^2(I,H)$. We want to conclude $u_t \in L^2(I,H)$. We know for sure that $\langle u_m', w_j\rangle_{V^*,V} = \langle f - Au_m, w_j\rangle_{V^*,V}$, so that muliplication by a test function and integration yields $\int_I \langle u_m', w_j\phi\rangle_{V^*,V} = \int_I \langle f - Au_m, w_j\phi\rangle_{V^*,V}$. Because $u_m \rightharpoonup u$ in $L^2(I,V)$ we observe that, by proposition A.2.1 applied on $A \in L(V,V^*)$, it holds $\int_I \langle u_m', w_j\phi\rangle_{V^*,V} \to \int_I \langle u', w_j\phi\rangle_{V^*,V}$.

What's more, is that $u'_m \rightharpoonup h$ in $L^2(I,H)$, so that $\int_I \langle h, w_j\rangle_{V^*,V}\phi = \int_I \langle u', w_j\rangle_{V^*,V}\phi$. It means that for almost all t, $\langle h, w_j\rangle_{V^*,V} = \langle u', w_j\rangle_{V^*,V}$. And now we can really say that $u' \in L^2(I,H)$, which even more precisely means $(i_V u)' = a^* r h$ almost everywhere.

We also obtain that u_t is bounded by $c(\alpha)(\|f_2\|_{L^\infty(I,V^*)} + \|f_2\|_{L^2(I,V^*)} + \|u_0\|_V + \|u\|_{L^2(I,V)})$.

Note that, by [27], theorem 2 of page 286, we can estimate $\|f_2\|_{L^\infty(I,V^*)}$ by $c(T)\,\|f_2\|_{H^1(I,V^*)}$, so that the claim for the time derivative u_t is proven.

□

For the case where $H = L^2$, $H^1 \supseteq V \supseteq H^1_0$, $f_2|_{H^1_0} = 0$ we have even more regularity available.

Theorem B.1.11 (Additional regularity)
Suppose assumption B.1.1 and assumption B.1.7.
Let additionally $H = L^2$, $H^1 \supseteq V \supseteq H^1_0$, $f_2|_{H^1_0} = 0$. Then $Au|_{H^1_0}$ extends to $\overline{Au_{H^1_0}} \in L^2(I,H)$ with:

$$\|u\|_{W(I,V)} + \|u\|_{C([0,T],H)} + \|u_t\|_{L^2(I,H)} + \left\|\overline{Au|_{H^1_0}}\right\|_{L^2(I,H)} \leq \tag{B.1.12}$$

$$c(\lambda, \alpha, \|A\|_{V^*}, T)(\|u_0\|_V + \|f_1\|_{L^2(I,H)} + \|f_2\|_{H^1(I,V^*)}) \tag{B.1.13}$$

Moreover $u_t + \overline{Au_{H^1_0}} = f_1$ in $L^2(0,T,L^2) \cong L^2(Q)$ and $\overline{Au|_{H^1_0}} = Au$ on H^1_0.

Proof.

For $v \in H^1_0$ we get $\langle Au, v\rangle_{V^*,V} = \langle f_1 - u_t, v\rangle_{V^*,V} = (f_1 - u_t, v)_H$, for almost all $t \in (0,T)$. From here we conclude that $Au(t)$ extends for a.a. t to an element of H with $(\overline{Au} - f_1 + u_t, v)_{L^2} = 0$ for all $v \in H^1_0$, almost all t. By density, $\overline{Au} - f_1 + u_t = 0$ in H for almost all t, so that $\overline{Au} = f_1 - u_t$ in $L^2(0,T,L^2) \cong L^2(Q)$.

This isometric isomorphism is stated in [59], page 144.

□

For our applications we also need to track the constants more precisely, which is accomplished in the next proposition.

Proposition B.1.14 (Tracking the costants)
With assumption B.1.1 there holds:

$$\|u\|^2_{C([0;T],H)} + \alpha\,\|u\|^2_{L^2(I,V)} \leq \exp(2\lambda T)(\|u_0\|^2_H + \alpha^{-1}\,\|f\|^2_{L^2(I,V^*)}) \tag{B.1.15}$$

$$\|u'\|_{L^2(I,V^*)} \leq \|A\|_{L(V,V^*)}\,\alpha^{-1/2}\sqrt{\exp(2\lambda T)}\,\|u_0\|_H + \tag{B.1.16}$$

$$\left(\|A\|_{L(V,V^*)}\,\alpha^{-1}\sqrt{\exp(2\lambda T)} + 1\right)\|f\|_{L^2(I,V^*)} \tag{B.1.17}$$

With additionally assumption B.1.7 we obtain:

$$C\,\|u'\|^2_{L^2(I,H)} \leq (1 + (1 + C_0)\alpha^{-1})\,\|f_2\|^2_{H^1(I,V^*)} + \tag{B.1.18}$$

$$(1 + \|A\|_{L(V,V^*)})\,\|u_0\|^2_V + C_0\,\|u_0\|^2_H + \tag{B.1.19}$$

$$\|f_1\|^2_{L^2(I,H)} + C_0\alpha^{-1}\,\|f_1\|^2_{L^2(I,V^*)} \tag{B.1.20}$$

with $C > 0$ a number independent of the problem.
Here $C_0 = 2^{-1}\max(1,\lambda)\max(1,\alpha^{-1})\exp(2\lambda T)$.

Proof.

No regularity

From page 21 of [34] we obtain that $\|u\|^2_{C([0;T],H)} + \alpha\,\|u\|^2_{L^2(I,V)} \leq \exp(2\lambda T)(\|u_0\|^2_H + \alpha^{-1}\,\|f\|^2_{L^2(I,V^*)})$. NOTA BENE, this is slightly wrong, i.e. a 2 is missing from the left hand side.

In particular, $\sqrt{\alpha}\,\|u\|_{L^2(I,V)} \leq \sqrt{\exp(2\lambda T)}(\|u_0\|_H + \alpha^{-1/2}\,\|f\|_{L^2(I,V^*)})$, or $\|u\|_{L^2(I,V)} \leq \alpha^{-1/2}\sqrt{\exp(2\lambda T)}(\|u_0\|_H + \alpha^{-1/2}\,\|f\|_{L^2(I,V^*)})$.

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:

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

and:

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

More regularity

We tie back to page 25 of [34]. 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, as in the proof of theorem B.1.8:

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

Also:

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

Putting all together:

$$\begin{aligned}\int_0^t \|u_n'\|^2_H + \frac{\alpha}{2} \, \|u_n(t)\|^2_V - \frac{\lambda}{2} \, \|u_n(t)\|^2_H - \frac{\|A\|}{2} \, \|u_{n0}\|_V \\ \frac{1}{2} \, \|f_2'\|^2_{L^2(I,V^*)} + \frac{1}{2} \, \|u_n\|^2_{L^2(I,V)} + \frac{\alpha}{4} \, \|u_n(t)\|^2_V + \\ + \frac{4}{\alpha} \, \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1}{2} \, \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1}{2} \, \|u_{n0}\|^2_V + \\ + \frac{1}{2} \, \|f_1\|^2_{L^2(I,H)} + \frac{1}{2}\int_0^t \|u_n'\|^2_H\end{aligned}$$

which brings us to:

$$\frac{1}{2}\int_0^t \|u_n'\|^2_H + \frac{\alpha}{4} \, \|u_n(t)\|^2_V - \frac{\lambda}{2} \, \|u_n(t)\|^2_H \leq \tag{B.1.21}$$

$$\frac{1}{2} \, \|f_2'\|^2_{L^2(I,V^*)} + \frac{1}{2} \, \|u_n\|^2_{L^2(I,V)} + \tag{B.1.22}$$

$$+ \frac{8+\alpha}{2\alpha} \, \|f_2\|^2_{L^\infty(I,V^*)} + \frac{1+\|A\|}{2} \, \|u_{n0}\|^2_V + \tag{B.1.23}$$

$$+ \frac{1}{2} \, \|f_1\|^2_{L^2(I,H)} \tag{B.1.24}$$

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:

$$\frac{1}{2}\int_0^T \|u'\|_H^2 \leq \frac{1}{2}\|f_2'\|_{L^2(I,V^*)}^2 + \frac{8+\alpha}{2\alpha}\|f_2\|_{L^\infty(I,V^*)}^2 + \frac{1+\|A\|}{2}\|u_0\|_V^2 + \frac{1}{2}\|f_1\|_{L^2(I,H)}^2 + \\ \text{limsup}_n\left(\frac{\lambda}{2}\|u_n\|_{C([0,T],H)}^2 + \frac{1}{2}\|u_n\|_{L^2(I,V)}^2\right)$$

Using a purely numeric constant C without dependences on the problem we can write:

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

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

$$\text{limsup}_n\left(\frac{\lambda}{2}\|u_n\|_{C([0,T],H)}^2 + \frac{1}{2}\|u_n\|_{L^2(I,V)}^2\right) \leq \tag{B.1.25}$$

$$2^{-1}\max(1,\lambda)\max(1,\alpha^{-1})\text{limsup}_n\left(\|u_n\|_{C([0,T],H)}^2 + \alpha\|u_n\|_{L^2(I,V)}^2\right) \leq \tag{B.1.26}$$

$$2^{-1}\max(1,\lambda)\max(1,\alpha^{-1})\exp(2\lambda T)(\|u_0\|_H^2 + \alpha^{-1}\|f_1+f_2\|_{L^2(I,V^*)}^2) \leq \tag{B.1.27}$$

$$2^{-1}\max(1,\lambda)\max(1,\alpha^{-1})\exp(2\lambda T)(\|u_0\|_H^2 + 2\alpha^{-1}\|f_1\|_{L^2(I,V^*)}^2 + 2\alpha^{-1}\|f_2\|_{L^2(I,V^*)}^2) \leq \tag{B.1.28}$$

$$CC_0(\|u_0\|_H^2 + \alpha^{-1}\|f_1\|_{L^2(I,V^*)}^2 + \alpha^{-1}\|f_2\|_{L^2(I,V^*)}^2) \tag{B.1.29}$$

where $C_0 = 2^{-1}\max(1,\lambda)\max(1,\alpha^{-1})\exp(2\lambda T)$ and C is a purely numeric constant without dependences on the problem.

Therefore:

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

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

Thus:

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

□

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

Proposition B.1.30 (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 [63], theorem 27.2, page 406. The proof is a simplification of his argument, since our operator A is for simplicity, independent in time. We also prove the proposition for the lowest order of differentiation, being the extension to higher derivatives tractable with equal arguments.

Consider the problem:

$$\begin{aligned} v_t + Av = f' \\ v(0) = f(0) - Au(0) \end{aligned}$$

By assumption, $f(0) - Au(0) \in H$, and $f' \in L^2(I, V^*)$, so that, by theorem B.1.5 we obtain $v \in W(I; V)$.

Define $w(t) := u(0) + \int_0^t v(s)ds$, an absolutely continuous V-valued function, being $u(0) \in V$ by assumption. We have $w_t = v$, so that $w \in H^1(I, V)$. We show that $w = u$.

Integrating the equation of v we obtain, with equalities holding in V^*, that:

$$\begin{aligned} w_t(t) = v(t) = \int_0^t f' - \int_0^t Av + v(0) = \\ f(t) - f(0) + f(0) - Au(0) - \int_0^t A(w_t) = \\ f(t) - f(0) + f(0) - Au(0) - Aw(t) + Au(0) = f(t) - Aw(t) \end{aligned}$$

Therefore, w solves the same equation as u and thus, $w = u$. From here we obtain both $u \in H^1(I, V)$, together with $u_{tt} = w_{tt} = v_t \in L^2(I, V^*)$, and the equation:

$$\begin{aligned} u_{tt} + Au_t = f' \\ u_t(0) = f(0) - Au(0) \end{aligned}$$

□

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 [48]). For such a choice we also have $H_0^1 = H^1 \cap \ker \mathrm{tr}$, see [43], 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 proposition 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 $H_0^1(U)$ is dense in H, so is V and we obtain a Gelfand triple. That V is a closed subspace of H^1 follows from the observation that if $u_n \to u$ in the V norm, then $\mathrm{tr}u_n \to \mathrm{tr}u$ in $L^2(\partial U)$. We can take an almost everywhere pointwise convergent sequence, so that $\mathrm{tr}u_n \to \mathrm{tr}u$ a.e., and by the fact that Γ_m has positive Hausdorff measure, we conclude $\mathrm{tr}u = 0$ on Γ_m.

We define $A := H^1 \to H^{1*}$ by $(Au)v := \int_u \nabla u \nabla v$. This operator can be the recast to $V \to H^{-1}$ and $V \to V^*$.

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)

$$u_0 \in W(I, H_0^1) \tag{B.2.1.13}$$
$$u_0' + Au_0 = -((\bar{u}', \cdot)_H + A\bar{u}) \text{ in } H^{-1} \text{ and for a.e. } t \in (0,T) \tag{B.2.1.14}$$
$$u_0(0) = 0 \tag{B.2.1.15}$$

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 $\implies$ $u - \bar{u}$ solves problem B.2.1.12, and if $u_0(\bar{u})$ solves problem B.2.1.12, then $\bar{u} + u_0(\bar{u})$ solves problem B.2.1.2.
Furthermore:

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

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 [35], page 20).

Reformulation (first part)

Consider the following commutative diagram, where $V = H^1_{0,m}$, $W = H^1_0$:

$$\begin{tikzcd}
H^1_{0,m} \arrow[dr, hook, "a"] & & & (H^1_{0,m})^* \arrow[ddd, hook, "c^*"] \\
& H \arrow[r, "r"] & H^* \arrow[ur, hook, "a^*"] \arrow[dr, hook, "b^*"'] & \\
& & & \\
H^1_0 \arrow[uuu, hook, "c"] \arrow[uur, hook, "b"'] & & & H^{-1}
\end{tikzcd}$$

Here, a, b, c are the trivial injections, r the Riesz isomorphism $h \mapsto (h, \cdot)_H$.

Now $(i_W(u - \bar{u}))' + A(u - \bar{u}) = (i_V u)'|_{H^{-1}} - (i_V \bar{u})'|_{H^{-1}} + Au - A\bar{u} = \{$ proposition A.2.7 $\} = (i_V u)'|_{H^{-1}} - (i_V \bar{u}_t)|_{H^{-1}} + Au - A\bar{u} = -(i_V \bar{u}_t)|_{H^{-1}} - A\bar{u}$ if u solves problem B.2.1.2, where $\bar{u}_t$ is the weak derivative of $\bar{u}$ in the $H^1(I, V)$ sense. Call $u_0 = u - \bar{u}$. By again proposition A.2.7, $u_0 \in W(I, H^1_0)$.

This motivates us to consider the problem:

$$u_0 \in W(I, H^1_0) \tag{B.2.1.17}$$

$$u_0' + Au_0 = -(f_1 + f_2) \text{ in } H^{-1} \text{ and for a.e. } t \in (0, T) \tag{B.2.1.18}$$

$$u_0(0) = 0 \tag{B.2.1.19}$$

Here, $f_1 := (i_V \bar{u}_t)|_{H^{-1}} = c^* a^* r a \bar{u}_t = b^* r(a\bar{u}_t) \in L^2(I, H)$.

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

Existence

By theorem B.1.11 we get a solution of the above problem with $u_0' \in L^2(I, H)$.

And now, let $u := \bar{u} + cu_0 = \bar{u} + u_0$. We claim it is a solution. The initial and boundary conditions are surely satisfied. We check it is in $W(I, V)$ and is satisfies the partial differential equation.

By proposition A.2.7, we have both $\bar{u}, cu_0 \in W(I, V)$. The derivative of $\bar{u}$ becomes $i_V \bar{u}_t$, see proposition A.2.7. Therefore $(i_V(\bar{u} + cu_0))'|_{H^1_0} = c^*(i_V(\bar{u} + cu_0))' = c^* i_V \bar{u}_t + c^* i_V(cu_0)' = b^* r(a\bar{u}_t) + i_W(u_0)'$ by proposition A.2.7.

Using the pde of u_0, ... $= b^* r(a\bar{u}_t) - Au_0 - f_1 - f_2 = -A(u_0 + \bar{u})$.

Uniqueness

For two solutions u_1, u_2 of *problem B.2.1.2* we can form $d := u_1 - u_2 \in W(I, H^1_0)$ by proposition A.2.7. Clearly, $d(0) = 0$. Moreover, $(i_{H^1_0} d)' = \{$ proposition A.2.7 $\} = (i_V u_1)'|_{H^1_0} - (i_V u_2)'|_{H^1_0} = A(u_1 - u_2)$.

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 $u = \bar{u} + u_0$ 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 u_0 as above and get $u = \bar{u} + u_0$ solving problem B.2.1.2.

Viceversa, let u solve problem B.2.1.2. Call $u_0 = u - \bar{u}$. Then, as seen above, $u_0 \in W(I, H^1_0)$ and $(i_V(u - \bar{u}))'|_{H^{-1}} + A(u - \bar{u}) = (i_V u)'|_{H^{-1}} - (i_V \bar{u})'|_{H^{-1}} + Au - A\bar{u} = \{$ proposition A.2.7 $\} = (i_V u)'|_{H^{-1}} - (i_V \bar{u}_t)|_{H^{-1}} + Au - A\bar{u} = -(i_V \bar{u}_t)|_{H^{-1}} - A\bar{u}$ if u solves problem B.2.1.2, where $\bar{u}_t$ is the weak derivative of $\bar{u}$ in the $H^1(I, V)$ sense. Call $u_0 = u - \bar{u}$. By again proposition A.2.7, $(i_W(u - \bar{u}))' + A(u - \bar{u}) = (i_V u)'|_{H^{-1}} - (i_V \bar{u})'|_{H^{-1}} + Au - A\bar{u} = (i_V u)'|_{H^{-1}} - (i_V \bar{u}_t)|_{H^{-1}} + Au - A\bar{u} = -(i_V \bar{u}_t)|_{H^{-1}} - A\bar{u} = -b^* r(a\bar{u}_t) - A\bar{u}$. Moreover, $u_0(0) = 0$, so that u_0 solves problem B.2.1.12.

Regularity

Let $u = \bar{u} + u_0$ be the unique solution, as before, of problem B.2.1.2. From proposition A.2.7 we know $(i_V(\bar{u}))' = i_V(\bar{u}_t) = a^* r(a\bar{u}_t)$, and $i_V(cu_0)' = a^* r(u_0')$, for $u_0' \in L^2(I, H)$ the representative of $(i_W(u_0))'$, equivalently, the weak derivative of u_0 in the $H^1(I, H)$ sense. It follows that $(i_V u)' = a^* r(a\bar{u}_t + u_0')$, 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 $\bar{u}(0) = 0$. Consider u_0. Then, by proposition B.1.14:

$$\|u_0\|^2_{C([0;T],H)} + \alpha \|u_0\|^2_{L^2(I,H^1_0)} \leq \exp(2\lambda T)\alpha^{-1} \left\|(\bar{u}', \cdot)_H + A\bar{u}\right\|^2_{L^2(I,H^{-1})}$$

$$\begin{aligned} C\left\|u_0'\right\|^2_{L^2(I,H)} \leq (1 + (1 + C_0)\alpha^{-1}) \|A\bar{u}\|^2_{H^1(I,H^{-1})} + \\ \left\|(\bar{u}', \cdot)_H\right\|^2_{L^2(I,H)} + C_0\alpha^{-1} \left\|(\bar{u}', \cdot)_H\right\|^2_{L^2(I,H^{-1})} \end{aligned}$$

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

We norm H^1_0 with the full H^1 norm too. Then:

$$\begin{aligned} \left\|(\bar{u}', \cdot)_H + A\bar{u}\right\|_{L^2(I,H^{-1})} \leq \\ \sup_{\|v\|_{L^2(I,H^1_0)}=1} \left\|\bar{u}'\right\|_{L^2(I,H)} \|v\|_{L^2(I,H)} + \|\nabla\bar{u}\|_{L^2(I,H)} \|\nabla v\|_{L^2(I,H)} \leq \\ C(\left\|\bar{u}'\right\|_{L^2(I,H)} + \|\nabla\bar{u}\|_{L^2(I,H)}) \end{aligned}$$

By proposition A.2.2, $\|A\bar{u}\|_{H^1(I,H^{-1})} \leq \|A\|_{L(V,H^{-1})} \|\bar{u}\|_{H^1(I,V)}$ (we could apply it since H^{-1} is separable, as a dual of a reflexive Banach space).

Finally, $\|(\bar{u}', \cdot)_H\|^2_{L^2(I,H^{-1})} \leq \|\bar{u}'\|^2_{L^2(I,H)}$.

We can then say:

$$\begin{aligned} \|u_0\|^2_{C([0;T],H)} + C\alpha \|u_0\|^2_{L^2(I,H^1_0)} \leq \exp(2\lambda T)\alpha^{-1} \|\bar{u}\|^2_{H^1(I,V)} \\ C\left\|u_0'\right\|^2_{L^2(I,H)} \leq ((1 + (1 + C_0)\alpha^{-1}) \|A\|^2_{L(V,H^{-1})} + 1 + C_0\alpha^{-1}) \|\bar{u}\|^2_{H^1(I,V)} \end{aligned}$$

Now, $\langle Av, v\rangle_{H^{-1},H^1_0} + 1 \cdot \|v\|^2_H = 1 \cdot \|v\|^2_{H^1_0}$, so that $\alpha = \lambda = 1$. Moreover, $\langle Au, v\rangle_{H^{-1},H^1_0} \leq \|u\|_V \|v\|_{H^1_0}$, i.e. $\|A\|_{L(V,H^{-1})} \leq 1$.

Therefore $\|u_0\|^2_{C([0;T],H)} + \|u_0\|^2_{L^2(I,H^1_0)} + \|u_0'\|^2_{L^2(I,H)} \leq C(T) \|\bar{u}\|^2_{H^1(I,V)}$ with $C > 1$, only dependent on T, smoothly, exploding for large T.

Now, let's analyse the norms of $\bar{u}$. Because $\bar{u} \in H^1(I, V)$, then, $\bar{u} \in C([0, T], V) \hookrightarrow C([0, T], H)$, where the embedding is non-expansive by the choice of the norm of V. Therefore $\|\bar{u}\|_{C([0;T],H)} \leq \|\bar{u}\|_{C([0;T],V)} \leq (1 + T) \|\bar{u}\|_{H^1(I,V)}$. We can therefore conclude that $\|u\|^2_{C([0;T],H)} + \|u\|^2_{L^2(I,H^1_0)} + \|u'\|^2_{L^2(I,H)} \leq C(T) \|\bar{u}\|^2_{H^1(I,V)}$ with $C > 1$, only dependent on T, smoothly, exploding for large T.

□

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 $L(V, H^{-1})$.

By proposition A.2.2, $G \in H^1(I, V^*)$. In fact, define $T : L^2(\Sigma_f) \to V^*$ by $\langle Tg, v\rangle_{V^*,V} := \int_{\Gamma_f} g\mathrm{tr} v d\sigma$. Then, $\langle Tg, v\rangle_{V^*,V} \leq \|g\|_{L^2(\Gamma_f)} \|v\|_V$ by trace theory. Now, $G(t) = Tg(t)$.

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:

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

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

Proof.

It is an application of theorem B.1.5, theorem B.1.8 and proposition B.1.14. □

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)

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

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

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

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

Remove the comment below

Note, for the regular case, we will be discussing only a homogeneous initial condition. This will suffice for our purposes. A generalization would entail handling more complicated compatibility conditions, see [45], chapter 2. Also note that the requirements imposed on the data below, are only sufficient, to ensure the desired regularity.

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 $G_D \in H^1(U)$ solving:

$$
\begin{cases}
-\Delta G_D(t) = 0 & \text{in } U\\
G_D(t) = g_D(t) & \text{on } \Gamma_D\\
G_D(t) = 0 & \text{on } \Gamma_N
\end{cases}
$$

We ask, aside from assumption B.2.3.2:
Make it more general, and hide the fact that this won't work unless I consider more general theories of compatibility conditions. In particular, just put the conditions in terms of the derivatives of u at initial time

1. $u_0 = 0$
2. $g_D \in H^{k+1}(I, H^{1/2}(\Gamma_D))$
3. $g_N \in H^k(I, L^2(\Gamma_N))$
4. $f \in H^k(I, H)$
5. $g_N^{(j)}(0) = 0$, for $j = 0, ..., k-1$
6. $f^{(j-1)}(0) - G_D^{(j)}(0) + \sum_{l=1}^{j-1}(-1)^l A^l f^{(j-l-1)}(0) \in V$, for $j = 0, ..., k-1$ (for $j = 0$ it is read $g_D(0) = 0$, which we already assumed)
7. $\sum_{j=1}^{k-1}(-1)^j A^j(f^{(k-j-1)}(0)) \in H$ (remember that $A : V \to V^*$, so that $Af \neq -\Delta f$, in general)

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:

- $g_N \in H^{k+1}(I, L^2(\Gamma_N))$
- $f^{(k-1)}(0) - G_D^{(k)}(0) + \sum_{l=1}^{k-1}(-1)^l A^l f^{(k-l-1)}(0) \in V$

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:

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

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 $1 \leq j \leq k$:

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

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 is (for a.e. t), a e.g. harmonic extension of g_D:

$$\begin{cases} -\Delta G_D(t) = 0 & \text{in } U \\ G_D(t) = g_D(t) & \text{on } \Gamma_D \\ G_D(t) = 0 & \text{on } \Gamma_N \end{cases}$$

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 proposition A.2.2.

We can therefore deduce the estimate:

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

Regularity: compatibility relations

$F := (f - \partial_t G_D, \cdot)_H + (g_N, \mathrm{tr}(\cdot))_{L^2(\Gamma_N)}$ is, thanks to the smoothness assumptions, in $H^k(I, V^*)$. We apply proposition B.1.30, to the problem:

$$\begin{cases}(\delta_t, v)_H + (\nabla\delta, \nabla v)_H = (F, v)_H \\ \delta(0) = \delta_0 \in V\end{cases}$$

for $\delta_0 = -G_D(0)$.

We check its hypothesis, for $k \geq 1$.

In particular $F^{(k-1)} = (f^{(k-1)} - G_D^{(k)}, \cdot)_H + (g_N^{(k-1)}, \mathrm{tr}(\cdot))_{L^2(\Gamma_N)}$.

Because $f \in H^k(I, H)$, and $g_N, G_D \in H^{k+1}(I, H^{1/2}(\Gamma_D)), H^{k+1}(I, H^1(U))$, we can define $F^{(k-1)}(0)$, which is $F^{(k-1)}(0) = (f^{(k-1)}(0) - G_D^{(k)}(0), \cdot)_H + (g_N^{(k-1)}(0), \mathrm{tr}(\cdot))_{L^2(\Gamma_N)}$. As $g_N^{(k-1)}(0) = 0$, we get:

$$F^{(k-1)}(0) = (f^{(k-1)}(0) - G_D^{(k)}(0), \cdot)_H$$

We now compute the terms g_k.

We have $g_k = \sum_{j=0}^{k-1}(-1)^j A^j F^{(k-j-1)}(0) + (-1)^k A^k(-G_D(0))$, $g_0 = -G_D(0)$.

Note, $AG_D(v) = (\nabla G_D, \nabla v) = 0$ for $v \in V$. Therefore, $A^j G_D(0) = 0$ and we get to $g_k = \sum_{j=0}^{k-1}(-1)^j A^j F^{(k-j-1)}(0)$, $k \geq 1$.

Let's start to check that $g_k \in H$. To do so, note that for $j = 0, ..., k-1$ we have that $A^j F^{(k-j-1)}(0) = A^j f^{(k-j-1)}(0) - A^j G_D^{(k-j)}(0)$.

So, for $j = 0$: $A^j F^{(k-j-1)}(0) = f^{(k-1)}(0) - G_D^{(k)}(0)$, whereas for $j \geq 1$: $A^j F^{(k-j-1)}(0) = A^j f^{(k-j-1)}(0) - A^{j-1} A G_D^{(k-j)}(0)$.

Because $f \in H^k(I, H), G_D \in H^{k+1}(I, H^1(U))$, the term for $j = 0$ is in H.

For $j \geq 1$. Note that, by calling $h : H^{1/2}(\Gamma_D) \to H^1(U)$ the operator $g_D \mapsto G_D$, thanks to the assumption $g_D \in H^{k+1}(I, H^{1/2}(\Gamma_D))$ and to proposition A.2.2, we have $\partial_{t^k} h g_D = h \partial_{t^k} g_D$, so that $AG_D^{(j)} = 0$, for all t and all $j \leq k$. Therefore $A^{j-1} A G_D^{(k-j)}(0) = 0$ for $j \geq 1$ without other assumptions, and we have to ask for $\sum_{j=1}^{k-1}(-1)^j A^j F^{(k-j-1)}(0) = \sum_{j=1}^{k-1}(-1)^j A^j(f^{(k-j-1)}(0)) \in H$.

It now remains to ask that $g_j \in V$ for $j = 1, ..., k-1$.

We have $g_j = \sum_{l=0}^{j-1}(-1)^l A^l F^{(j-l-1)}(0)$, for $j = 1, ..., k-1$, and, as seen before, $AG_D^{(j-l)} = 0$, so that we must ensure:

$$f^{(j-1)}(0) - G_D^{(j)}(0) + \sum_{l=1}^{j-1}(-1)^l A^l f^{(j-l-1)}(0) \in V$$

Regularity: time smoothness

So, proposition B.1.30 ensures then that $\delta \in H^k(I, V)$, $\delta^{(k+1)} \in L^2(I, V^*)$. Because we $G_D \in H^{k+1}(I, H^1(U))$ 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.1.30 we also have:

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

We ask for $g_k \in V$.

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 theorem B.1.8 to obtain $\delta \in H^{k+1}(I, H)$.

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, for a.e. $t \in (0, T)$:

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

which is the variational counterpart to:

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

This holds for $0 \leq j \leq k$.

H^2 regularity results that can be found in chapter 2 of [35] let us conclude the proof.

□

An application of this, please

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 proposition 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 [38], theorem 1.31 at page 39).

We are now ready to restrict both state and adjoint space.

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. There holds that the $W(I,V)$ derivative is represented by the $H^1(I,H)$ derivative and $\langle u', v\rangle_{V^*,V} = (u',v)_H$, with the suitable interpretations of u' (on the left, we have $i_V(u)'$, i_V the Gelfand triple embedding; on the right we have u, seen in H, and then weakly differentiated in the $H^1(I,H)$ sense)
- 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.

Completeness

We have the inclusions $L^2(I,H) \subseteq L^2(I,V) \cap H^1(I,H) \subseteq H^1(I,V)$.

If q_n is Cauchy in Q, then it is Cauchy in the individual norms of $L^2(I,V), H^1(I,H)$, so that q_n convergens to two limits, one in $L^2(I,V)$ and one in $H^1(I,H)$. The convergence is common in $L^2(I,H)$, which implies that the two limits coincide at $q \in Q(I,V)$. The convergence in $Q(I,V)$ of q_n to Q follows from the individual convergences of $q_n, \nabla q_n, q_{nt}$ in $L^2(I,H), L^2(I,H), L^2(I,H)$.

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 [38], page 39, lemma 1.9.

Continuity

Follows from the embedding $H^1(I,H) \hookrightarrow C([0,T],H)$, as seen in [27], theorem 2 of page 286.

More density

We can therefore speak of initial values. In particular, $C_c^\infty(I,V) \subseteq Q_0(I,V) \subseteq L^2(I,V)$, and as before, the density result follows.

Relationship with $W(I,V)$

Consider the chain:

$$V \xhookrightarrow{a} H \xrightarrow{r} H^* \xhookrightarrow{a^*} V^*$$

where a is the trivial embedding and r the Riesz isomorphism.

We claim that for $v \in Q(I,V)$, then $(a^* rav)' = a^* r(av)'$, where $av \in H^1(I,H)$. In fact, for $\phi \in C_c^\infty(I)$, we get $\int_I a^* rav\phi' = \{$ proposition A.2.1 $\} = a^* r \int_I av\phi' = -a^* r \int_I (av)'\phi = -\int_I a^* r(av)'\phi$.

Now, let $u \in W(I,V)$, with $(a^* rau)' = a^* rh$, $h \in L^2(I,H)$. Then $a^* r \int_I h\phi = \{$ proposition A.2.1 $\} = \int_I a^* rh\phi = \int_I (a^* rau)'\phi = a^* r(-\int au\phi')$.

We know that a^* is injective and so is r, so that $\int_I h\phi = -\int_I au\phi'$ as we wanted.

Integration by parts

We note that for $v, w \in Q(I,V) \subseteq W(I,V)$, we have $\int_I \langle (a^* rav)', w\rangle_{V^*,V} = \int_I \langle a^* r(av)', w\rangle_{V^*,V} = \int_I ((av)', aw)_H$. We can now apply theorem 3.11 at page 148 of [59] to conclude that $\int_I (v_t, w)_H = -\int_I ((aw)_t, av)_H + ((av)(T), (aw)(T))_H - ((av)(0), (aw)(0))_H$

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 proposition 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:

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

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 we can draw a similar diagram:

$$Q(I,V) \xhookrightarrow{j} H^1(I,H) \xrightarrow{\partial_t} L^2(I,H)$$

We therefore obtain $(\partial_t q_k, p)_{L^2(I,H)} \to (\partial_t q, p)_{L^2(I,H)}$ for all $p \in L^2(I,H)$.

The convergence $(q_k, p)_{L^2(I,H)} \to (q, p)_{L^2(I,H)}$ for all $p \in L^2(I,H)$ follows 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:

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

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, this is equivalent to:

$$
\begin{aligned}
w \in W_0(I, H^1_{0,m}), \bar{u} + v_0 \in W_0(I, H^1_{0,m}), v_0 \in W_0(I, H^1_0) \\
\int_I \langle w', q \rangle_{H^{1*}_{0,m}, H^1_{0,m}} + (\nabla w, \nabla q)_H = \int_I (g, \mathrm{tr} q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, H^1_{0,m}) \\
\int_I \langle v_0', p \rangle_{H^{-1}, H^1_0} + (\nabla v_0, \nabla p)_H = -\int_I (\bar{u}', p)_H + (\nabla \bar{u}, \nabla p)_H, \quad \forall p \in Q^0(I, H^1_0)
\end{aligned}
$$

By regularity, see theorem B.2.1.11, theorem B.2.2.10, and thanks to proposition B.3.3 this implies:

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

where now the derivatives are in the $H^1(I, H)$ sense. Indeed we have proved in proposition B.3.3 that $u \in W(I, V)$ with $L^2(I, H)$ derivative, is actually $Q(I, V)$, with weak derivative in the $H^1(I, H)$ sense equal to the $L^2(I, H)$ representative of u' in the $W(I, V)$ sense. There, we also proved the representation of the duality bracket.

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 we can get to:

$$
\begin{aligned}
w \in W_0(I, H^1_{0,m}), \bar{u} + v_0 \in W_0(I, H^1_{0,m}), v_0 \in W_0(I, H^1_0) \\
\int_I \langle w', q \rangle_{H^{1*}_{0,m}, H^1_{0,m}} + (\nabla w, \nabla q)_H = \int_I (g, \mathrm{tr} q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, H^1_{0,m}) \\
\int_I \langle v_0', p \rangle_{H^{-1}, H^1_0} + (\nabla v_0, \nabla p)_H = -\int_I (\bar{u}', p)_H + (\nabla \bar{u}, \nabla p)_H, \quad \forall p \in Q^0(I, H^1_0)
\end{aligned}
$$

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

Proposition C.1.1 (Measurability of composition)
Define $\mathcal{M} := \{\tau : \mathbb{R}^n \to \mathbb{R}^n$ Lebesgue measurable $\}/\sim$, the quotient being the almost everywhere equal relation (according to the Lebesgue measure).
Consider also U from $\mathcal{M}_c := \{\tau : \mathbb{R}^n \to \mathbb{R}^n$ continuous $\}/\sim$, the application "unique continuous representative", and $\mathcal{M}_{BL} := \{\tau : \mathbb{R}^n \to \mathbb{R}^n$ Lipschitz homeomorphism$\}/\sim \subseteq \mathcal{M}_c$.
We can then define $\circ : \mathcal{M} \times \mathcal{M}_{BL}, \mathcal{M}_c \times \mathcal{M} \to \mathcal{M}$ by, respectively, $[f] \circ g := [f \circ U(g)], f \circ [g] := [U(f) \circ g]$. These definitions are well posed.

Proof.

$\underline{\mathcal{M}_c}$

$U(f)$ is Borel measurable, so the preimage of a Borel set is Borel measurable, and g is Lebesgue measurable, so his preimage of such Borel set is Lebesgue measurable (see here for the different notions of measurability).

This shows that $U(f) \circ g$ is measurable.

To complete the well posedness, if $h = g$ a.e., then clearly $U(f) \circ g = U(f) \circ h$ a.e..

$\underline{\mathcal{M}_{BL}}$

Consider $f \circ U(g)$. We need to prove it is measurable and that is only depends on $[f]$.

For the measurability: the preimage of a Borel set, by f, is Lebesgue measurable L. $U(g)$ has a Lipschitz inverse, which will map this set to a Lebesgue set. Indeed, $L = B \cup N$, with B Borel and N Lebesgue measurable and null (see here). Image and unions commute, so, $U(g)^{-1}(L) = U(g)^{-1}(B) \cup U(g)^{-1}(N)$. The first set is Lebesgue measurable by measurability of $U(g)$, the second one is null, because Lipschitz maps map null sets into null sets, see 9.54 at page 271 of [43].

□

Throughout, D is a bounded Lipschitz domain. We define as in [54] the following spaces of transformations:

Definition C.1.2 (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 $U(\tau^{-1}) = U(\tau)^{-1}$

Observation C.1.3 (A technicality).
Technically, in the original definition of [54], τ need not to be a continuous function, although this is suggested e.g. in remarque 2.1 at page II-4.

Going to equivalence classes of τ makes the identification with continuous functions more precise, as we now show.

One implication

Let $\tau : \mathbb{R}^n \to \mathbb{R}^n$ with $[\tau - \mathrm{Id}] \in W^{k,\infty}$. Then τ is equal a.e. to a (Lebesgue) measurable function, hence also (Lebesgue) measurable, and thus $[\tau] \in \mathcal{V}^k$ as we have defined it (this is proved here; note that $\{g \neq f\}$ is measurable as the Lebesgue measure is complete).

Now, suppose τ is a bijection, and $[\tau^{-1} - \mathrm{Id}] \in W^{k,\infty}$ too. Then $\tau = \mathrm{Id} + g = G, \tau^{-1} = \mathrm{Id} + h = H$ almost everywhere. Here, G, H are at least Lipschitz. But then $\tau \circ H = \mathrm{Id}$ a.e., and since H is Lipschitz, we can conclude also $G \circ H = \mathrm{Id}$ a.e., so, everywhere. With a symmetric reasoning, we are lead to $G = H^{-1}$, so that G is bi-Lipschitz.

Thus, $[\tau] \circ [\tau^{-1}] := [U(\tau) \circ U(\tau^{-1})] = [G \circ G^{-1}] = \mathrm{Id}$ and an analogous reasoning leads to $[\tau] \in \mathcal{T}^k$ as we have defined it.

The other implication

It is immediate for $\mathcal{V}^k$ and for $\mathcal{T}^k$, in the equivalence class of $\tau \in \mathcal{T}^k$ there is a unique $U(\tau)$ at least bi-Lipschitz, hence invertible, with $[U(\tau)] = \tau$.

This shows that:

1. $\{\tau : \mathbb{R}^n \to \mathbb{R}^n \text{ with } [\tau - \mathrm{Id}] \in W^{k,\infty}\}/\sim = \mathcal{V}^k$
2. $\{\tau : \mathbb{R}^n \to \mathbb{R}^n \text{ bijection with } [\tau^{\pm 1} - \mathrm{Id}] \in W^{k,\infty}\}/\sim = \mathcal{T}^k$

We need to check the well-posedness of $\circ$.

Proposition C.1.4
$\circ : \mathcal{V}^1 \times \mathcal{V}^1 \to \mathcal{V}^1$ and $\circ : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \times \mathcal{V}^1 \to W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ are well defined.

Proof.

We start by $\circ : W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \times \mathcal{V}^1 \to \mathcal{V}^1$. We have $\theta \circ \tau = [U(\theta) \circ U(\tau)]$ for instance (see proposition C.1.1); the latter is a bounded Lipschitz map, so it remains in $W^{1,\infty}$.

For the second claim, just write $\eta \circ \tau - \mathrm{Id} = (\eta - \mathrm{Id}) \circ \tau + \tau - \mathrm{Id}$ and use the first part.

□

Proposition C.1.5 (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 $D(f \circ \psi) = Df \circ \psi D\psi$. The equality holds a.e. also for the classical derivatives.
- $D(\psi^{-1}) = (D\psi)^{-1} \circ \psi^{-1}$, where $(D(\psi^{-1}))^{-1} := [(DU(\psi^{-1}))^{-1}]$, the representative being a.e. invertible. The equality holds a.e. also for the classical derivatives.
- $|\det(D\psi)|$ is an essentially bounded measurable function with $|\det(D\psi)| \geq \delta > 0$ a.e..

Proof.

Weak derivatives

We notice that $f \circ \phi$ has a unique Lipschitz representative, that is $U(f) \circ U(\phi)$. The desired formula follows as in [54], lemme 2.1 at page II-6, for the classical derivatives, because Lipschitz function are almost everywhere differentiable by the Rademacher theorem (see here). The chain rule holds for functions differentiable only at one point.

Now, to identify the weak derivatives:

- $U(f)$ is Lipschitz, so that $DU(f)$, the classical derivative, is also the weak derivative Df (note that f need not to be essentially bounded to state this). The latter is a measurable function, as a.e. limit of difference quotients.
- $DU(f) \circ U(\psi)$, is measurable, see proposition C.1.1. It is also essentially bounded.
- By proposition C.1.1 we observe that $DU(f) \circ U(\psi)$ represents $Df \circ \psi$
- $D\psi = [DU(\psi)]$ as seen above
- the product of equivalence classes is always defined as the product of their representatives

Therefore $Df \circ \psi D\psi = [DU(f) \circ U(\psi) DU(\psi)]$.

And now, because $f \circ \phi$ is Lipschitz, it has weak derivatives, $D(f \circ \phi)$, equal to the classical derivatives $DU(f \circ \phi) = D(U(f) \circ U(\psi)) = DU(f) \circ U(\psi) DU(\psi)$, where the last equality holds a.e., as mentioned at the beginning of the proof.

This let us conclude the first claim.

Inverse Jacobian

For the second one, put $f = \psi^{-1}$. Then, for the classical derivatives, $I = DU(\psi) \circ U(\psi)^{-1} DU(\psi^{-1})$ a.e., so that both $DU(\psi) \circ U(\psi)^{-1}, DU((\psi)^{-1})$ are invertible as matrices, a.e..

Determinant

We have defined $|\det(D\psi)| := [|\det DU(\psi)|]$, see proposition C.1.1. The claim follows as in lemme 4.2, pag. IV-7 of [54], and because det is a polynomial of essentially bounded functions.

□

We go on to define the space of admissible transformations.

Definition C.1.6 (Admissible transformations)
We define $\Theta := \{\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \text{ with } \theta = 0 \text{ on } \mathbb{R}^n \setminus D\}$, a Banach subspace of $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$.
We also define $\mathcal{T} := \{\tau \in \mathcal{T}^1, \tau^{\pm 1}|_{\mathbb{R}^n \setminus D} = \mathrm{Id}\}$.

Proposition C.1.7 (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
- $\eta^{-1} \in \mathcal{T}$

Proof.

Stability under inversion

It is trivial, because the definition of $\mathcal{T}$ is symmetric with respect to inversion.

Stability under composition ($\mathcal{T}^1$)

$\eta \circ \tau$ is surely in $\mathcal{V}^1$ by proposition C.1.1. Now, by the above point, $\tau^{-1} \circ \eta^{-1}$ is in $\mathcal{V}^1$ too, and the composition yields: $(\eta \circ \tau) \circ (\tau^{-1} \circ \eta^{-1}) = [U(\eta) \circ U(\tau)] \circ [(U\tau)^{-1} \circ (U\eta)^{-1}] = \mathrm{Id}$.

□

Proposition C.1.8 (Small perturbations of $\mathcal{T}$)
Let $\theta \in \Theta$ with small enough $\|\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$. Then, $\mathrm{Id} + \theta \in \mathcal{T}$.
Let $\delta\theta \in \Theta$ with small enough $\|\delta\theta\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)}$, and $\tau \in \mathcal{T}$. Then, $\tau + \delta\theta \in \mathcal{T}$.

Proof.

Perturbation of identity

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

$U(\tau)^{-1}$ exists and is Lipschitz, see the proof of lemme 2.4 of [54], page II-16. We can therefore define τ^{-1} and we obtain that it is $\mathcal{V}^1$. So, $\tau \in \mathcal{T}^1$. The fact that $\tau = \mathrm{Id}$ outside of D automatically implies $\tau^{-1} = \mathrm{Id}$ outside of D, which can be seen more precisely by going to the smooth representatives of τ, τ^{-1}.

Perturbation, not of identity

We solve the equation $\tau + \delta\theta = \eta \circ \tau$, i.e., we define $\eta := \mathrm{Id} + \delta\theta \circ \tau^{-1}$. Because $\tau^{-1} \in \mathcal{T}$ and $\delta\theta \in \Theta$ we observe that $\delta\theta \circ \tau^{-1} \in \Theta$, thanks to proposition C.1.7.

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

But by proposition C.1.5 this follows immediately. One can alternatively apply point i) of lemme 2.2, [54].

□

Theorem C.1.9
Small perturbations of identity, Lipschitz property Let $U \subset\subset D$ be Lipschitz bounded. There exists $0 < C(U) < 1$ such that, for $\tau \in W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)$ and $\|\tau - \mathrm{Id}\|_{W^{1,\infty}(\mathbb{R}^n;\mathbb{R}^n)} \leq C(U)$, then $T(U)$ is also bounded Lipschitz, where T is $U(\tau)$, the unique Lipschitz continuous representative of τ (see proposition A.1.3).
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 [2], lemma 3, page 629. □

C.2. Transforming Sobolev spaces

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

1. $f \in L^p(T(U)) \iff f \circ T \in L^p(U)$ and there holds, for $f \in L^p(T(U))$:
$$\|f\|_{L^p(T(Q))} \leq \left(\|\det DT\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \|f \circ T\|_{L^p(Q)}$$
2. $f \in W^{1,p}(T(U)) \iff f \circ T \in W^{1,p}(U)$ and there holds, for $f \in W^{1,p}(T(U))$:
$$Df \circ T = (Df)^{-t} D(f \circ T)$$
$$\|Df\|_{L^p(T(Q);\mathbb{R}^n)} \leq \left(\|\det DT\|_{L^\infty(\mathbb{R}^n)}\right)^{1/p} \left\|(DT)^{-1}\right\|_{L^\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})} \|D(f \circ T)\|_{L^p(Q;\mathbb{R}^n)}$$
3. add the rest of this proposition
4. if $p \in (1, \infty)$, $f \in W_0^{1,p}(T(U)) \iff f \circ T \in W_0^{1,p}(U)$
5. therefore, composition by T is a linear isomorphism between $W^{k,p}(T(U)) \to W^{k,p}(U)$ for $k = 0, 1$, and between $W_0^{1,p}(T(U)) \to W_0^{1,p}(U)$ for $k = 0, 1$, $p \in (1, \infty)$
6. for D a bounded Lipschitz domain and $\mathcal{T}, \Theta$ defined before, we get, for $f \in H^1(D)$, that $\mathrm{tr} f = \mathrm{tr}(f \circ T)$
7. if moreover, $\Omega, T(\Omega) \subset\subset D$ are also bounded Lipschitz domains, letting $U := D \setminus \Omega$, another bounded Lipschitz domain, for $f \in H^1(T(U))$ and $\mathrm{tr}_{T(U)} f = 0$ on $\partial T(\Omega)$, then $\mathrm{tr}_U f \circ T = 0$ on $\partial\Omega$ and $\mathrm{tr}_{T(U)} f = \mathrm{tr}_U f \circ T$ on ∂D
8. so, $\circ T$ is a linear isomorphism of $H^1_{0,m}(U)$ and $H^1_{0,m}(T(U))$ ($H^1_{0,m}$ 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 [54], pages IV.4, IV.5, IV.6.

Static strace

To do so, let $f_n \in C(\overline{D}) \cap H^1(D)$ converging in $H^1(D)$ to f. By point 4, we have $f_n \circ T \to f \circ T$ in $H^1(D)$ (rememeber, $T(D) = D$ by invertibility of T and the fact that $T(x) = x$ outside of D). Therefore we have:

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

Zero moving trace

First of all, as T is a homeomorphism of $\mathbb{R}^n$, $TU = D \setminus T(\Omega)$, $T\partial U = \partial D \sqcup \partial\Omega$, $T\partial\Omega = \partial T\Omega$.

Now, an application of theorem A.1.1 yields that the extension to 0 in $T\Omega$ of f, call it $\bar{f}$, is $H^1(D)$, with $\partial_i \bar{f} = \partial_i f$ in TU, 0 in $T(\Omega)$.

We claim that $\mathrm{tr}_D \bar{f} = \mathrm{tr}_{T(U)} f|_{\partial D}$. In fact, approximate $\bar{f}$ by restrictions to D of $C_c^\infty(\mathbb{R}^n)$ functions f_n (see theorem 3.18 of [1], page 54), which also approximate f on $T(U)$, by the observation that $\left\|f_n|_{T(U)}\right\|_{H^1(T(U))} \leq \|f_n|_D\|_{H^1(D)}$. Then:

$$\mathrm{tr}_{T(U)}(f_n|_{T(U)})|_{\partial D} = (f_n|_{T(U)})|_{\partial T(U)}|_{\partial D} = f_n|_{\partial D} = \mathrm{tr}_D(f_n|_D)$$

Now, by what we observed before, $\mathrm{tr}_{T(U)}(f_n|_{T(U)}) \to \mathrm{tr}_{T(U)}(f)$ in $L^2(\partial T(U))$, so that $\mathrm{tr}_{T(U)}(f_n|_{T(U)})|_{\partial D} \to \mathrm{tr}_{T(U)}(f)|_{\partial D}$. On the other hand $\mathrm{tr}_D(f_n|_D) \to \mathrm{tr}_D \bar{f}$, which yields the claim.

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

We can now also say that $\mathrm{tr}_U f \circ T = 0$ on $\partial\Omega$.

$$(\eta\phi_n)|_{\partial\Omega} = \mathrm{tr}_U(\phi_n|_U)_{\partial\Omega} \to \mathrm{tr}_U(f \circ T)_{\partial\Omega}$$

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

We claim that, for $\psi \in W^{1,\infty}(\mathbb{R}^n;\mathbb{R})$ and $f \in H^1(U)$, then $f\psi$ has the same trace as f as long as $\psi = 1$ in a neighbourhood of ∂U.

Note that $f\psi \in H^1(U)$ still. Now: approximate f by restriction of test functions f_n. Then $f_n\psi$ is $C(\overline{U}) \cap H^1(U)$ (thanks also to corollary A.1.4), so that $\text{tr}_U(f_n\psi) = \text{tr}_U(f_n)$. Because $f_n\psi \to f\psi$ is $H^1(U)$ the claim is valid.

This last convergence follows from $\|(f_n - f)\psi\|_{L^2} \leq \|(f_n - f)\|_{L^2} \|\psi\|_{L^\infty}$, the chain rule $\partial_i(f_n\psi) = \partial_i f_n \psi + \partial_i \psi f_n$ (see corollary 4.1.18 here) and again $\|\partial_i(f_n - f)\psi\|_{L^2} \leq \|\partial_i(f_n - f)\|_{L^2} \|\psi\|_{L^\infty}$, $\|(f_n - f)\partial_i\psi\|_{L^2} \leq \|(f_n - f)\|_{L^2} \|\partial_i\psi\|_{L^\infty}$.

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 $\partial T\Omega$, $\beta = 0$ close to ∂D and 1 close to $\partial T\Omega$. This can be accomplished by e.g. building a suitable partition of unity of the compact sets $\partial\Omega$ and ∂D. (can I do this? Yes, see bachelor's thesis, take $K = \partial\Omega$ etc. Also, be careful with all of these equalities...).

$f\beta$ has zero trace, as it can be verified by approximating f by smooth functions again:

$$\text{tr}_{T(U)} f\beta \leftarrow_{L^2(\partial T(U))} \text{tr}_{T(U)} f_n\beta$$

where the latter quantity is $\text{tr}_{T(U)} f_n$ on $\partial T(U)$ and 0 on ∂D. By restricting the convergence to first ∂D and then to $\partial T(U)$, and using almost everywhere convergent subsequences, we conclude that $\text{tr}_{T(U)} f\beta = \text{tr}_{T(U)} f$ on $\partial T(U)$ and $\text{tr}_{T(U)} f\beta = 0$ on ∂D, i.e. $f\beta$ has zero trace.

Domain transformation

But zero trace functions in $H^1(T(U))$, since $T(U)$ is assumed to be bounded Lipschitz, are exactly the functions $H^1_0(T(U))$ (theorem 18.7 at page 595 of [43]).

By then point 4, $(f\beta) \circ T \in H^1_0(U)$.

Because T is bi-Lipschitz, we can write $(f\beta) \circ T = f \circ T\beta \circ T$ almost everywhere.

We have that $\beta \circ T + \eta \circ T$ is $W^{1,\infty}$ and 1 near ∂U.

So, $\text{tr}_U f \circ T = \text{tr}_U f \circ T(\beta \circ T + \eta \circ T) = \text{tr}_U(f \circ T\beta \circ T) + \text{tr}_U(f \circ T\eta \circ T)$.

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

Hence $\text{tr}_U f \circ T|_{\partial\Omega} = tr_U f \circ T(\beta \circ T)|_{\partial\Omega} = 0$.

□

C.3. Transforming Bochner spaces

Proposition C.3.1 (Isomorphism between Q spaces)

$$\circ T : Q(I, V_T) \to Q(I, V)$$

is a linear isomorphism, and so is:

$$\circ T : Q_0(I, V_T) \to Q_0(I, V)$$

In particular, $(u \circ T)' = u' \circ T$ (under suitable identifications, see the proof).

Proof.

Existence of derivative

Consider the following commutative diagram:

$$\begin{tikzcd}
V_T \arrow[r, hook, "a_T"] \arrow[d, "\circ T_H =: t_V"'] & H_T \arrow[r, "r_T"] \arrow[d, "\circ T_H =: t_H"] & H_T^* \arrow[r, hook, "a_T^*"] & V_T^* \\
V \arrow[r, hook, "a"] & H \arrow[r, "r"] & H^* \arrow[r, hook, "a^*"] & V^*
\end{tikzcd}$$

We know that $f \in Q(I, V_T)$ satisfies $a_T f \in H^1(I, H_T)$. Therefore, by proposition A.2.2, $t_H a_T f = a t_V f \in H^1(I, H)$, and $t_v \in L^2(I, V)$, so that $t_V : Q(I, V_T) \to Q(I, V)$ is well defined.

Boundedness

We have that $t_V : V_T \to V$ is linear bounded, so that $t_V : L^2(I, V_T) \to L^2(I, V)$ is also linear and bounded. Still by proposition A.2.2, we have $(a t_V f)' = (t_H a_T f)' = t_H (a_T f)'$.

Thus $\|t_V f\|_{L^2(I,V)} \leq C(T) \|f\|_{L^2(I,V_T)}$, together with $\|(a t_V f)'\|_{L^2(I,H)} \leq C(T) \|(a_T f)'\|_{L^2(I,H_T)}$.

By noting that $(t_V)^{-1} = (\circ T)^{-1}$ is bijective, and by the bounded inverse theorem:

$$\circ T : Q(I, V_T) \to Q(I, V)$$

is a linear isomorphism.

Zero initial value

Consider $a t_V f$. It has a unique $C([0, T], H)$ representative, $U(a t_V f)$. Also, $a_T f$ has a unique continuous representative $U(a_T f)$. Now, $a t_V f = t_H a_T f$, so that $[U(a t_V f)] = [t_H U(a_T f)]$. By continuity, $U(a t_V f) = t_H U(a_T f)$ on $[0, T]$ and thus, whenever $U(a_T f)(0) = 0$, so is $U(a t_V f)$, informally, also $t_V f(0) = 0$.

So, $t_V(Q_0(I, V_T)) \subseteq Q_0(I, V)$.

$(t_V)^{-1} = (\circ T)^{-1}$ and we can conclude that $t_V^{-1}(Q_0(I, V)) \subseteq Q_0(I, V_T)$.

$\square$

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 continue from proposition B.3.5.

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

We are working under the assumption:

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

Suppose the problem is formulated on $T(U)$. To ease the notation, call $H^1_{0,m}(T(U)) = \mathtt{W}_T, H^1_{0,m}(U) = \mathtt{W}, H^1_0(U) = \mathtt{V}$ and analogously for the other spaces.

We write the problem as:

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

Applying a change of variables, we get equivalently:

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

Here $A_T = |\det(DT)| DT^{-1}(DT)^{-t}$.

Now, we note that:

- $\mathrm{tr}_{T(U)} q = \mathrm{tr}_U (q \circ T)$ on Σ_f by theorem C.2.1
- $w_t^T \circ T = (w^T \circ T)_t$ by the proof of proposition C.3.1 and analogously for v_0
- by proposition C.3.1,$\circ T$ is a bijection between $Q^0(I, \mathtt{W}_T)$ and $Q^0(I, \mathtt{W})$ and analogously for $\mathtt{V}$
- $\bar{u} \in H^1(I, \mathtt{W}_T)$ and that $\bar{u}'$ denoted the weak derivative in the $H^1(I, \mathtt{W}_T)$ sense, so that proposition A.2.1 yields $\bar{u} \circ T \in H^1(I, \mathtt{W})$ and $(\bar{u} \circ T)' = \bar{u}' \circ T$

We therefore get, equivalently:

$$\begin{aligned}
&w^T \in Q_0(I, \mathtt{W}_T), v_0^T \in Q_0(I, \mathtt{V}_T)\\
&\int_I ((w^T \circ T)_t, q|\det(DT)|)_H + (A_T \nabla(w^T \circ T), \nabla q)_H =\\
&\int_I (g, \mathrm{tr}_U q)_{L^2(\Gamma_f)}, \quad \forall q \in Q^0(I, \mathtt{W})\\
&\int_I ((v_0^T \circ T)_t, p|\det(DT)|)_H + (A_T \nabla(v_0^T \circ T), \nabla p)_H =\\
&-\int_I ((\bar{u} \circ T)', p|\det(DT)|)_H + (A_T \nabla(\bar{u} \circ T), \nabla p)_H, \quad \forall p \in Q^0(I, \mathtt{V})
\end{aligned}$$

and by proposition C.3.1, we also get $w^T \circ T \in Q_0(I, \mathtt{W}), v_0^T \circ T \in Q_0(I, \mathtt{V})$.

On the other hand, consider:

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

Then, we note the following:

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

Therefore we obtain, equivalently:

$$\begin{aligned} w \circ T^{-1} \in Q_0(I, \mathtt{W}_T), v_0 \circ T^{-1} \in Q_0(I, \mathtt{V}_T) \\ \int_I ((w \circ T^{-1})_t, q^T)_{H_T} + (\nabla(w \circ T^{-1}), \nabla q^T)_{H_T} = \\ \int_I (g, \mathrm{tr}_{T(U)} q^T)_{L^2(\Gamma_f)}, \quad \forall q^T \in Q^0(I, \mathtt{W}_T) \\ \int_I ((v_0 \circ T^{-1})_t, p^T)_{H_T} + (\nabla(v_0 \circ T^{-1}), \nabla p^T)_{H_T} = \\ -\int_I (\bar{u}', p^T)_{H_T} + (\nabla \bar{u}, \nabla p^T)_{H_T}, \quad \forall p^T \in Q^0(I, \mathtt{V}_T) \end{aligned}$$

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

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 again, T is the unique Lipschitz representative of $\tau \in \mathcal{T}$.

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

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

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

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

We have the following:

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

Here, $A_T := (DT)^{-1}(DT)^{-t}|\det(DT)|$.

D. Inhomogenous FEM 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 [58]): an example of this in a setting close to ours, is contained in [39].

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 [64]. This requires complete knowledge of the (curved) boundary of the computational domain. Optimal order estimates are also observed in [9]. 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 [58]: 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. [16] for the elliptic case, or, more generally, the discussion in [17], and that in [7] 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 ([32]), and powerful finite element libraries can be directly used to simulate the partial differential equations, we used Fenics ([47]).

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. [6].

The approach we took is based on the work of [25], [24], [8] and [23].

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.

please make precise the mesh assumptions

D.1. Elliptic problems

We consider a finite element method for approximating problems of the following form.

Assumption D.1.1 (Basic assumptions for elliptic problems)
Consider $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$, with C^2 boundary, and data $f \in L^2(\Omega), g_D \in H^{3/2}(\Gamma_D), g_N \in H^{1/2}(\Gamma_N)$, where $\Gamma_D \sqcup \Gamma_N = \partial\Omega$ and $\overline{\Gamma_D} \cap \overline{\Gamma_N} = \emptyset$. We assume Γ_D to be non-empty.

Problem D.1.2 (Inhomogeneous elliptic problem)
Under assumption D.1.1, the problem is:

$$\begin{cases} -\Delta u + ku = f & \text{on } \Omega \\ u = g_D & \text{on } \Gamma_D \\ \partial_\nu u = g_N & \text{on } \Gamma_N \end{cases}$$

where $k \geq 0$ is a constant.
By this we mean to find $u \in H^1(\Omega)$ with:

$$a(u,v) = l(v), \text{ for all } v \in H^1_{0,D}$$

where $a(u,v) = \int_\Omega \nabla u \nabla v + k \int_\Omega uv$, and $l(v) = \int_\Omega fv + \int_{\Gamma_N} g_N v$ and $H^1_{0,D}$ is the space of all H^1 functions with vanishing trace on Γ_D.
Add existence, uniqueness, regularity

We define a polygonal/polyhedral meshing Ω_h (open) of Ω, which has boundary nodes on $\partial\Omega$. We denote by $\Gamma_{D_h}, \Gamma_{N_h}$ the discrete Dirichlet and Neumann boundaries, and by $S^1_{h,0,D_h}$ 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.1.3 (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 [25])
- 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.

This proof is lacking a bound on the quasiconvexity constant and the fact that G_h is surjective

See section 4.1 of [25] for the first two points, which follow from the definition of G_h. See also Lemma 8.16 of [24].

The last one is contained in Lemma 8.12, [24]. We give more detail for the third and fourth points which is not addressed in [24], [25].

<u>G_h is a bi-Lipschitz homeomorphism</u>

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 $\phi \in C^\infty_c(\Omega_h)$.

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 [24] shows that $\|\mathrm{Id} - G_h\|_{W^{1,\infty}(\Omega_h)} \lesssim h$. Thanks to proposition A.1.3, 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 $\mathrm{Lip}(\mathrm{Id} - G_h) \lesssim \|\mathrm{Id} - G_h\|_{W^{1,\infty}(\Omega_h)}$. (This is not trivial: one could use quasiconvexity a sin Heinonen, and then bound the quasiconvexity constant uniformly)

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 [61]) 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 [24] (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. [36], chapter 1 and wikipedia) 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.1.4 (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 [25]).
There holds:

- if $v \in H^m(Q)$ if and only if $v^{-l} \in H^m(G_h(Q))$, for $m = 0, 1$, and $Q \subseteq \Omega_h$ open
- for $v_h \in S^1_{h,0,D_h}$, we have $v_h^l \in H^1(\Omega)$, with zero trace on Γ_D
- for $v_h \in S^1_h$, one has the following norm equivalences, which don't depend on h:
    1. $\|v_h\|_{L^2(\partial\Omega_h)} \sim \|v_h^l\|_{L^2(\partial\Omega)}$
    2. $\|v_h\|_{L^2(\Omega_h)} \sim \|v_h^l\|_{L^2(\Omega)}$
    3. $\|\nabla v_h\|_{L^2(\Omega_h)} \sim \|\nabla v_h^l\|_{L^2(\Omega)}$
- consequently, the lifting operator $S^1_{h,0,D_h} \to H^k_{0,D}(\Omega)$ is bounded, for the L^2 norms if $k = 0$, and H^1 norms if $k = 1$

Proof.

The first point follows by the fact that G_h is bi-Lipschitz, see proposition D.1.3, and theorem 11.53 of [43].

The second point follows by applying the arguments about conformity outlined in section 5 of [8]. Following Example 2 therein, we discover that we can apply proposition and corollary 5.1.

The last point can be found in [25], see e.g proposition 4.9 and 4.13.

□

Now, define $f_h \in S^1_h, g_{N,h} \in S^1_h(\Gamma_{N_h})$ to be any finite element approximations of f, g_N. Note, here $S^1_h(\Gamma_{N_h})$ means the usual piecewise linear FEM space over Γ_{N_h}.

We can now define the discrete approximation of problem D.1.2.

Problem D.1.5 (FEM approximation of problem D.1.2)
We find $u_h \in S^1_h$ with $u_h(p) = g_D(p)$ for all p external nodes of $\partial\Omega_h$, and solving:

$$a_h(u_h, v_h) = l_h(v_h), \text{ for all } v_h \in S^1_{h,0,D_h}$$

where $a_h(u_h, v_h) = \int_{\Omega_h} \nabla u_h \nabla v_h + k \int_{\Omega_h} u_h v_h$, and $l_h(v_h) = \int_{\Omega_h} f_h v_h + \int_{\Gamma_{N_h}} g_{h,N} v_h$
Add existence, uniqueness, connection with FEniCS

Note, we assumed $g_D \in H^{3/2}(\partial\Omega)$. Thanks to the C^2 smoothness of $\partial\Omega$ we can apply theorem 1.5.1.2 of [35] and obtain a $G \in H^2(\Omega)$ with $\text{tr}_2 G = g_D$. Here tr_2 denotes the trace operator from $H^2(\Omega)$. By Sobolev embeddings, $G \in C(\overline{\Omega})$.

Now, we can pick $G_k \in C^\infty(\overline{\Omega}) \cap H^2(\Omega)$ converging in $H^2(\Omega)$ to G. We can do so by [1], theorem 3.18 at page 54. Then: $G_k|_{\partial\Omega} = \text{tr}_2 G_k \to \text{tr}_2 G = g_D$, and by $H^2(\Omega) \hookrightarrow C(\overline{\Omega})$ we obtain $G|_{\partial\Omega} = g_D$, so that g_D is continuous in both $n = 2, 3$ and so we can define its pointwise interpolation.

Alternatively we could have used Sobolev embeddings on manifolds to arrive to the same conclusion.

Proposition D.1.6 (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_h^1.
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 [25]. □

Proposition D.1.7 (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), $\delta\theta \in W^{1,\infty}(\Omega;\mathbb{R}^d)$. Then:

1. $\left|\int_\Omega v_h^l w_h^l - \int_{\Omega_h} v_h w_h\right| \lesssim h \|v_h\|_{L^2(\Omega_h)} \|w_h\|_{L^2(\Omega_h)}$
2. $\left|\int_\Omega v_h^l w_h^l - \int_{\Omega_h} v_h w_h\right| \lesssim h^2 \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)}$
3. $\left|\int_{\partial\Omega} v_h^l w_h^l - \int_{\partial\Omega_h} v_h w_h\right| \lesssim h^2 \|v_h\|_{L^2(\partial\Omega_h)} \|w_h\|_{L^2(\partial\Omega_h)}$
4. $\left|\int_\Omega \nabla v_h^l \nabla w_h^l - \int_{\Omega_h} \nabla v_h \nabla w_h\right| \lesssim h \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)}$
5. $\left|\int_\Omega \nabla v \nabla w - \int_{\Omega_h} \nabla v^{-l} \nabla w^{-l}\right| \lesssim h^2 \|v\|_{H^2(\Omega)} \|w\|_{H^2(\Omega)}$
6. $\left|\int_\Omega v_h^l w_h^l \mathrm{div}(\delta\theta_h^l) - \int_{\Omega_h} v_h w_h \mathrm{div}(\delta\theta_h)\right| \lesssim h \|v_h\|_{L^2(\Omega_h)} \|w_h\|_{L^2(\Omega_h)} \|\mathrm{div}(\delta\theta_h)\|_{L^\infty(\Omega_h)}$
7. $\left|\int_\Omega (A'(\delta\theta_h^l)\nabla v_h^l)\nabla w_h^l - \int_{\Omega_h} (A'(\delta\theta_h)\nabla v_h)\nabla w_h\right| \lesssim h \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)} \|D\delta\theta_h\|_{L^\infty(\Omega_h)}$
8. $\left|\int_\Omega v_h^l w_h^l \mathrm{div}(\delta\theta_h^l) - \int_{\Omega_h} v_h w_h \mathrm{div}(\delta\theta_h)\right| \lesssim h^2 \|v_h\|_{H^1(\Omega_h)} \|w_h\|_{H^1(\Omega_h)} \|\mathrm{div}(\delta\theta_h)\|_{L^\infty(\Omega_h)}$

Proof.

See [23], and in particular, for the third point, Lemma 5.6 of [41]. Only the last two points are not already present in the literature.

<u>Proof of $6, 8$</u>

We can reason as in section 6 of [25]. To this end, we perform integration by parts:

$$\begin{aligned}\int_{\Omega_h} v_h w_h \mathrm{div}(\delta\theta_h) = \int_\Omega v_h^l w_h^l \mathrm{tr}(D(\delta\theta_h^l)(D(G_h^{-1}))^{-1})|\det(D(G_h^{-1}))| =\\ \int_\Omega v_h^l w_h^l \mathrm{tr}(D(\delta\theta_h^l)(D((G_h^{-1}))^{-1} - \mathrm{Id}))|\det(D(G_h^{-1}))| +\\ \int_\Omega v_h^l w_h^l \mathrm{tr}(D(\delta\theta_h^l))(|\det(D(G_h^{-1}))| - 1) +\\ \int_\Omega v_h^l w_h^l \mathrm{tr}(D(\delta\theta_h^l))\end{aligned}$$

The conclusion now follows from proposition D.1.3 and the fact that, for square matrices A, B, we have $|\mathrm{tr}(AB)| \leq \|A\|_F \|B\|_F$, and $\|\cdot\|_F$ is the Frobenius norm.

By noting that the first and second integrals are zero on the interior elements, and upon using the "narrow band" inequality Lemma 6.3, [25], as suggested in Lemma 6.4 of [25], we are able to also conclude that 8 must hold.

Proof of $7, 9$

It is very similar to the previous ones. The only peculiarity is the appearance of a term like $A'(\delta\theta_h) \circ G_h^{-1} - A'(\delta\theta_h^l)$. This is estimated, in the L^∞ norm, as follows:

$$\begin{aligned}\left\|A'(\delta\theta_h) \circ G_h^{-1} - A'(\delta\theta_h^l)\right\|_{L^\infty(\Omega_h)} &\leq \\ 2\left\|D(\delta\theta_h^l)(D(G_h^{-1}))^{-1} - D(\delta\theta_h^l)\right\|_{L^\infty(\Omega_h)} &+ \\ \left\|\mathrm{tr}(D(\delta\theta_h^l)(D((G_h^{-1}))^{-1} - \mathrm{Id}))\right\|_{L^\infty(\Omega_h)}&\end{aligned}$$

and we can now use proposition D.1.3 to conclude.

$\square$

Theorem D.1.8 (H^1 estimate)
For h small enough, we have $\left\|u - u_h^l\right\|_{H^1(\Omega)} \lesssim h + \left\|f - f_h^l\right\|_{L^2(\Omega)} + \left\|g_N - g_{h,N}^l\right\|_{L^2(\Gamma_N)}$

Proof.

We partially follow the structure of the arguments in [23], making some simplifications, and modifications to adapt them to our case.

Conclusion

$\left\|u - u_h^l\right\|_{H^1(\Omega)} \leq \|u - \Pi_c u\|_{H^1(\Omega)} + \left\|\Pi_c u - u_h^l\right\|_{H^1(\Omega)}$. The interpolation estimates proposition D.1.6 allow us to worry only about the second term. It is $\left\|(\Pi_h u - u_h)^l\right\|_{H^1(\Omega)} \lesssim \|\Pi_h u - u_h\|_{H^1(\Omega_h)}$ by proposition D.1.4. We estimate the latter quantity, calling $e_h := u_h - \Pi_h u$, which is zero on Γ_{D_h}.

Defect, e_h and u

Let $d_h \in S^1_{h,0,D_h}$ be the unique solution to $a_h(d_h, v_h) = l_h(v_h) - a_h(\Pi_h u, v_h)$, $v_h \in S^1_{h,0,D_h}$.

Using $0 = l_h(v_h) - a_h(u_h, v_h)$, $v_h \in S^1_{h,0,D_h}$, we come to $a_h(d_h - e_h, v_h) = 0$, $v_h \in S^1_{h,0,D_h}$. Testing with $d_h - e_h = 0$ on Γ_{D_h} and using the connectedness of Ω_h, we conclude that $e_h = d_h$.

Moreover, by proposition D.1.4, we have $v_h^l \in H^1_{0,D}$, so that $a(u, v_h^l) = l(v_h^l)$ and thus :

$$a_h(e_h, v_h) = l_h(v_h) - l(v_h^l) + a(u, v_h^l) - a_h(\Pi_h u, v_h)$$

Estimation of e_h

The form a_h is H^1 coercive, $h-$uniformly. This we show by the following estimate, C not depending on h:

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

We used, in order:

- 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 [22])
- proposition D.1.4 on $\left\|v_h^l\right\|_{H^1(\Omega)}^2$
- proposition 4.6 of [23]

Therefore $\|e_h\|_{H^1(\Omega_h)}^2 \lesssim a_h(e_h, e_h) = l_h(e_h) - l(e_h^l) + a(u, e_h^l) - a_h(\Pi_h u, e_h)$, where we can test by $e_h = 0$ on Γ_{D_h}.

This last term is estimated exactly as in proposition 5.5 of [23]. In particular, we make use of th H^2 regularity of u, and we extend $g_{N,h}, g_N$ to zero, on Γ_{D_h}, Γ_D

□

Note, the assumption of non-emptiness of the Dirichlet boundary is not strictly necessary, and can be removed, when $k > 0$. In this case, we have to modify the above arguments because a is not coercive anymore, but this is possible by consider a slightly different defect equation, where an L^2 scalar product is added.

For an L^2 error estimate we apply the Aubin-Nitsche trick, following [28] and [23].

Theorem D.1.9 (L^2 estimate)
Assume either that $f \in H^1(\Omega)$ or that $\left\|f_h^l\right\|_{H^1(\Omega)} \lesssim \|f\|_{L^2(\Omega)}$. Then, for h small enough, we have $\left\|u - u_h^l\right\|_{L^2(\Omega)} \lesssim h^2 + \left\|f - f_h^l\right\|_{L^2(\Omega)} + \left\|g_N - g_{h,N}^l\right\|_{L^2(\Gamma_N)} + \|g_D - \Pi_c g_D\|_{L^2(\Gamma_D)} + A$, where $A = 0$ if $\left\|f_h^l\right\|_{H^1(\Omega)} \lesssim \|f\|_{L^2(\Omega)}$ and $A = h^2 \left\|f - f_h^l\right\|_{H^1(\Omega)}$ otherwise.

Proof.

Define $e := u - u_h^l$ (whose boundary values at Γ_D are not necessarily 0!), and z solving the dual problem:

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

This problem possesses H^2 regularity, so that we can write, after multiplying both sides by $e \in H^1$ (thanks to proposition D.1.4):

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

Using that $z \in H^2$ we have that $\partial_\nu z = 0$ on Γ_N, together with the estimate $\|z\|_{H^2(\Omega)} \lesssim \|e\|_{L^2(\Omega)}$ (check!! It's done at page 92 of Grisvard) and thus:

$$\begin{aligned} \|e\|_{L^2(\Omega)}^2 &= a(z, e) + \|e\|_{L^2(\Gamma_D)} \|\partial_\nu z\|_{L^2(\partial\Omega)} \\ &\leq a(z, e) + C\|e\|_{L^2(\Gamma_D)} \|e\|_{L^2(\Omega)} \end{aligned}$$

Only $a(z, e)$ remains to be estimated, and this is done in the proof of theorem 5.3 of [23], and in remark 5.6.

□

Corollary D.1.10 (Actual estimates)
By assuming f, g_N, g_D in H^2 we conclude $\left\|u - u_h^l\right\|_{H^1(\Omega)} \lesssim h, \left\|u - u_h^l\right\|_{L^2(\Omega)} \lesssim h^2$.

Proof.

It suffices to take $f_h := \Pi_h f$, $g_{N,h} = \Pi_h g$ and employ proposition D.1.6. □

Unfortunately the smoothness assumptions to obtain optimal order of convergence are quite strict. However, the advantage of this approach is that it is straightforward to implement, and works in both dimensions $n = 2, 3$.

If one is concerned with just H^1 error estimates, without taking numerical integration into account, we can relax the requirements on f. Incidentally, how we are about to choose f, is more in line with the implementation of FEniCS.

Proposition D.1.11 (H^1 estimate with rougher f)
We choose $f_h = f$ on $\Omega \cap \Omega_h$ and 0 otherwise, assuming $f \in H^1(\Omega)$. Then we obtain, for h small enough, $\|u - u_h^l\|_{H^1(\Omega)} \lesssim h + \|g_N - g_{h,N}^l\|_{L^2(\Gamma_N)}$

Proof.

Analysing the proof of proposition 5.5 in [23] we see that we only need to prove that $\left|\int_\Omega f v_h^l - \int_{\Omega_h} f_h v_h\right| \lesssim h \left\|v_h^l\right\|_{H^1(\Omega)}$, for $v_h \in S^1_{h,0,D_h}$.

We can rewrite the difference as follows:

$$\begin{aligned}\int_\Omega f v_h^l - \int_{\Omega_h} f_h v_h &= \\ \int_{\Omega\cap\Omega_h} f v_h^l - \int_{\Omega_h\cap\Omega} f_h v_h + \int_{\Omega\setminus\Omega_h} f v_h^l - \int_{\Omega_h\setminus\Omega} f_h v_h &= \\ \int_{\Omega\cap\Omega_h} f v_h^l - \int_{\Omega_h\cap\Omega} f_h v_h + \int_{\Omega\setminus\Omega_h} f v_h^l &= \\ \int_{\Omega\cap\Omega_h^\partial} f(v_h^l - v_h) + \int_{\Omega\setminus\Omega_h} f v_h^l\end{aligned}$$

where we used that $f = 0$ outside of Ω, that $f = f_h$ in $\Omega \cap \Omega_h$ and that $v_h^l = v_h$ for all simplices with at most one node on $\partial\Omega$ (by the definition of G_h). The set of all the other (straight) simplices is denoted by Ω_h^∂.

For the first integral we have that for h small enough, $\Omega \setminus \Omega_h \subseteq N_{ch^2}$ (see [58] for this), for $N_\delta := \{x \in \Omega, 0 < \text{dist}(x, \partial\Omega) < \delta\}$.

Using the assumption $f \in H^1(\Omega)$, together with Lemma 4.10 of [25], we conclude that:

$$\left|\int_{\Omega\setminus\Omega_h} f v_h^l\right| \leq \|f\|_{L^2(N_\delta)} \left\|v_h^l\right\|_{L^2(N_\delta)} \lesssim \delta \|f\|_{H^1(\Omega)} \left\|v_h^l\right\|_{H^1(\Omega)}$$

To control the other integral, we note that $\Omega \cap \Omega_h^\partial \subseteq N_h$, also for h small enough. Then:

$$\begin{aligned}\left|\int_{\Omega\cap\Omega_h^\partial} f(v_h^l - v_h)\right| &\leq \|f\|_{L^2(N_h)} \left(\left\|v_h^l\right\|_{L^2(N_h)} + \|v_h\|_{L^2(\Omega\cap\Omega_h^\partial)}\right) \\ &\lesssim h^{1/2} \|f\|_{H^1(\Omega)} \left(h^{1/2} \left\|v_h^l\right\|_{H^1(\Omega)} + \|v_h\|_{L^2(\Omega\cap\Omega_h^\partial)}\right)\end{aligned}$$

But $\|v_h\|_{L^2(\Omega\cap\Omega_h^\partial)} \leq \|v_h\|_{L^2(\Omega_h^\partial)} \lesssim \|v_h^l\|_{L^2(G_h(\Omega_h^\partial))}$, the last inequality resulting upon a change of variables applied elementwise, and an application of (4.10b) from [25] to estimate the appearing determinant.

Because $G_h(\Omega_h^\partial) \subseteq N_h$ (this is said in lemma 8.24 of 9, see edelmann), the proof is concluded.

□

This same strategy brings us to an optimal L^2 error estimate, too.

Proposition D.1.12 (L^2 estimate with rougher f)
We choose $f_h = f$ on $\Omega \cap \Omega_h$ and 0 otherwise, assuming $f \in H^1(\Omega)$. Then we obtain, for h small enough, we have $\|u - u_h^l\|_{L^2(\Omega)} \lesssim h^2 + \|g_N - g_{h,N}^l\|_{L^2(\Gamma_N)} + \|g_D - \Pi_c g_D\|_{L^2(\Gamma_D)}$.

Proof.

Analyizing the proof of the L^2 estimate, and of theorem 5.3 in [23], we see that we only need to prove that $\left|\int_\Omega f\Pi_c z - \int_{\Omega_h} f_h \Pi_h z\right| \lesssim h^2 \|e\|_{L^2(\Omega)}$.

Just like before, we arrive at:

$$\int_\Omega f\Pi_c z - \int_{\Omega_h} f_h \Pi_h z = \int_{\Omega\cap\Omega_h^\partial} f(\Pi_c z - \Pi_h z) + \int_{\Omega\setminus\Omega_h} f\Pi_c z$$

Here, proposition D.1.6 lets us estimate $\|\Pi_c z\|_{H^1(\Omega)} \lesssim \|z\|_{H^2(\Omega)}$, for h small, so that, just like in the previous proof, and using the H^2 regularity of z:

$$\left|\int_{\Omega\setminus\Omega_h} f\Pi_c z\right| \lesssim h^2 \|f\|_{H^1(\Omega)} \|z\|_{H^2(\Omega)} \lesssim h^2 \|f\|_{H^1(\Omega)} \|e\|_{L^2(\Omega)}$$

Now, Ω is smooth enough for the existence of a bounded extension operator $E : H^2(\Omega) \to H^2(\mathbb{R}^n)$ (see [43], theorem 13.17 at page 425, 13.13 at page 424, and definition 9.57 at page 273). Therefore:

$$\left|\int_{\Omega\cap\Omega_h^\partial} f(\Pi_c z - \Pi_h z)\right| \lesssim h^{1/2} \|f\|_{H^1(\Omega)} \|\Pi_c z - \Pi_h z\|_{L^2(\Omega\cap\Omega_h^\partial)}$$

But $\|\Pi_c z - \Pi_h z\|_{L^2(\Omega\cap\Omega_h^\partial)} \le \|\Pi_c z - z\|_{L^2(\Omega)} + \|Ez - \Pi_h Ez\|_{L^2(\Omega_h)}$.

By proposition D.1.6 and by theorem 3.1.6 of [18], with constants independent of h, we obtain $\|\Pi_c z - \Pi_h z\|_{L^2(\Omega\cap\Omega_h^\partial)} \le Ch^2(\|z\|_{H^2(\Omega)} + \|Ez\|_{H^2(\Omega_h)}) \le Ch^2(\|z\|_{H^2(\Omega)} + \|Ez\|_{H^2(\mathbb{R}^n)}) \lesssim h^2 \|z\|_{H^2(\Omega)} \le h^2 \|e\|_{L^2(\Omega)}$.

Hence $\left|\int_{\Omega\cap\Omega_h^\partial} f(\Pi_c z - \Pi_h z)\right| \lesssim h^{5/2} \|e\|_{L^2(\Omega)}$ and the proof is concluded.

□

Summing up, here are the assumptions we used to obtain optimal order estimates.

Assumption D.1.13 (Assumptions for optimal order estimates)
On top of assumption D.1.1 we have assumed:

- quasi-uniformity of the mesh
- h small enough (all the estimates are asymptotic)
- $g_D, g_N \in H^2$
- $f \in H^1$

D.2. Parabolic problems

D.2.1. Semidiscrete estimates

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

Add a more precise reference to the triangulation, quasi uniformity...

Problem D.2.1.1 (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 [57] in e.g. theorem 1.2. To deal with the polygonal/polyhedral domain approximation we adapt some arguments contained in [24], 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.2.1.2 (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.2.1.3 (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.

Well posedness and stability

Consider $\delta_h := R_h z - \Pi_h z$. Then, $a_h(\delta_h, v_h) = a(z, v_h^l) - a_h(\Pi_h z, v_h), v_h \in S^1_{h,0,D_h}$, $\delta_h = 0$ on Γ_{D_h}.

The right hand side is a bounded functional on S_h^1, also by proposition D.1.4, and a_h is (h-uniformly) coercive on $S^1_{h,0,D_h}$ by the proof of theorem D.1.8.

Therefore, δ_h exists, and we see that $\delta_h + \Pi_h z$ satisfies the equation for $R_h z$. Defining $R_h z := \delta_h + \Pi_h z$ is a well posed operation, since we can check that $R_h z$ doesn't depend on the (discrete) extension of $\Pi_h z|_\Gamma$: if we had two candidates $R^i hz$, $i = 1, 2$, we could form a difference, 0 on Γ_{D_h}, that would qualify as a test function in both variational formulations. Coercivity of a_h would then yield $R_h^1 = R_h^2$.

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 $\|R_h z\|_{H^1(\Omega_h)} \lesssim \|\delta_h\|_{H^1(\Omega_h)} + \|\Pi_h z\|_{H^1(\Omega_h)}$.

For the second term.

Employing proposition D.1.4 $\|\Pi_h z\|_{H^1(\Omega_h)} \lesssim \|\Pi_c z\|_{H^1(\Omega)} \leq \|\Pi_c z - z\|_{H^1(\Omega)} + \|z\|_{H^1(\Omega)} \lesssim (1+h)\,\|z\|_{H^2(\Omega)}$, where in the last step we used proposition D.1.6.

For the first term, we know that $\|\delta_h\|^2_{H^1(\Omega_h)} \lesssim a_h(\delta_h,\delta_h) = a(z,\delta_h^l) - a_h(\Pi_h z,\delta_h)$. We can insert a 0 term: $\|\delta_h\|^2_{H^1(\Omega_h)} \lesssim a(z - \Pi_c z, \delta_h^l) + a(\Pi_c z,\delta_h^l) - a_h(\Pi_h z,\delta_h)$ and use proposition D.1.6, proposition D.1.4 and proposition D.1.7, to get:

$$\|\delta_h\|^2_{H^1(\Omega_h)} \lesssim h\,\|z\|_{H^2(\Omega)}\,\|\delta_h\|_{H^1(\Omega_h)} + h\,\|\Pi_h z\|_{H^1(\Omega_h)}\,\|\delta_h\|_{H^1(\Omega_h)}$$

For the second term, we obtain, for h small, that $\|\delta_h\|_{H^1(\Omega_h)} \lesssim \|z\|_{H^2(\Omega)}$, and the stability is shown.

Error bounds

We start from the H^1 error bound.

We follow [24] closely here, adapting the proof of Lemma 3.8 at page 1720, where in particular we make sure that H^2 stability of R_h is sufficient, instead of the stronger H^1 stability they use. We are also using a slightly different bilinear form and function spaces.

Calling $F_h(v) := a(z - R_c z, v)$ for $v \in H^1$, we readily obtain:

$$|F_h(v_h^l)| \lesssim h\,\left\|v_h^l\right\|_{H^1(\Omega)}\,\|z\|_{H^2(\Omega)}$$

For $\eta \in H^2(\Omega)$ we instead have:

$$|F_h(\eta)| \lesssim \left(h^2\,\|z\|_{H^2(\Omega)} + h\,\|z - R_c z\|_{H^1(\Omega)}\right)\|\eta\|_{H^2(\Omega)}$$

The above estimates are shown in detail in [24].

Using again the same arguments of [24] we come to:

$$\|z - R_c z\|^2_{H^1(\Omega)} \lesssim h\,\|z - R_c z\|_{H^1(\Omega)}\,\|z\|_{H^2(\Omega)} + h\,\|z\|_{H^2(\Omega)}\left(h\,\|z\|_{H^2(\Omega)} + \|z - R_c z\|_{H^1(\Omega)}\right)$$

Appying Young's inequality brings us finally to:

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

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.1.4), and define w, just like in theorem D.1.9, by:

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

As in the proof of theorem D.1.9:

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

and:

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

For the first term we can employ the estimates derived at the beginning and the H^1 error norm, so as to obtain:

$$|F_h(w)| \lesssim h^2\,\|z\|_{H^2(\Omega)}\,\|w\|_{H^2(\Omega)}$$

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 proposition 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.1.4.

□

Assumption D.2.1.4 (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 as we can see in chapter 2, we can get away with asking particular smoothness and compatibility assumptions on the problem data, see SOME FUTURE CHAPTER and theorem B.2.3.6. For more general problems with non-null initial conditions, a finer analysis is most likely necessary.

We now can attempt an error estimate for problem D.2.1.1, for the following spatial semidiscrete formulation.

Problem D.2.1.5 (Spatially semidiscrete approximation of problem D.2.1.1)
We look for $u_h \in H^1(I, S_h^1)$ satisfying:

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

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

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

We are making the following assumptions on the data:

Assumption D.2.1.6 (Assumptions for the spatial semidiscretization)

- $\partial\Omega \in C^2$
- $g_N \in L^2(I, H^2(\Omega))$, 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 $G_D := E g_D \in H^1(I, H^2(\Omega))$ and therefore (see proposition 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 $\left\|f - f_h^l\right\|_{L^2(\Omega_h)} \lesssim C_f h^2$, 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.2.1.7 (Well posedness of problem D.2.1.5)
There exists a unique solution to problem D.2.1.5, 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.

<u>Existence</u>

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.2.1.5 with the basis functions v_{hj} we obtain the problem:

$$M_h d_h'(t) + A_h d_h(t) = F_h(t), \text{ a.e. } t \tag{D.2.1.8}$$
$$d_h(0) = d_{h,0} \tag{D.2.1.9}$$

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 [52], 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 by energy estimates

Uniqueness (and hence, independence on the particular extension $G_{D,h}$) follows by proving an energy estimate at first. In fact, let $e := u_h^1 - u_h^2$ be the difference of two solutions. It satisfies:

$$(\partial_t e_h, v_h)_{L^2(\Omega_h)} + a_h(e_h, v_h) = 0, v_h \in S^1_{h,0,D_h}, a.e.t$$
$$e_h = 0 \text{ for a.e. } t, \text{ on } \Gamma_{D_h}$$
$$e_h(0) = 0$$

We can test the equation by e_h, use that $a_h(v_h, v_h) = \|v_h\|^2_{H^1(\Omega_h)} - \|v_h\|^2_{L^2(\Omega_h)}$, that $e_h(0) = 0$ and Gronwall's lemma to conclude the desired uniqueness.

Stability

Following [34], page 20, 21, we can prove, for δ_h, that:

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

so that, 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.2.1.6:

- $\|g_{N,h}\|_{L^2(I,L^2(\Gamma_{N_h}))} \lesssim \|g_N\|_{L^2(I,H^2(\Gamma_N))}$ (here is suffices to use proposition D.1.6))
- because the Lagrange interpolator is linear bounded $H^2(\Omega) \to S^1_h$ there holds, by proposition D.1.6: $\partial_t G_{D,h} = \Pi_h \partial_t G_D$, 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.1.6 and proposition D.1.4. Thanks to the properties of G_D, and the fact that the extension E of proposition A.2.6 commutes with Π_h (by proposition 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.2.1.10 (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.2.1.4, assumption D.2.1.6 and assumption B.2.3.2 must be fulfilled.

Proof.

Also here, we adapt the argument from [24], in particular, those of pages 1727, 1728, 1729, which are modifications of standard techniques that can be traced in e.g. [57], theorem 1.2. We make it clear where one could use other approximations of the data, provided that they enjoy similar properties.

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.2.1.3.

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 we obtain:

$$\begin{aligned}(\partial_t \theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h) = (\partial_t R_h u, v_h)_{L^2(\Omega_h)} &- (\partial_t u, v_h^l)_{L^2(\Omega)} \\ +(f, v_h^l)_{L^2(\Omega)} &- (f_h, v_h)_{L^2(\Omega_h)} \\ +(g_N, v_h^l)_{L^2(\Gamma_N)} &- (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}\end{aligned}$$

Adding and subtracting $(\partial_t R_c u, v_h^l)_{L^2(\Omega)}$:

$$(\partial_t \theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h) = (\partial_t R_h u, v_h)_{L^2(\Omega_h)} - (\partial_t R_c u, v_h^l)_{L^2(\Omega)} \tag{D.2.1.11}$$
$$-(\partial_t \rho, v_h^l)_{L^2(\Omega)} \tag{D.2.1.12}$$
$$+(f, v_h^l)_{L^2(\Omega)} - (f_h, v_h)_{L^2(\Omega_h)} \tag{D.2.1.13}$$
$$+(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})} \tag{D.2.1.14}$$

This means that we can estimate the right hand sides of the above equation to quantify the size of θ_h.

Estimating the size of θ_h: right hand sides

By proposition 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.1.7, and proposition D.2.1.3.

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.2.1.3. By the choice of $g_{D,h}$ and by proposition D.1.6, $|(\partial_t\rho, v_h^l)_{L^2(\Omega)}| \lesssim h^2(\|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \|v_h\|_{H^1(\Omega_h)}$.

Moreover:

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

By proposition D.1.7 and trace theorems there holds:

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

Using the choice of $g_{N,h}$ and also proposition D.1.6, proposition D.1.4, we obtain:

$$|(g_N, v_h^l)_{L^2(\Gamma_N)} - (g_{N,h}, v_h)_{L^2(\Gamma_{N_h})}| \lesssim h^2 \|g_N\|_{H^2(\Gamma_N)} \|v_h\|_{H^1(\Omega_h)}$$

Analogously:

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

We used throughout assumption D.2.1.6.

Calling $E_h(v_h) := (\partial_t\theta_h, v_h)_{L^2(\Omega_h)} + a_h(\theta_h, v_h)$, we discovered that:

$$|E_h(v_h)| \lesssim h^2 \|v_h\|_{H^1(\Omega_h)} (C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \tag{D.2.1.15}$$

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:

$$\frac{1}{2}\frac{d}{dt} \|\theta_h\|_{L^2(\Omega_h)}^2 + \|\theta_h\|_{H^1(\Omega_h)}^2 - \|\theta_h\|_{L^2(\Omega_h)}^2 = E_h(\theta_h)$$

Hence:

$$\frac{1}{2}\frac{d}{dt} \|\theta_h\|_{L^2(\Omega_h)}^2 + \|\theta_h\|_{H^1(\Omega_h)}^2 \lesssim \|\theta_h\|_{L^2(\Omega_h)}^2 + Qh^2 \|\theta_h\|_{H^1(\Omega_h)}$$

Here we called $Q := C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}$.

By Young's inequality:

$$\frac{1}{2}\frac{d}{dt} \|\theta_h\|_{L^2(\Omega_h)}^2 + \|\theta_h\|_{H^1(\Omega_h)}^2 \lesssim \|\theta_h\|_{L^2(\Omega_h)}^2 + 2Q^2h^4 + \frac{1}{2} \|\theta_h\|_{H^1(\Omega_h)}^2$$

Re-arranging:

$$\frac{1}{2}\frac{d}{dt}\|\theta_h\|^2_{L^2(\Omega_h)} + \frac{1}{2}\|\theta_h\|^2_{H^1(\Omega_h)} \lesssim \|\theta_h\|^2_{L^2(\Omega_h)} + 2Q^2h^4$$

We now integrate from 0 to t:

$$\frac{1}{2}\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \frac{1}{2}\int_0^t \|\theta_h\|^2_{H^1(\Omega_h)} \lesssim 2\int_0^t \frac{1}{2}\|\theta_h\|^2_{L^2(\Omega_h)} + 2h^4\int_0^t Q^2 + \frac{1}{2}\|\theta_h(0)\|^2_{L^2(\Omega_h)}$$

Adding non-negative terms on the right hand side yields:

$$\frac{1}{2}\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \frac{1}{2}\int_0^t \|\theta_h\|^2_{H^1(\Omega_h)} \lesssim 2\left(\int_0^t \frac{1}{2}\|\theta_h\|^2_{L^2(\Omega_h)} + \int_0^t \frac{1}{2}\int_0^s \|\theta_h\|^2_{H^1(\Omega_h)}\, dsdt\right) + 2h^4\int_0^t Q^2 + \frac{1}{2}\|\theta_h(0)\|^2_{L^2(\Omega_h)}$$

Gronwall's inequality (25, page 19 of [34]) now yields:

$$\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \int_0^t \|\theta_h\|^2_{H^1(\Omega_h)} \lesssim e^{2t}\left(4h^4\int_0^t Q^2 + \|\theta_h(0)\|^2_{L^2(\Omega_h)}\right)$$

Therefore, for all $t \in [0,T]$ we have:

$$\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \int_0^T \|\theta_h\|^2_{H^1(\Omega_h)} \lesssim 8h^4\int_0^T Q^2 + 2\|\theta_h(0)\|^2_{L^2(\Omega_h)} \tag{D.2.1.16}$$

We can apply also proposition D.1.4 to obtain an estimate in spaces that don't depend on h:

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

Conclusion

We have, for $e = u - u_h^l$ (and $h < 1$, at least), that:

$$\begin{aligned}\|e(t)\|^2_{L^2(\Omega)} + h^2\int_0^T \|e\|^2_{H^1(\Omega)} &\lesssim \\ \|\rho(t)\|^2_{L^2(\Omega)} + h^2\int_0^T \|\rho\|^2_{H^1(\Omega)} + \left\|\theta_h^l(t)\right\|^2_{L^2(\Omega)} + \int_0^T \left\|\theta_h^l\right\|^2_{H^1(\Omega)} &\lesssim \{\text{ proposition D.2.1.3 }\} \\ h^4\|u(t)\|^2_{H^2(\Omega)} + h^4\|g_D(t)\|^2_{L^2(\Gamma_D)} + h^2h^2\int_0^T \|u\|^2_{H^2(\Omega)} + h^4\int_0^T Q^2 + \left\|\theta_h^l(0)\right\|^2_{L^2(\Omega)}\end{aligned}$$

A triangle inequality applied to $\left\|\theta_h^l(0)\right\|^2_{L^2(\Omega)}$, an application of proposition D.2.1.3 and the definition of Q bring us to:

$$\begin{aligned}h^{-4}\|e(t)\|^2_{L^2(\Omega)} + h^{-2}\int_0^T \|e\|^2_{H^1(\Omega)} &\lesssim \\ \|u(t)\|^2_{H^2(\Omega)} + \|g_D(t)\|^2_{L^2(\Gamma_D)} + \int_0^T \|u\|^2_{H^2(\Omega)} + \|u_0\|^2_{H^2(\Omega)} \\ + \int_0^T C_f^2 + \int_0^T \|f_h\|^2_{H^1(\Omega_h)} + \int_0^T \|g_N\|^2_{H^2(\Gamma_N)} + \int_0^T \|\partial_t u\|^2_{H^2(\Omega)} + \int_0^T \|\partial_t g_D\|^2_{H^2(\Gamma_D)}\end{aligned}$$

This means that:

$$
\begin{aligned}
h^{-4}\left\|e(t)\right\|_{L^2(\Omega)}^2 + h^{-2}\int_0^T \|e\|_{H^1(\Omega)}^2 \lesssim \\
\|u\|_{H^1(I,H^2(\Omega))}^2 + \|g_D\|_{H^1(I,H^2(\Gamma_D))}^2 + \|u_0\|_{H^2(\Omega)}^2 + \int_0^T C_f^2 + \int_0^T \|f_h\|_{H^1(\Omega_h)}^2 + \int_0^T \|g_N\|_{H^2(\Gamma_N)}^2
\end{aligned}
$$

□

We can also prove convergence of the derivatives in a rather strong norm.

Corollary D.2.1.17 (Refined error estimate)
Apart from assumption D.2.1.4, assumption D.2.1.6 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 $B := \|u\|_{H^1(I,H^2(\Omega))}^2 + \|g_D\|_{H^1(I,H^2(\Gamma_D))}^2 + \int_0^T C_f^2 + \|f_h\|_{L^2(I,L^2(\Omega_h))}^2 + \|g_N\|_{H^1(H^2(\Gamma_N))}^2 + \|u_0\|_{H^2(\Omega)}^2$.

Proof.

We employ again the error decomposition $e = \rho + \theta_h^l$.

Another estimate for θ_h

Consider again eq. (D.2.1.11):

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

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 [38], (1.61), page 42. Integrate from 0 to t to obtain:

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

Estimating the left hand side:

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

For the terms with $g_N, g_{N,h}$ we integrate by parts and find:

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

For the right hand side, estimating every piece but the first two, with the help of proposition D.1.7, and C independent of h and t:

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

Applying Young's inequality several times, with possibly a different C, still independent of h and t:

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

We re-arrange, and apply eq. (D.2.1.16) to the term $\|\theta_h(t)\|^2_{L^2(\Omega_h)} + \int_0^t \|\theta_h\|^2_{H^1(\Omega_h)}$.

Calling $q = \int_0^T \left[\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)} + C_f^2 + \|f_h\|^2_{L^2(\Omega_h)} + Q^2 + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t g_N\|^2_{H^2(\Gamma_N)}\right]$ we read:

$$
\frac{1}{2}\int_0^t \|\partial_t \theta_h\|^2_{L^2(\Omega_h)} + \frac{1}{4}\|\theta_h(t)\|^2_{H^1(\Omega_h)} \lesssim \|\theta_h(0)\|^2_{H^1(\Omega_h)} + h^4 q
$$

or also, upon using proposition D.1.4, proposition D.2.1.3 and proposition D.1.6:

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

<u>Conclusion</u>

There holds

$$
\begin{aligned}
\|e(t)\|^2_{H^1(\Omega)} + \int_0^T \|\partial_t e\|^2_{L^2(\Omega)} \leq \\
\int_0^T \|\partial_t \rho\|^2_{L^2(\Omega)} + h^2\|\rho(t)\|^2_{H^1(\Omega)} + \int_0^T \left\|\partial_t \theta_h^l\right\|^2_{L^2(\Omega)} + \left\|\theta_h^l(t)\right\|^2_{H^1(\Omega)} \leq \{\text{ above, and proposition D.2.1.3 }\} \leq \\
h^2\int_0^T \left(\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}\right) + h^2\|u(t)\|^2_{H^2(\Omega)} + h^2\|u_0\|^2_{H^2(\Omega)} + h^4 q
\end{aligned}
$$

□

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. [5].

Corollary D.2.1.18 (Order two convergence of derivatives in dual norm)
Under assumption D.2.1.4, assumption D.2.1.6 and assumption B.2.3.2 we have, for all $w \in L^2(I, H^1_{0,D}(\Omega))$:

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

Proof.

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

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

The definition is remimniscent of that of the Ritz projection. We will prove well-posedness and H^k stability of such projection, i.e. $\|\pi_h w\|_{H^k(\Omega_h)} \lesssim \|w\|_{H^k(\Omega)}$, for $k = 0, 1$.

First, let us show how this projection helps in the estimate.

Conclusion

For $w \in H^1_{0,D}(\Omega)$ we estimate $(\partial_t(\theta_h^l), w)_{L^2(\Omega)} = (w, (\partial_t \theta_h^l))_{L^2(\Omega)} = (\pi_h w, \partial_t \theta_h)_{L^2(\Omega_h)}$. We have also used that lifting and differentiating with respect to time commute, by proposition D.1.4 and proposition A.2.2. We can now apply eq. (D.2.1.11):

$$\begin{aligned}
(\partial_t(\theta_h^l), w)_{L^2(\Omega)} = a_h(\theta_h, \pi_h w) - E_h(\pi_h w) \lesssim \{ \text{ eq. (D.2.1.15) } \} \lesssim \\
\|\theta_h\|_{H^1(\Omega_h)} \|\pi_h w\|_{H^1(\Omega_h)} + h^2(\|\pi_h w\|_{H^1(\Omega_h)} C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \lesssim \\
\|\theta_h\|_{H^1(\Omega_h)} \|w\|_{H^1(\Omega)} + h^2 \|w\|_{H^1(\Omega)} (C_f + \|f_h\|_{H^1(\Omega_h)} + \|g_N\|_{H^2(\Gamma_N)} + \|\partial_t u\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)})
\end{aligned}$$

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

$$\begin{aligned}
\left| \int_I (\partial_t(\theta_h^l), w)_{L^2(\Omega)} \right|^2 \lesssim \\
\left(\int_I \|\theta_h\|^2_{H^1(\Omega_h)} + h^4 \int_I (C_f^2 + \|f_h\|^2_{H^1(\Omega_h)} + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}) \right) \int_I \|w\|^2_{H^1(\Omega)} \lesssim \{ \text{ eq. (D.2.1.16) } \} \lesssim \\
h^4 \left(\int_I Q^2 + \|u_0\|^2_{H^2(\Omega)} + \int_I (C_f^2 + \|f_h\|^2_{H^1(\Omega_h)} + \|g_N\|^2_{H^2(\Gamma_N)} + \|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}) \right) \|w\|^2_{L^2(I,H^1(\Omega))}
\end{aligned}$$

We can also estimate:

$$\begin{aligned}
\left| \int_I (\rho_t, w)_{L^2(\Omega)} \right| \lesssim \{ \text{ as in the proof of theorem D.2.1.10 } \} \lesssim \\
\int_I h^2(\|\partial_t w\|_{H^2(\Omega)} + \|\partial_t g_D\|_{H^2(\Gamma_D)}) \|w\|_{H^1(\Omega_h)} \lesssim \{ \text{ Cauchy-Schwarz } \} \lesssim \\
h^2 \sqrt{\|\partial_t u\|^2_{H^2(\Omega)} + \|\partial_t g_D\|^2_{H^2(\Gamma_D)}} \|w\|_{L^2(I,H^1(\Omega))}
\end{aligned}$$

and by the usual splitting $e = \rho + \theta_h^l$ we can conclude.

L^2 projection: well-posedness

From the definition of π_h we obtain:

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

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.

To be precise we don't know whether G_h takes measurable functions into measurable functions. But for L^2 arguments, we can reason as follows: w^{-l} we know to be piecewise in L^2, so we can glue it to an L^2 fcn by in case modifying it on a null set. Also ξ is piecewise measurable (it is peicewise C^1). So $w^{-l}\xi$ is measurable and L^2. Well actually now we know it...

L^2 projection: stability

L^2 stability of π_h follows by testing with $\pi_h w$ itself and using proposition D.1.4.

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.1.7 and of proposition D.1.4 (4.6 still applies here, do the reasonings elementwise and use lemma 8.16 of [24]) 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 [4] 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, $\left\|\pi_h^* v\right\|_{L^2(\Omega_h)} \leq \left\|v\right\|_{L^2(\Omega_h)}$, so that $|\pi_h^* w^{-l}|_{H^1(\Omega_h)} \lesssim h^{-1} \left\|w^{-l} - w_h\right\|_{L^2(\Omega_h)} + \left\|w_h\right\|_{H^1(\Omega_h)}$

So, if there holds $\left\|w^{-l} - w_h\right\|_{L^2(\Omega_h)} \lesssim h \left\|w\right\|_{H^1(\Omega)}$ and $\left\|w_h\right\|_{H^1(\Omega_h)} \lesssim \left\|w\right\|_{H^1(\Omega)}$, then we are done.

what is h??? Also throughout the rest of the thesis... I checked this, it is the maximum h_K in the linear triangulation for Ranner, and a parameter that I can choose to be h of Ranner, in Bernardi

Finding w_h

Such w_h will be the optimal order interpolator with boundary conditions described in (5.9) at page 1230, [8]. We need to check that our framework matches that of [8] to apply such a result.

But this is ensured by the construction outlined in [24], 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 [24], whereas all the other properties are already discussed in [8] following example 2 (see pages 1216, 1221, 1228, and remark 5.2 at page 1230).

Applying corollary 5.1 of [8] to $\Gamma_0 = \Gamma_D$ (Γ_0 is in the notation of [8]) we find $w_h \in S^1_{h,0,D_h}$ (true by proposition and corollary 5.1, [8]), with:

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

Therefore we also get $\left\|w_h^l\right\|_{H^1(\Omega)} \lesssim (C(1+h)+1) \left\|w\right\|_{H^1(\Omega)}$.

Applying proposition D.1.4 we see that w_h satisfies all the requirements. Note, is is essential here that $w = 0$ on Γ_D.

□

D.2.2. Fully discrete estimates

Here, we attempt at deriving fully discrete estimates given the semidiscrete results just above. We found difficulties in adapting the arguments of [57], and this is the main reason for passing through the semidiscrete world at first. In particular, one would have to compare at some point quantities similar to $(\partial_t u, e_h^l)_{L^2(\Omega)}$ and $(\partial_t u_h, e_h)_{L^2(\Omega_h)}$, for e_h the discretization error we want to bound. This difference is $O(h^2)$, but then H^1 norms of e_h appear, which makes it difficult to apply some algebraic manipulations to bound the weaker L^2 norm. To keep only L^2 norms, one has to content himself with an $O(h)$ discrepancy in the aforementioned term, which would yield suboptimal results.

Assumption D.2.2.1 (Assumptions for full discretization)

We discuss the implicit Euler method ($\theta = 1$) and the Crank-Nicolson method ($\theta = 1/2$).
We ask assumption D.2.1.6.
We further assume:

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

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

Problem D.2.2.2 (Numerical scheme)
Under assumption D.2.2.1, it is:

$$\begin{aligned}\left(\frac{u_h^{k+1}-u_h^k}{\delta t}, v_h\right)_{L^2(\Omega_h)} + a_h(\theta u_h^{k+1} + (1-\theta)u_h^k, v_h) =\\ (\theta f_h^{k+1} + (1-\theta)f_h^k, v_h)_{L^2(\Omega_h)} + (\theta g_{N,h}^{k+1} + (1-\theta)g_{N,h}^k, v_h)_{L^2(\Gamma_{N_h})}, \quad v_h \in S^1_{h,0,D_h}, 1 \le k \le K\\ u_h^{k+1} = g_{D,h}^{k+1}, \quad 1 \le k \le K, \text{ on } \Gamma_{D_h}\\ u_h^0 = u_{0h}\end{aligned}$$

Proposition D.2.2.3 (Discrete versus semidiscrete)
We are working under assumption D.2.2.1.
Call $e_h^k := u_h^k - u_h(t^k)$ and $\delta f_h^k := f_h^k - f_h(t^k)$. Then, for $\theta = 1, 1/2$, we have $u_h \in H^{1/\theta+1}(I, S_h^1)$ and, for $1 \le n \le K$:

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

where $C^2 := \int_I \left\|f_h^{(1/\theta)}\right\|^2_{-1,h} + \int_I \left\|g_N^{(1/\theta)}\right\|^2_{H^2(\Gamma_N)} + \int_I \left\|g_D^{(1/\theta+1)}\right\|^2_{H^{3/2}(\Gamma_D)} + \left\|\delta_h(0)^{(1/\theta)}\right\|^2_{L^2(\Omega_h)}$.
Moreover, $D_n^2 := \delta t \sum_{k=0}^{n-1}\left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|^2_{L^2(\Omega_h)}$.
We refer to the proof of proposition D.2.1.7 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.2.1.5, for $u_h \in H^1(I, S_h^1)$:

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

For the L^2 estimate we closely follow [53] here, page 385 and following, in particular, theorem 11.3.1 and 11.3.2.

Error equation

We note that the sole smoothness assumptions allow us to conclude that $u_h \in H^2(I, S_h^1)$, so that $\partial_t u_h$ admits pointwise values. Then we have: A θ is probably missing from ∂_t

$$\left(\frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t}, v_h\right)_{L^2(\Omega_h)} + a_h(\theta u_h(t^{k+1}) + (1-\theta)u_h(t^k), v_h) = \left(\frac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} - \partial_t u_h(t^{k+1}) - (1-\theta)\partial_t u_h(t^k), v_h\right)_{L^2(\Omega_h)} + (\theta f_h(t^{k+1}) + (1-\theta)f_h(t^k), v_h)_{L^2(\Omega_h)} + (\theta g_{N,h}(t^{k+1}) + (1-\theta)g_{N,h}(t^k), v_h)_{L^2(\Gamma_{N_h})}$$

By the equations for the fully discrete problem, and calling $e_h^k := u_h^k - u_h(t^k)$, and $\delta f_h^k := f_h^k - f_h(t^k)$:

$$\left(\frac{e_h^{k+1} - e_h^k}{\delta t}, v_h\right)_{L^2(\Omega_h)} + a_h(\theta e_h^{k+1} + (1-\theta)e_h^k, v_h) = (\theta \delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k, v_h)_{L^2(\Omega_h)} \tag{D.2.2.4}$$

$$e_h^{k+1} = 0, \text{ on } \Gamma_{D_h} \tag{D.2.2.5}$$

$$e_h^0 = 0 \tag{D.2.2.6}$$

where we defined $Q_h^k := \dfrac{u_h(t^{k+1}) - u_h(t^k)}{\delta t} - \partial_t u_h(t^{k+1}) - (1-\theta)\partial_t u_h(t^k)$.

Stability

We test the above error equation with $\theta e_h^{k+1} + (1-\theta)e_h^k \in S_{h,0,D_h}^1$ to obtain, also thanks to the h uniform coercivity of a_h we have shown in theorem D.1.8:

$$\left\|e_h^{k+1}\right\|_{L^2(\Omega_h)}^2 - \left\|e_h^k\right\|_{L^2(\Omega_h)}^2 + (2\theta - 1)\left\|e_h^{k+1} - e_h^k\right\|_{L^2(\Omega_h)}^2 + 2C\delta t\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{H^1(\Omega_h)}^2 \leq 2\delta t\left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|_{L^2(\Omega_h)}\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{L^2(\Omega_h)} + 2\delta t\left\|Q_h^k\right\|_{-1,h}\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{H^1(\Omega_h)}$$

where C is independent of h, k. Here $\|w\|_{-1,h} := \sup_{0 \neq v_h \in S_{h,0,D_h}^1} \dfrac{(w, v_h)_{L^2(\Omega_h)}}{\|v_h\|_{H^1(\Omega_h)}}$. We now apply Young's inequality and leave out a non-negative term on the left to obtain:

$$\left\|e_h^{k+1}\right\|_{L^2(\Omega_h)}^2 - \left\|e_h^k\right\|_{L^2(\Omega_h)}^2 + 2(C - 2\epsilon)\delta t\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{H^1(\Omega_h)}^2 \leq 2\delta t\epsilon^{-1}\left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|_{L^2(\Omega_h)}^2 + 2\delta t\epsilon^{-1}\left\|Q_h^k\right\|_{-1,h}^2$$

ϵ must be of course chosen small enough. We then sum from $k = 0$ to $n - 1$ to obtain:

$$\|e_h^n\|_{L^2(\Omega_h)}^2 + \delta t\sum_{k=0}^{n-1}\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{H^1(\Omega_h)}^2 \lesssim \delta t\sum_{k=0}^{n-1}\left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|_{L^2(\Omega_h)}^2 + \delta t\sum_{k=0}^{n-1}\left\|Q_h^k\right\|_{-1,h}^2$$

Conclusion: L^2 estimate

It remains to qualify Q_h^k.

In the case $\theta = 1/2$, from the smoothness assumptions on the data we obtain $u_h \in H^3(I, S_h^1)$, together with:

$$(u_h''', v_h)_{L^2(\Omega_h)} + a_h(u_h'', v_h) = (f_h'', v_h)_{L^2(\Omega_h)} + (g_{N,h}'', v_h)_{L^2(\Gamma_{N_h})}$$

By the smoothness of u_h we obtain $(Q_h^k, v_h) = \dfrac{1}{2\delta t}\left(\displaystyle\int_{t^k}^{t^{k+1}} (t^{k+1}-s)(t^k-s)u_h'''(s)ds, v_h\right)_{L^2(\Omega_h)}$, which means that:

$$|(Q_h^k, v_h)| \leq \frac{1}{2\delta t}\sqrt{\int_{t^k}^{t^{k+1}} (t^{k+1}-s)^2(t^k-s)^2 ds}\sqrt{\int_{t^k}^{t^{k+1}} (u_h'''(s), v_h)^2_{L^2(\Omega_h)} ds} \leq C\delta t^{3/2}\sqrt{\int_{t^k}^{t^{k+1}} \|u_h'''(s)\|^2_{-1,h}\, ds}\, \|v_h\|_{H^1(\Omega_h)}$$

This means that:

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

Differentiating problem D.2.1.5 twice we obtain:

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

We therefore only need to estimate the very last piece. This is done by energy estimates, as in proposition D.2.1.7. We consider the splitting $u_h = \delta_h + G_{D,h}$, see assumption D.2.1.6, and estimate $\|\delta_h''\|_{H^1(\Omega_h)}$. We find out in particular that:

$$\begin{aligned} &\|\delta_h''\|_{C([0,T],L^2(\Omega_h))} + \|\delta_h''\|_{L^2(I,H^1(\Omega_h))} \lesssim \\ &\|f_h''\|_{L^2(I,(S^1_{h,0,D_h})^*)} + \left\|g_{N,h}''\right\|_{L^2(I,L^2(\Gamma_{N_h}))} + \left\|G_{D,h}'''\right\|_{L^2(I,H^1(\Omega_h)))} + \|\delta_h(0)''\|_{L^2(\Omega_h)} \end{aligned}$$

and by definition of u_h:

$$\|u_h''\|_{L^2(I,H^1(\Omega_h))} \lesssim \tag{D.2.2.7}$$

$$\|f_h''\|_{L^2(I,(S^1_{h,0,D_h})^*)} + \left\|g_{N,h}''\right\|_{L^2(I,L^2(\Gamma_{N_h}))} + \left\|G_{D,h}'''\right\|_{L^2(I,H^1(\Omega_h)))} + \|\delta_h(0)''\|_{L^2(\Omega_h)} \tag{D.2.2.8}$$

We only need to estimate the term on the right. Using eq. (D.2.1.8) we find out that:

$$\begin{aligned} d_h'(0) &= -M_h^{-1}(A_h d_h(0) + F_h(0)) \\ d_h''(0) &= -M_h^{-1}(A_h d_h'(0) + F_h'(0)) \end{aligned}$$

Under our hypothesis assumption D.2.2.1, we have that $\|\delta_h''(0)\|^2_{L^2(\Omega_h)} = |M_h^{1/2} d_h(0)''| \lesssim C$. This, and assumption D.2.1.6, yield a bound, uniform on h, on $\displaystyle\int_I \|u_h'''\|^2_{-1,h}$.

This bound is:

$$\int_I \|u_h'''(t)\|^2_{-1,h} \lesssim \int_I \|f_h''\|^2_{-1,h} + \int_I \left\|g_{N,h}''\right\|^2_{L^2(\Gamma_{N_h})} + \int_I \left\|G_{D,h}'''\right\|^2_{H^1(\Omega_h)} + \|\delta_h(0)''\|^2_{L^2(\Omega_h)}$$

But $\left\|g_{N,h}''\right\|_{L^2(\Gamma_{N_h})} = \|\Pi_h g_N''\|_{L^2(\Gamma_{N_h})}$, where Π_h is the nodal interpolator (see assumption D.2.1.6). By proposition D.1.7, $\left\|g_{N,h}''\right\|_{L^2(\Gamma_{N_h})} \lesssim \|\Pi_c g_N''\|_{L^2(\Gamma_N)} \leq (1+h^2)\,\|g_N''\|_{H^2(\Gamma_N)}$, where we also used proposition D.1.6.

Moreover $\left\|G_{D,h}'''\right\|_{H^1(\Omega_h)} = \|\Pi_h G_D'''\|_{H^1(\Omega_h)} \lesssim \|\Pi_c G_D'''\|_{H^1(\Omega)} \lesssim (1+h)\,\|G_D'''\|_{H^2(\Omega)} \lesssim \|g_D'''\|_{H^{3/2}(\Gamma_D)}$.

Therefore:

$$\int_I \|u_h'''(t)\|_{-1,h}^2 \lesssim \int_I \|f_h''\|_{-1,h}^2 + \int_I \|g_N''\|_{H^2(\Gamma_N)}^2 + \int_I \|g_D'''\|_{H^{3/2}(\Gamma_D)}^2 + \|\delta_h(0)''\|_{L^2(\Omega_h)}^2$$

The proof for $\theta = 1$ is very similar.

Conclusion: estimates for the difference quotient

We go back to eq. (D.2.2.4). We employ the L^2 projection π_h^* as in the proof of corollary D.2.1.18, where we proved its stabilities properties. Consider then any $v \in H^1_{0,D}(\Omega)$, so that $v^{-l} \in H^1_{0,D_h}(\Omega_h)$ (i.e. $v^{-l} = 0$ on Γ_{D_h}) are you sure :D?.

Then:

$$\left(\frac{e_h^{k+1} - e_h^k}{\delta t}, v^{-l}\right)_{L^2(\Omega_h)} = \left(\frac{e_h^{k+1} - e_h^k}{\delta t}, \pi_h^* v^{-l}\right)_{L^2(\Omega_h)} = \tag{D.2.2.9}$$

$$-a_h(\theta e_h^{k+1} + (1-\theta)e_h^k, \pi_h^* v^{-l}) + (\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k, \pi_h^* v^{-l})_{L^2(\Omega_h)} \tag{D.2.2.10}$$

which leads us to:

$$\left\|\frac{e_h^{k+1} - e_h^k}{\delta t}\right\|_{(H^1_{0,D_h}(\Omega_h))^*} \lesssim$$
$$\left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|_{H^1(\Omega_h)} + \left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k + Q_h^k\right\|_{-1,h}$$

We thus have:

$$\delta t \sum_{k=0}^{n-1} \left\|\frac{e_h^{k+1} - e_h^k}{\delta t}\right\|^2_{(H^1_{0,D_h}(\Omega_h))^*} \lesssim$$
$$\delta t \sum_{k=0}^{n-1} \left\|\theta e_h^{k+1} + (1-\theta)e_h^k\right\|^2_{H^1(\Omega_h)} + \delta t \sum_{k=0}^{n-1} \left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|^2_{L^2(\Omega_h)} + \delta t \sum_{k=0}^{n-1} \left\|Q_h^k\right\|^2_{-1,h} \lesssim$$
$$\delta t \sum_{k=0}^{n-1} \left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|^2_{L^2(\Omega_h)} +$$
$$(\delta t)^{2/\theta}\left(\int_I \left\|f_h^{(1/\theta)}\right\|^2_{-1,h} + \int_I \left\|g_N^{(1/\theta)}\right\|^2_{H^2(\Gamma_N)} + \int_I \left\|g_D^{(1/\theta+1)}\right\|^2_{H^{3/2}(\Gamma_D)} + \left\|\delta_h(0)^{(1/\theta)}\right\|^2_{L^2(\Omega_h)}\right)$$

□

Theorem D.2.2.11 (Fully discrete estimates)
With the hypothesis and notation of theorem D.2.1.10, proposition D.2.2.3, corollary D.2.1.17, corollary D.2.1.18, there holds:

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

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

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

where $D^2 := \delta t \sum_{k=0}^{K-1} \left\|\theta\delta f_h^{k+1} + (1-\theta)\delta f_h^k\right\|^2_{L^2(\Omega_h)}$. 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 $H^1_{0,D}(\Omega)$. If we put $w \in H^(I, H^1_{0,D})$ this probably still works, by choosing to evaluate the sum on the right on the local averages of w, and employing dual estimates for such projection.

Proof.

<u>L^2 norm</u>

By theorem D.2.1.10, $\left\|u(t) - u_h^l(t)\right\|_{L^2(\Omega)}^2 \lesssim h^4 A^2$. Combining this with the L^2 estimates proved in proposition D.2.2.3 we see, thanks to proposition D.1.4:

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

<u>H^1 norm</u>

Using proposition D.2.2.3 and proposition D.1.4:

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

For the case $\theta = 1/2$ one could argue by noticing that $\dfrac{e_h(t^k) + e_h(t^{k+1})}{2} = \dfrac{1}{\delta t}\displaystyle\int_{t^k}^{t^{k+1}} \Pi e_h(s)ds$, bounding the first sum by $\|\Pi u - u\|_{L^2(I,H^1(\Omega))}^2 + \|\Pi u_h^l - u_h^l\|_{L^2(I,H^1(\Omega))}^2 + \|e_h\|_{L^2(I,H^1(\Omega))}^2$, Πe_h being the Lagrangian linear interpolator of $e_h := u - u_h^l$, and then using the $O(\delta t^2)$ approximation power of Π, thus obtaining s bound that is $O(\delta t^4 + h^2)$.

But by employing corollary D.2.1.17 the proof simplifies and is fine for both values of θ. In fact:

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

<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:

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

For the first term we can use corollary D.2.1.18. For the second one we can write, thanks to proposition D.1.4 (one is not a FEM function, are we sure this holds? Also, is w^{-l} of zero value??????????):

$$\begin{aligned}
&\left|\delta t \sum_{k=0}^{K-1} \left(\frac{(e_h^{k+1})^l - (e_h^k)^l}{\delta t}, w_k \right)_{L^2(\Omega)} \right| \lesssim \\
&\delta t h \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{L^2(\Omega_h)} \|w_k\|_{H^1(\Omega)} + \delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{-1,h} \|w_k\|_{H^1(\Omega)} \leq \\
&\left(h \sqrt{\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{L^2(\Omega_h)}} + \sqrt{\sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{-1,h}} \right) \|w\|_{L^2(I, H^1(\Omega))}
\end{aligned}$$

If we can control $\delta t \sum_{k=0}^{K-1} \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{L^2(\Omega_h)}$ we are done, also by the estimates in proposition D.2.2.3.

We now test eq. (D.2.2.4) by $\frac{e_h^{k+1} - e_h^k}{\delta t}$. Then:

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

Applying an additional Young's inequality in the case $\theta = 1$ this reads:

$$\left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|^2_{L^2(\Omega_h)} + \frac{\left\|\nabla e_h^{k+1}\right\|^2_{L^2(\Omega_h)}}{2\delta t} - \frac{\left\|\nabla e_h^k\right\|^2_{L^2(\Omega_h)}}{2\delta t} \leq \left(\left\| \theta \delta f_h^{k+1} + (1-\theta) \delta f_h^k \right\|_{L^2(\Omega_h)} + \left\| Q_h^k \right\|_{-1,h} \right) \left\| \frac{e_h^{k+1} - e_h^k}{\delta t} \right\|_{H^1(\Omega_h)}$$

or also, as $e_h^0 = 0$:

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

Applying inverse inequalities and by the proof of proposition D.2.2.3, for h small:

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

□

Corollary D.2.2.12 (Further estimates for A, B, C, D)
Assume that f_h^k and f_h are the, respectively, fully discrete and semidiscrete solutions (see problem D.2.2.2 and problem D.2.1.5) of problem D.2.1.1, for which all the assumptions of theorem D.2.2.11 hold (in particular, all the continuous and discrete compatibility conditions).
We assume for simplicity, for the right hand side of the equation of f, call it F, that $F \in H^{1/\theta}(I, H^2(\Omega))$ and we take $F_h = \Pi_h F$ and $F_h^k = F_h(t^k)$.
We can therefore say that:

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

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

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

and w_K is as in theorem D.2.2.11.
Note, the Dirichlet and Neumann boundaries need not to be the same for f, u.

Proof.

We start to establish semidiscrete and fully discrete estimates for f.

We assume the following notation for its problem, see problem D.2.1.1:

$$\begin{cases} \partial_t f - \Delta f = F & \text{on } \Omega \times I \\ f = \gamma_D & \text{on } \Gamma'_D \times I \\ \partial_\nu f = \gamma_N & \text{on } \Gamma'_N \times I \\ f(0) = f_0 \end{cases}$$

By our hypothesis, we can apply theorem D.2.2.11 to f and obtain error bounds with constants $A(f), B(f), C(f), D(f)$ which we now show to be bounded, uniformly with respect to $h, \delta t$.

In particular, by the choice of F_h^k, we see that $D(f) = 0$.

For $C(f)$, the requirement of compatibilty leaves only one last bound to be made, that on $\int_I \left\| F_h^{(1/\theta)} \right\|_{-1,h}^2$. This one is surely bounded with h, by the choice of $F_h = \Pi_h F$, the time smoothness of F, and proposition D.1.6.

For $A(f), B(f)$ we only need to estimate $\int_I C_F^2$ and $\int_I \|F_h\|_{H^1(\Omega_h)}^2$. The latter term is done as above. Morevoer, by proposition D.1.6, C_F is just $\|F\|_{H^2(\Omega)}$, whose integral in time is bounded by assumption.

Therefore, proposition D.2.2.3 yields the estimate:

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

and $C_f = A_f$ by theorem D.2.1.10.

There remains to check that A, B, C are also bounded with $h, \delta t$.

For C, the assumed compatibility requirements leave us only the estimation of $\int_I \left\| f_h^{(1/\theta)} \right\|_{-1,h}^2$. To avoid complications with the fact that this dual norm $\{-1, h\}$ might not actually be the same dual norm of the problem of f (in fact, the Dirichlet and Neumann boundaries may not be the same between f and u), we proceed to estimate the stronger $L^2(\Omega_h)$ norm. This can be done as above eq. (D.2.2.7). The bound uniform on h is again a consequence of the assumed compatibility conditions, and the fact that $\left\| F_h^{(2/\theta)} \right\|_{L^2(I, L^2(\Omega_h))}$ is bounded, by the requirements on F.

There remains to bound A, B. Our smoothness assumptions allow us to only check A, where we see that we need to bound $\int C_f^2$ (already done, by above $C_f = A_f$) and $\int_I \|F_h\|^2_{H^1(\Omega_h)}$. This term is bounded by basic energy estimates on f_h.

This concludes the proof of 7, that of 9 follows just like 6 implied 8, see above.

□

Make a comment on why imposing BCs with interpolation of nodal values exactly on the boundary, is the right thing to do, in shape optimization... for instance, when the boundary moves, a projected bc would also move and we would need to know the exact transformation etc

One could be extraprecise and track the dependence on Ω too, this is very difficult though

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