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A TRANSFORMATION APPROACH IN SHAPE OPTIMIZATION: EXISTENCE AND REGULARITY RESULTS

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Abstract. In this paper we consider a model shape optimization problem. The state variable solves an elliptic equation on a star-shaped domain where the radius is given via a control function. First we reformulate the problem on a fixed reference domain, where we put a focus on the regularity which is needed to ensure the existence of an optimal solution. Second, we introduce the Lagrangian and use it to show that the optimal solution possesses a higher regularity, which allows for the explicit computation of the derivative of the reduced cost functional as a boundary integral. We finish the paper with some second order optimality conditions.

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Introduction

In this paper we consider the following shape optimization problem governed by a linear elliptic equation:

$$\min \tilde{J}(q,u) = \frac{1}{2}\left\|u - u_d^q\right\|^2_{\mathrm{L}^2(\Omega_q)} + \frac{\alpha}{2}\left\|q\right\|^2_{\mathrm{H}^2((0,2\pi))},$$

subject to

$$\begin{cases} -\Delta u + u = f^q & \text{in } \Omega_q, \\ u = 0 & \text{on } \Gamma_q = \partial\Omega_q, \end{cases}$$

where the domain Ω_q is star-shaped with respect to the origin with radius given by the control q, see Figure 1. The data functions u_d^q and f^q are restrictions of functions defined on a sufficiently large (holding-all) domain $\hat{\Omega}$. The problem is analyzed by using a transformation T_q onto a reference domain Ω_0. The precise formulation including a functional analytic setting is presented in Section 1.

Similar shape optimization problems, where the unknown part of the boundary is parametrized as the graph of a function, are considered in various publications, see e.g., [17, 18, 27, 35]. The problem formulation in these publications involves a bound on an appropriate norm of q. Our formulation utilizes a Tikhonov-type term $\|q\|^2_{\mathrm{H}^2((0,2\pi))}$ instead. In [26] the authors consider a similar approach with a simpler domain, where the transformation T_q is given explicitly. Generally speaking, our approach leads to a problem on a fixed domain where the coefficients of the differential operator are variable. In a more abstract setting, such types of problems

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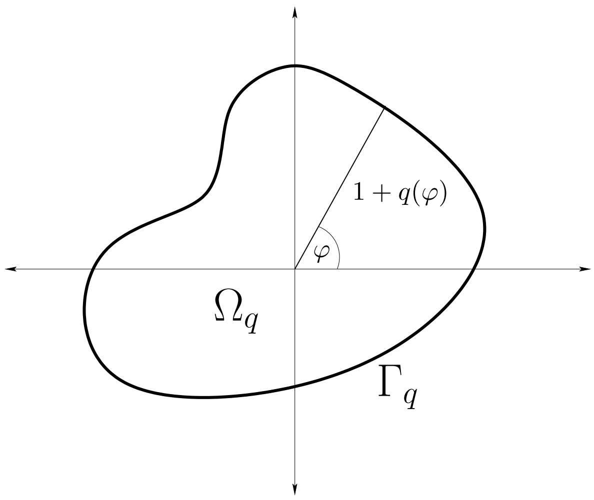

FIGURE 1. The domain Ω_q

have already been considered in [8]. Concerning the existence of optimal shapes in a general setting, we would like to refer to [6, 19].

The main contribution of this paper is the implementation of the standard control theoretic approach for optimization with partial differential equations as presented in [37] and the references cited therein. In the context of shape optimization, calculus is often carried out formally, the needed regularity of the domain and the involved functions is often left unclear or has to be kind of C^k, whereas within the theory of optimal control one mainly has a look at regularity results with respect to Sobolev Spaces. Within this paper we state the exact requirements regarding the Sobolev regularity that ensure that the transformation actually exists, is bijective and that the derivative of the reduced cost functional can be computed via a boundary integral. Our approach also aims at providing the theoretical background for a numerical implementation and related error estimates. For this very reason, we are using a transformation approach, which avoids remeshing, is therefore easier to implement and allows for the comparison of states corresponding to different controls. Choosing the H^2-norm for regularization is due to computational aspects, our approach can also be carried out using the weaker $\mathrm{H}^{3/2+\varepsilon}$-norm instead. We would also like to mention that our approach can also be carried out in three dimensions. In that case one has to use the $\mathrm{H}^{2+\varepsilon}$-norm for regularization in order to ensure that the domain Ω_q is Lipschitz.

In papers which follow a similar approach, cf. [5, 13, 21, 22], the existence of such a transformation with the desired regularity is very often just assumed. Within the setting of the Level set method, as considered in [1, 20] one defines the domain Ω_q as the zero level set of a function ϕ, which evolves in time according to a descent direction of the cost functional. Again, the needed regularity is often just assumed to hold.

The paper is organized as follows: In the next section we discuss a precise formulation of the shape optimization problem under consideration, reformulate the problem using a transformation to a reference domain Ω_0 and show the existence of at least one globally optimal solution applying standard techniques. In Section 2 we first show the differentiability of the control-to-state operator and the reduced cost functional. In order to introduce the Lagrangian, we first present the concept of the very weak formulation. Using the first-order optimality conditions we show higher regularity of the optimal control $\overline{q}$, i.e. $\overline{q} \in \mathrm{H}^{9/2}((0, 2\pi))$ and the corresponding state, which allows for the definition of the derivative as a boundary integral. Similar ideas have already been used in [7, 29, 30]. Due to the fact that the considered optimization problem is not convex in general, we also deal with second order optimality conditions, where we adapt the technique from [10].

Throughout the paper, Id shall denote the identity function, whereas I shall denote the identity matrix. With c and c_i we will denote generic constants which are — if not stated otherwise — independent of the other variables and have different values on different appearances. With ε we will denote a positive real number which can be made arbitrarily small. For $1 \le p \le \infty$, $k, n \in \mathbb{N}$ and $\Omega \subset \mathbb{R}^n$ let $\mathrm{L}^p(\Omega)$ and $\mathrm{W}^{k,p}(\Omega)$ denote the usual Lebesgue spaces with norm $\|\cdot\|_{\mathrm{W}^{k,p}(\Omega)}$ and seminorm $|\cdot|_{\mathrm{W}^{k,p}(\Omega)}$. It is well known that on $\mathrm{W}_0^{k,p}(\Omega)$, the set of all functions in $\mathrm{W}^{k,p}(\Omega)$ whose derivatives up to order $k-1$ vanish on the boundary in the trace sense, $\|\cdot\|_{\mathrm{W}_0^{k,p}(\Omega)} = |\cdot|_{\mathrm{W}^{k,p}(\Omega)}$ is equivalent to $\|\cdot\|_{\mathrm{W}^{k,p}(\Omega)}$. Furthermore, we set $\mathrm{H}^k(\Omega) = \mathrm{W}^{k,2}(\Omega)$. If $s \notin \mathbb{N}$, $s = k + \sigma$ with $k = \lfloor s \rfloor \in \mathbb{N}_0$, $\sigma \in (0,1)$ and $p \in (1,\infty)$, let $\mathrm{W}^{s,p}(\Omega)$ be the space of all functions $u \in \mathrm{W}^{k,p}(\Omega)$ with

$$\|u\|^p_{\mathrm{W}^{s,p}(\Omega)} = \|u\|^p_{\mathrm{W}^{k,p}(\Omega)} + |u|^p_{\mathrm{W}^{s,p}(\Omega)} < \infty,$$

where

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

If V is a Banach space, its dual will be denoted with V'. For any Hilbert space X, $(\cdot,\cdot)_X$ shall denote the corresponding scalar product. As in most cases we will be dealing with the Hilbert space L^2, let $(\cdot,\cdot)_\Omega$ denote the L^2-scalar product over the domain Ω, whereas $\langle\cdot,\cdot\rangle_\Gamma$ shall denote the L^2-scalar product over the boundary Γ. If the domain is clear, we skip the subindices. For $k \in \mathbb{N}_0$ and $\alpha \in (0,1]$, let $\mathrm{C}^{k,\alpha}(\Omega)$ be the set of all k-times continuously differentiable functions whose derivatives of order k are Hölder continuous with exponent α.

1. Optimization problem

1.1. Problem formulation

In this section we first describe the shape optimization problem under consideration. The control variable q is an element of the control space $Q = \mathrm{H}^2_{\mathrm{per}}(I)$ with $I = (0, 2\pi)$ and

$$\mathrm{H}^2_{\mathrm{per}}(I) = \overline{\mathrm{C}^\infty_{\mathrm{per}}(I)}^{\|\cdot\|_{\mathrm{H}^2(I)}}, \tag{1}$$

equipped with the standard H^2-norm, where

$$\mathrm{C}^\infty_{\mathrm{per}}(I) = \left\{ v \in \mathrm{C}^\infty(I) |\ v^{(n)}(0) = v^{(n)}(2\pi) \quad \forall n \in \mathbb{N}_0 \right\}.$$

The control q characterizes the domain Ω_q through

$$\Omega_q = \left\{ (x,y) \in \mathbb{R}^2 |\ r < 1 + q(\varphi),\ r = \sqrt{x^2+y^2},\ \varphi = \arg(x+iy) \right\}.$$

To exclude a possible degeneracy of the domain Ω_q, we fix $\overline{\varepsilon} > 0$ and define the set

$$\overline{Q}^{\mathrm{ad}} = \left\{ q \in Q |\ q(\varphi) \ge -1 + \overline{\varepsilon} \text{ for all } \varphi \in I \right\}. \tag{2}$$

Because of $\mathrm{H}^2(I) \hookrightarrow \mathrm{C}^{1,1/2}(\overline{I})$, (2) is well-defined. For each $q \in \overline{Q}^{\mathrm{ad}}$ the domain Ω_q is a Lipschitz domain, which allows for the definition of the state variable $u \in \mathrm{H}^1_0(\Omega_q)$ being the weak solution of the state equation

$$\begin{cases} -\Delta u + u = f^q & \text{in } \Omega_q, \\ \qquad\quad u = 0 & \text{on } \Gamma_q = \partial\Omega_q. \end{cases} \tag{3}$$

The shape optimization problem is then given as:

$$\text{Minimize } \tilde{J}(q,u) = \frac{1}{2}\|u - u_d^q\|^2_{\mathrm{L}^2(\Omega_q)} + \frac{\alpha}{2}\|q\|^2_{\mathrm{H}^2(I)}, \quad q \in \overline{Q}^{\mathrm{ad}}, u \in \mathrm{H}^1_0(\Omega_q), \tag{4}$$

subject to (3), where $\alpha > 0$ is fixed.

We define the solution operator $\tilde{S}$, which assigns to each $q \in \overline{Q}^{\mathrm{ad}}$ the unique solution $\tilde{S}(q) = \tilde{u}(q)$ of (3). This allows to introduce the reduced cost functional $j\colon \overline{Q}^{\mathrm{ad}} \to \mathbb{R}$ by

$$j(q) = \tilde{J}(q, \tilde{S}(q)).$$

In order to prove the existence of an optimal solution to (4), we need to bound $\overline{Q}^{\mathrm{ad}}$ in $\mathrm{H}^2(I)$.

Lemma 1.1. *There exists $\tilde{C} = \tilde{C}(\alpha) > 0$ such that the search for a solution to* (4) *can be restricted to the set*

$$Q^{\mathrm{ad}} = \left\{ q \in \overline{Q}^{\mathrm{ad}} \,\middle|\, \|q\|_{\mathrm{H}^2(I)} \le \tilde{C} \right\}. \tag{5}$$

Furthermore it holds that $\lim_{\alpha\to\infty} \tilde{C}(\alpha) = 0$.

Proof. We set $q_0 = 0 \in \overline{Q}^{\mathrm{ad}}$. A necessary condition for $q \in \overline{Q}^{\mathrm{ad}}$ to be a solution to (4) is

$$j(q) \le j(q_0),$$

which reads as

$$\frac{1}{2}\left\|\tilde{S}(q) - u_d^q\right\|^2_{\mathrm{L}^2(\Omega_q)} + \frac{\alpha}{2}\|q\|^2_{\mathrm{H}^2(I)} \le j(q_0),$$

or equivalently

$$\|q\|^2_{\mathrm{H}^2(I)} \le \frac{2}{\alpha}\left(j(q_0) - \frac{1}{2}\left\|\tilde{S}(q) - u_d^q\right\|^2_{\mathrm{L}^2(\Omega_q)}\right) \le \frac{2}{\alpha} j(q_0).$$

Setting $\tilde{C}(\alpha) = \sqrt{\frac{2}{\alpha} j(q_0)}$ finishes the proof. □

Due to the boundedness of Q^{ad} in $\mathrm{C}^1(\bar{I})$ it follows that there exists a bounded so-called holding-all domain $\hat{\Omega}$, such that $\overline{\Omega_q} \subset \hat{\Omega}$ for all $q \in Q^{\mathrm{ad}}$. Throughout we assume for the data

$$u_d^q = u_d|_{\Omega_q}, \; f^q = f|_{\Omega_q}, \text{ with } u_d, f \in \mathrm{C}^{2,1}(\hat{\Omega}), \tag{6}$$

we will therefore just write f and u_d instead of f^q and u_d^q.

The rest of this paper is mainly devoted to show the following theorems concerning the existence of an optimal solution and the improved regularity of every optimal solution. The first theorem is proven in Subsection 1.3, the second theorem is proven in Subsection 2.4.

Theorem 1.2. *If the constant $\tilde{C}$ from* (5) *is chosen sufficiently small in the sense of Assumption 1.16, then the problem* (4) *has a global solution.*

Theorem 1.3. *Let $\overline{q}$ be an optimal solution to problem* (4) *which lies in the interior of Q^{ad}. Then it holds that $\overline{q} \in \mathrm{H}^{9/2}(I)$.*

1.2. **Transformation of the problem**

The aim of the following subsection is to reformulate the original problem (4) on a fixed reference domain Ω_0. This method is called the method of mapping, a short overview can be found in [12, 36]. We define Ω_0 to be the unit circle and then compute a transformation T_q such that the domain Ω_q is just the image of Ω_0 under that transformation, $\Omega_q = T_q(\Omega_0)$. All the results remain true if Ω_0 is replaced by any other sufficiently smooth domain sufficiently close to Ω_q in the sense of Assumption 1.16. In order to compute T_q it is often necessary to solve an additional partial differential equation like the equations of linear elasticity or the Laplace equation. Within this paper we will focus on the Laplace equation. Our results remain true as long as Theorem 1.5 holds for the chosen equation.

If one worked locally near the optimal shape instead of transforming the whole domain, then one would have to remesh the working domain every step, which is costly. As already mentioned, we bypass this remeshing at the cost of two additional Laplace equations. The reason why we choose this approach is the fact that it allows for comparing states corresponding to different shapes, which is important in the context of error estimation. Furthermore, from a practical point of view, adding some Laplace equations to the numerical solver is often less complicated than including a remeshing step.

Let $F = (F_1, F_2)^T$ be the weak solution of the following boundary value problem.

$$\begin{cases} -\Delta F = 0 & \text{in } \Omega_0, \\ \quad F = q\,n & \text{on } \Gamma_0, \end{cases} \tag{7}$$

where n shall denote the outer unit normal to Γ_0 and the Laplacian shall act on each component separately. If $F = F(q)$ solves (7) for a given $q \in Q$, then define $T_q = T_{F(q)} = \mathrm{Id} + F(q)$. This transformation will now be used to reformulate the original problem (4) on Ω_0. In order to do so, we will need regularity results for elliptic partial differential equations of various types. Here we state them all at once.

Theorem 1.4. *Let $\Omega \subset \mathbb{R}^2$ be bounded with Lipschitz boundary Γ, $f \in \mathrm{H}^{-1}(\Omega)$, and let the matrix A be symmetric and uniformly elliptic with coefficients $a_{i,j} \in \mathrm{L}^\infty(\Omega)$. Furthermore, let $u \in \mathrm{H}^1_0(\Omega)$ be the weak solution of*

$$\begin{cases} -\operatorname{div}(A \cdot \nabla u) = f & \text{in } \Omega, \\ \qquad u = 0 & \text{on } \Gamma. \end{cases}$$

(1) If $1/2 \geq t > s > 0$ and the coefficients of A belong to $\mathrm{C}^{0,t}(\overline{\Omega})$, then for all $f \in \mathrm{H}^{-1+s}(\Omega)$ it holds $u \in \mathrm{H}^{1+s}_0(\Omega)$ and there exists $c_s > 0$ with $\|u\|_{\mathrm{H}^{1+s}(\Omega)} \leq c_s \|f\|_{\mathrm{H}^{-1+s}(\Omega)}$.

(2) If the coefficients of A are Lipschitz and $f \in \mathrm{H}^{-1/2+\varepsilon}(\Omega)$, then $u \in \mathrm{H}^{3/2}(\Omega)$. In addition, if $f \in \mathrm{L}^2(\Omega)$, then there exists $c > 0$ with $\|u\|_{\mathrm{H}^{3/2}(\Omega)} \leq c \|f\|_{\mathrm{L}^2(\Omega)}$.

(3) If Ω is convex, the coefficients of A are Lipschitz and $f \in \mathrm{L}^2(\Omega)$, then $u \in \mathrm{H}^2(\Omega)$ and there exists $c > 0$, depending only on the diameter of Ω, with $\|u\|_{\mathrm{H}^2(\Omega)} \leq c \|f\|_{\mathrm{L}^2(\Omega)}$.

(4) If Ω is sufficiently smooth, the coefficients of A are Lipschitz and $f \in \mathrm{L}^p(\Omega)$ for a $p < \infty$ then it holds that $u \in \mathrm{W}^{2,p}(\Omega)$ and there exists $c_p > 0$, depending on p and the Lipschitz-constant of A, such that $\|u\|_{\mathrm{W}^{2,p}(\Omega)} \leq c_p \|f\|_{\mathrm{L}^p(\Omega)}$.

Proof. Part (1) can be found in [33], (2) can be found in [23, 24, 34], part (3) is proven in [14, 25] and the proof of the last part can be found in [14]. □

The following regularity result can be found in [16], Theorem 9.1.20.

Theorem 1.5. *Let $\Omega \subset \mathbb{R}^2$ be a bounded and open domain with C^∞-boundary Γ. Assume $s \geq 0$, $s \neq 1/2$ and $g \in \mathrm{H}^{s+1/2}(\Gamma)$. Then the weak solution u of*

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ \quad u = g & \text{on } \Gamma, \end{cases}$$

belongs to $\mathrm{H}^{s+1}(\Omega)$*, and there holds the estimate* $\|u\|_{\mathrm{H}^{s+1}(\Omega)} \le c_s \|g\|_{\mathrm{H}^{s+1/2}(\Gamma)}$.

Furthermore, we will also need the Trace Theorem several times. The following version can be found in [14], Theorem 1.5.1.2.

Theorem 1.6. *Let* Ω *be a bounded and open subset of* $\mathbb{R}^2$ *with a* $\mathrm{C}^{k,1}$ *boundary* Γ *for* $k \ge 0$. *Let* $1 < p < \infty$ *and assume that* $s - 1/p$ *is not an integer,* $s \le k+1$, $s - 1/p = l + \sigma$, $0 < \sigma < 1$ *and* l *is a nonnegativ integer. Then the mapping*

$$u \mapsto \left\{ u|_\Gamma, \left.\frac{\partial u}{\partial n}\right|_\Gamma, \dots, \left.\frac{\partial^l u}{\partial n^l}\right|_\Gamma \right\},$$

which is defined for $u \in \mathrm{C}^{k,1}(\overline{\Omega})$*, has a unique continuous extension as an operator from*

$$\mathrm{W}^{s,p}(\Omega) \text{ onto } \prod_{j=0}^{l} \mathrm{W}^{s-j-1/p,p}(\Gamma).$$

This operator has a continuous right inverse which does not depend on p.

Corollary 1.7. *For* $q \in Q^{\mathrm{ad}}$*, the solution* $u \in \mathrm{H}_0^1(\Omega_q)$ *defined via* (3) *possesses the higher regularity* $u \in \mathrm{H}^{3/2}(\Omega_q)$.

Proof. This corollary follows from Theorem 1.4, part (2). □

Corollary 1.8. *For* $q \in Q$ *it holds that* $F = F(q)$ *as the weak solution to* (7) *possesses the regularity* $F \in \left(\mathrm{H}^{5/2}(\Omega_0)\right)^2 \hookrightarrow \left(\mathrm{C}^{1,1/2}(\overline{\Omega_0})\right)^2$ *and* $\|F\|_{\left(\mathrm{H}^{s+1/2}(\Omega_0)\right)^2} \le c_s \|q\|_{\mathrm{H}^s(I)}$ *for* $s > 1$.

Proof. As the outer unit normal n of the unit circle is uniformly bounded in $\left(\mathrm{C}^2(\Gamma_0)\right)^2$, we get

$$\|q\, n\|_{(\mathrm{H}^2(\Gamma_0))^2} \le c \|n\|_{(\mathrm{C}^2(\Gamma_0))^2} \|q\|_{\mathrm{H}^2(I)} \le c \|q\|_{\mathrm{H}^2(I)},$$

cf. [14], Theorem 1.4.1.1, and the result follows with Theorem 1.5. □

Remark 1.9. For $q \in Q$, $F(q)$ shall always denote the unique solution to (7) for that given q.

Remark 1.10. With a slight abuse of notation we will just write $F \in \mathrm{W}^{k,p}(\Omega)$ instead of $F \in \left(\mathrm{W}^{k,p}(\Omega)\right)^2$, for both components of F possess the same regularity. This kind of notation will be applied throughout to vector-valued functions.

Let

$$\mathcal{F} = \left\{ F \in \mathrm{H}^{5/2}(\Omega_0) \,\middle|\, \exists q \in Q \text{ such that } F = F(q) \text{ solves (7)} \right\}, \tag{8}$$

$$\mathcal{F}^{\mathrm{ad}} = \left\{ F \in \mathrm{H}^{5/2}(\Omega_0) \,\middle|\, \exists q \in Q^{\mathrm{ad}} \text{ such that } F = F(q) \text{ solves (7)} \right\}, \tag{9}$$

where $\mathcal{F}^{\mathrm{ad}}$ is a bounded set in $\mathrm{H}^{5/2}(\Omega_0)$ due to Corollary 1.8 and (5). Note that $\mathcal{F}^{\mathrm{ad}}$ need not be closed in $\mathrm{H}^{5/2}(\Omega_0)$ for the trace is not surjective as an operator from $\mathrm{H}^{k+1/2}(\Omega_0)$ to $\mathrm{H}^k(\Gamma_0)$ for $k \in \mathbb{N}_0$ as follows from Theorem 1.6.

Before we can proceed, we need some results concerning the regularity of the product of functions. The following lemma can be found in [14], Theorem 1.4.4.2 and the comment afterward.

Lemma 1.11. *Let* $\Omega \subset \mathbb{R}^n$ *be bounded, open, with sufficiently regular boundary* Γ*, let* $s_1, s_2 \ge s \ge 0$ *and* $p_1, p_2, p \in (1, \infty)$ *such that either*

$$s_1 + s_2 - s \ge n\left(\frac{1}{p_1} + \frac{1}{p_2} - \frac{1}{p}\right) \ge 0, \qquad s_j - s > n\left(\frac{1}{p_j} - \frac{1}{p}\right), \qquad j = 1, 2,$$

or

$$s_1 + s_2 - s > n\left(\frac{1}{p_1} + \frac{1}{p_2} - \frac{1}{p}\right) \geq 0, \qquad s_j - s \geq n\left(\frac{1}{p_j} - \frac{1}{p}\right), \qquad j = 1, 2.$$

Then $u, v \mapsto uv$ is a continuous bilinear form from $\mathrm{W}^{s_1,p_1}(\Omega) \times \mathrm{W}^{s_2,p_2}(\Omega)$ into $\mathrm{W}^{s,p}(\Omega)$.

In what follows we will also have to work with the inverse transformation T_F^{-1}. The following two lemmas ensure that the multiplicative inverse of a functions also possess a desired regularity.

Lemma 1.12. *Let $\Omega \subset \mathbb{R}^n$ be open an bounded. Let $v \in \mathrm{H}^1(\Omega)$ and $k \in \mathbb{N}$. If there exists $c_0 > 0$ such that $v(x) \geq c_0$ for almost every $x \in \Omega$, then $v^{-k} \in \mathrm{H}^1(\Omega)$.*

Proof. We only have to show that

$$\nabla\left(v^{-k}\right) = -kv^{-k-1}\nabla v \in \mathrm{L}^2(\Omega),$$

which follows from the generalized Hölder inequality and

$$v^{-k-1} \in \mathrm{L}^\infty(\Omega),\ \nabla v \in \mathrm{L}^2(\Omega).$$

□

Lemma 1.13. *Let $\Omega \subset \mathbb{R}^n$, $n \leq 2$, be open an bounded. Let $s \geq 0$ and $v \in \mathrm{H}^s(\Omega)$. If there exists $c_0 > 0$, such that $v(x) \geq c_0$ for almost every $x \in \Omega$, then $v^{-1} \in \mathrm{H}^s(\Omega)$.*

Proof. Let $s = k + \sigma$, where $k \in \mathbb{N}_0$ and $\sigma \in [0, 1)$. First, consider the case $k = 0$. For $\sigma = 0$ the result is clear. If $\sigma \in (0, 1)$, then

$$\begin{aligned}
\left|v^{-1}\right|^2_{\mathrm{H}^s(\Omega)} &= \int_\Omega \int_\Omega \frac{\left|v(x)^{-1} - v(y)^{-1}\right|^2}{|x-y|^{n+2\sigma}} \,\mathrm{d}x\,\mathrm{d}y \\
&= \int_\Omega \int_\Omega \left|\frac{1}{v(x)v(y)}\right|^2 \frac{|v(x) - v(y)|^2}{|x-y|^{n+2\sigma}} \,\mathrm{d}x\,\mathrm{d}y \\
&\leq \frac{1}{a^4}\, |v|^2_{\mathrm{H}^s(\Omega)}\,.
\end{aligned}$$

Now consider the case $s = 1+\sigma$, $v \in \mathrm{H}^{1+\sigma}(\Omega)$. Due to Lemma 1.12 it remains to consider the case $\sigma \in (0, 1)$. As $\nabla v \in \mathrm{H}^\sigma(\Omega)$ and $v^{-3} \in \mathrm{H}^1(\Omega)$ due to Lemma 1.12, it follows from Lemma 1.11 that $-2v^{-3}\nabla v = \nabla\left(v^{-2}\right) \in \mathrm{H}^\varepsilon(\Omega)$ for $\varepsilon < \sigma$. Hence, $v^{-2} \in \mathrm{H}^{1+\varepsilon}(\Omega)$, and again with Lemma 1.11 it follows that $-v^{-2}\nabla v = \nabla\left(v^{-1}\right) \in \mathrm{H}^\sigma(\Omega)$, and $v^{-1} \in \mathrm{H}^{1+\sigma}(\Omega)$.

The next case is $s = 2$. Due to Lemma 1.12 we only have to show that

$$\nabla^2\left(v^{-1}\right) = 2v^{-3}\nabla v \cdot \nabla v^T - v^{-2}\nabla^2 v \in \mathrm{L}^2(\Omega),$$

which follows from $v^{-2}, v^{-3} \in \mathrm{L}^\infty(\Omega)$, $\nabla v \in \mathrm{H}^1(\Omega) \hookrightarrow \mathrm{L}^4(\Omega)$, and $\nabla^2 v \in \mathrm{L}^2(\Omega)$.

We finish this proof with induction. Assume that the statement has been shown for all $s < k$ for some $k \in \mathbb{N}$ with $k \geq 2$. Let $s = k + \sigma$, $\sigma \in [0, 1)$ and $v \in \mathrm{H}^{k+\sigma}(\Omega)$. We can further assume that $\sigma > 0$ if $k = 2$. As $v^{-1} \in \mathrm{H}^{(k-1)+\sigma}(\Omega)$ by induction hypothesis, we get $v^{-2} \in \mathrm{H}^{(k-1)+\sigma}(\Omega)$ with Lemma 1.11. Furthermore, $\nabla v \in \mathrm{H}^{(k-1)+\sigma}(\Omega)$, and again with Lemma 1.11 we end up with $-v^{-2}\nabla v = \nabla\left(v^{-1}\right) \in \mathrm{H}^{(k-1)+\sigma}(\Omega)$, which leads to $v^{-1} \in \mathrm{H}^{k+\sigma}(\Omega)$. □

With those results at hand, we can now proceed in transforming the optimization problem. For $F \in \mathcal{F}^{\mathrm{ad}}$, $\delta F, \tau F \in \mathcal{F}$, the following functions derived from the transformation

$$T_F = \mathrm{Id} + F \tag{10}$$

will be used in the sequel. Some regularity as well as stability results concerning these functions can be found in the Annex, Section 3.

$$\mathrm{D}T_F(x,y) = \mathrm{I} + \mathrm{D}F(x,y) = \begin{pmatrix} 1+\partial_x F_1(x,y) & \partial_y F_1(x,y) \\ \partial_x F_2(x,y) & 1+\partial_y F_2(x,y) \end{pmatrix}, \tag{11}$$

$$\gamma_F(x,y) = \det\left(\mathrm{D}T_F(x,y)\right), \tag{12}$$

$$\gamma'_{F,\delta F}(x,y) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\gamma_{F+t\cdot\delta F}(x,y)\right|_{t=0}, \tag{13}$$

$$\gamma''_{F,\delta F,\tau F}(x,y) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\gamma'_{F+t\cdot\tau F,\delta F}(x,y)\right|_{t=0}, \tag{14}$$

$$A_F(x,y) = \left(\gamma_F \mathrm{D}T_F^{-1}\cdot \mathrm{D}T_F^{-T}\right)(x,y), \tag{15}$$

where $\mathrm{D}T_F^{-1} = (\mathrm{D}T_F)^{-1}$,

$$A'_{F,\delta F}(x,y) = \left.\frac{\mathrm{d}}{\mathrm{d}t}A_{F+t\cdot\delta F}(x,y)\right|_{t=0}, \tag{16}$$

$$A''_{F,\delta F,\tau F}(x,y) = \left.\frac{\mathrm{d}}{\mathrm{d}t}A'_{F+t\cdot\tau F,\delta F}(x,y)\right|_{t=0}. \tag{17}$$

Lemma 1.14. *There exist $c_0 > 0$, $0 < c_1 < c_2$ and $0 < c_3 < c_4$ such that for $\|q\|_{\mathrm{H}^2(I)} < c_0$ it holds that $\gamma_{F(q)} \in [c_1, c_2]$ and the two Eigenvalues of $A_{F(q)}$ are elements of the interval $[c_3, c_4]$. If $c_0 \to 0$, then $c_1, c_2, c_3, c_4 \to 1$.*

Proof. This lemma follows from Lemma 3.2 and the fact that the Eigenvalues of a matrix continuously depend on its entries. □

As we use the transformation $T_{F(q)}$ to map Ω_0 onto Ω_q, it is desirable that this transformation is one-to-one.

Lemma 1.15. *For $\|q\|_{\mathrm{H}^2(I)}$ sufficiently small, the transformation $T_{F(q)}\colon \Omega_0 \to \Omega_q$ is bijective.*

Proof. As $\Gamma_q = T_{F(q)}(\Gamma_0)$ by definition of $F(q)$, surjectivity follows by continuity and injectivity follows from Lemma 3.2. □

Assumption 1.16. We assume that the constant $\tilde{C}$ in (5) is chosen sufficiently small such that Lemma 1.14 and Lemma 1.15 hold for all $q \in Q^{\mathrm{ad}}$.

Remark 1.17. With Lemma 1.1 it follows that Assumption 1.16 holds if α is sufficiently large. Furthermore, within practical applications like computing the optimal shape of an airfoil, a good approximation of the optimal shape is very often already known a priori.

For the ease of notation, for $F \in \mathcal{F}^{\mathrm{ad}}$, $u, z \in \mathrm{H}^1(\Omega_0)$ we will make use of the following bilinear forms

$$a(F)(u,z) = \int_{\Omega_0} \nabla u^T \cdot A_F \cdot \nabla z + uz\gamma_F \,\mathrm{d}x, \tag{18}$$

$$l(F)(z) = \int_{\Omega_0} (f\circ T_F) z\gamma_F \,\mathrm{d}x. \tag{19}$$

Lemma 1.18. *Let $F \in \mathcal{F}^{\mathrm{ad}}$. Then there exists a unique $u \in \mathrm{H}^1_0(\Omega_0)$ such that*

$$a(F)(u,z) = l(F)(z) \qquad \forall z \in \mathrm{H}^1_0(\Omega_0), \tag{20}$$

and $\|u\|_{\mathrm{H}^1_0(\Omega_0)} \le c\,\|f\|_{\mathrm{L}^2(\Omega_q)}$.

Proof. As the bilinear form $a(F)(\cdot,\cdot)$ is continuous and coercive due to Lemma 3.8, this lemma is a direct consequence of the Theorem of Lax-Milgram. □

For more stability results concerning the forms (18) and (19) we refer to the Annex, Section 3.

Remark 1.19. For $q_1, q_2 \in Q^{\text{ad}}$ and $F_3 \in \mathcal{F}^{\text{ad}}$, $u(q_1)$, $u(F_2)$ and $u(F_3)$ shall denote the unique solutions to (20) for $F = F(q_1)$, $F = F_2 = F(q_2)$ and $F = F_3$, respectively.

Lemma 1.18 motivates the introduction of another solution operator S which assigns to each control $q \in Q^{\text{ad}}$ the "transported" solution, i.e. let $S(q) = u(q) \in \mathrm{H}_0^1(\Omega_0)$ be the solution of (20) for $F = F(q)$.

Lemma 1.20. *Let $q \in Q^{\text{ad}}$, $F = F(q) \in \mathcal{F}^{\text{ad}}$ and $v \in \mathrm{L}^2(\Omega_q)$. Then it holds that $v \in \mathrm{H}^1(\Omega_q)$ if and only if $v \circ T_F \in \mathrm{H}^1(\Omega_0)$. Furthermore, the two norms $\|\cdot\|_{\mathrm{H}^1(\Omega_q)}$ and $\|\cdot \circ T_F\|_{\mathrm{H}^1(\Omega_0)}$ are equivalent.*

Proof. Let $v \in \mathrm{H}^1(\Omega_q)$. We have

$$
\begin{aligned}
\|v\|^2_{\mathrm{H}^1(\Omega_q)} &= \int_{\Omega_q} v^2 + |\nabla v|^2 \,\mathrm{d}x = \int_{\Omega_0} (v \circ T_F)^2 \gamma_F + |\nabla v \circ T_F|^2 \gamma_F \,\mathrm{d}x \\
&\le c \int_{\Omega_0} (v \circ T_F)^2 + \left|\mathrm{D}T_F^T \cdot \nabla v \circ T_F\right|^2 \,\mathrm{d}x \\
&= c \,\|v \circ T_F\|^2_{\mathrm{H}^1(\Omega_0)} \\
&\le c \int_{\Omega_0} (v \circ T_F)^2 + |\nabla v \circ T_F|^2 \,\mathrm{d}x \le c \int_{\Omega_0} (v \circ T_F)^2 \gamma_F + |\nabla v \circ T_F|^2 \gamma_F \,\mathrm{d}x \\
&= c \int_{\Omega_q} v^2 + |\nabla v|^2 \,\mathrm{d}x = c \,\|v\|^2_{\mathrm{H}^1(\Omega_q)} ,
\end{aligned}
$$

where we also used Assumption 1.16. □

Lemma 1.21. *Let $F \in \mathcal{F}^{\text{ad}}$, $u^q \in \mathrm{H}_0^1(\Omega_q)$, $u = u^q \circ T_F \in \mathrm{H}_0^1(\Omega_0)$. Then the following two variational formulations are equivalent*

$$
\int_{\Omega_q} \left((\nabla u^q)^T \cdot \nabla z^q + u^q z^q\right) \,\mathrm{d}x = \int_{\Omega_q} f z \,\mathrm{d}x \qquad \forall z^q \in \mathrm{H}_0^1(\Omega_q), \tag{21}
$$

$$
\int_{\Omega_0} \left(\nabla u^T \cdot A_F \cdot \nabla z + u z \gamma_F\right) \,\mathrm{d}x = \int_{\Omega_0} (f \circ T_F)\, z \gamma_F \,\mathrm{d}x \qquad \forall z \in \mathrm{H}_0^1(\Omega_0). \tag{22}
$$

Proof. In order to proof this lemma one has to use integration by substitution and Lemma 1.20. □

We are now able to reformulate problem (4) on the reference domain.

$$
\min J(q, u, F) = \frac{1}{2} \int_{\Omega_0} (u - u_d \circ T_F)^2 \gamma_F \,\mathrm{d}x + \frac{\alpha}{2} \|q\|^2_{\mathrm{H}^2(I)} , \tag{23}
$$

subject to

$$
\begin{cases} -\Delta F = 0 & \text{in } \Omega_0, \\ \quad F = q\, n & \text{on } \Gamma_0, \end{cases} \qquad \begin{cases} -\operatorname{div}(A_F \cdot \nabla u) + u \gamma_F = f \circ T_F \gamma_F & \text{in } \Omega_0, \\ \quad u = 0 & \text{on } \Gamma_0. \end{cases}
$$

Theorem 1.22. *The two problems (4) and (23) are equivalent.*

Proof. Let $q \in Q^{\text{ad}}$, $u^q = u(q) \circ T_{F(q)} \in \mathrm{H}_0^1(\Omega_q)$. This theorem now follows from the fact that $\tilde{J}(q, u^q) = J(q, u(q), F(q))$ and the fact that the state equations on Ω_q and Ω_0, (3) and (20), respectively, are uniquely solvable. □

1.3. **Existence of an optimal solution**

Within this subsection we are going to proof Theorem 1.2. The following proof relies on Assumption 1.16 which can be omitted as mentioned in Remark 1.25. Due to Theorem 1.22 it is sufficient to show that (23) has a global solution.

Proof. Let $j(q) = J(q, u(q), F(q)) \geq 0$ be the reduced cost functional. There exists a minimizing sequence $(q_n, u_n = u(q_n), F_n = F(q_n))_{n\in\mathbb{N}}$ with

$$j = \inf_{q\in Q^{\mathrm{ad}}} j(q) = \lim_{n\to\infty} j(q_n) = \lim_{n\to\infty} J(q_n, u_n, F_n).$$

As Q^{ad} is a convex, closed and bounded subset of the Hilbert space $\mathrm{H}^2(I)$ there exists $\overline{q} \in Q^{\mathrm{ad}}$ such that, up to extracting a subsequence, it holds that

$$\begin{aligned} q_n &\rightharpoonup \overline{q} && \text{in } \mathrm{H}^2(I), \\ q_n &\to \overline{q} && \text{in } \mathrm{H}^{2-\varepsilon}(I) && \text{for } n\to\infty, \end{aligned}$$

due to the compact embedding of $\mathrm{H}^2(I)$ into $\mathrm{H}^{2-\varepsilon}(I)$. Let $\overline{F} = F(\overline{q}) \in \mathcal{F}^{\mathrm{ad}}$ and $\overline{u} = u(\overline{F})$. Due to Corollary 1.8 it follows that $F_n \to \overline{F}$ in $\mathrm{H}^{5/2-\varepsilon}(\Omega_0)$. Hence, $u(F_n) \to u(\overline{F}) = \overline{u}$ in $\mathrm{H}^1(\Omega_0)$ by Lemma 3.11. In addition, $\gamma_{F_n} \to \gamma_{\overline{F}}$ and $u_d \circ T_{F_n} \to u_d \circ T_{\overline{F}}$ in $\mathrm{L}^\infty(\Omega_0)$ due to Lemma 3.3, which leads to

$$\lim_{n\to\infty} \left(\int_{\Omega_0} \left(u(F_n) - u_d \circ T_{F_n}\right)^2 \gamma_{F_n} \,\mathrm{d}x \right) = \int_{\Omega_0} \left(u(\overline{F}) - u_d \circ T_{\overline{F}}\right)^2 \gamma_{\overline{F}} \,\mathrm{d}x. \tag{24}$$

As the squared norm is continuous and convex it is lower semicontinuous,

$$\liminf_{n\to\infty} \|q_n\|^2_{\mathrm{H}^2(I)} \geq \|\overline{q}\|^2_{\mathrm{H}^2(I)}, \tag{25}$$

and by adding (24) and (25) we arrive at

$$J(\overline{q}, \overline{u}, \overline{F}) \leq \liminf_{n\to\infty} J(q_n, u_n, F_n) = j, \tag{26}$$

and conclude that $J(\overline{q}, \overline{u}, \overline{F}) = j$. Hence $\left(\overline{q}, \overline{u}, \overline{F}\right)$ is a global solution to (23). □

Corollary 1.23. *Every minimizing sequence $(q_n)_{n\in\mathbb{N}} \subset Q^{\mathrm{ad}}$ contains a subsequence $(q_{n_k})_{k\in\mathbb{N}}$ such that $q_{n_k} \to \overline{q}$ in $\mathrm{H}^2(I)$ for $k\to\infty$, where $\overline{q}$ is an optimal solution to* (23).

Proof. In the proof of Theorem 1.2 we have already shown the existence of such a subsequence with $q_{n_k} \rightharpoonup \overline{q}$ in $\mathrm{H}^2(I)$. As $J(q_{n_k}, u(q_{n_k}), F(q_{n_k})) \to J(\overline{q}, \overline{u}, \overline{F})$ it follows that $\|q_{n_k}\|_{\mathrm{H}^2(I)} \to \|\overline{q}\|_{\mathrm{H}^2(I)}$. It is well-known that within Hilbert spaces weak convergence plus convergence of the norm implies strong convergence, and the result follows. □

Remark 1.24. Although the state equation (20) is linear, the mapping $q \mapsto u(q)$ is highly nonlinear and one cannot expect the reduced cost functional j to be convex. Therefore uniqueness of an optimal solution cannot be shown in general.

Remark 1.25. Although the proof of Theorem 1.2 depends on Assumption 1.16, this assumption can be omitted. In [17], Theorem 2.8, the authors show existence of an optimal solution for a similar shape optimization problem where they just need some sort of compactness of Q^{ad} in Q. As the proof mentioned in the source cited above is more invloved than the one presented here, and as Assumption 1.16 is needed throughout the paper, we decided to include the proof as stated.

2. The optimality system

2.1. Differentiability of the control-to-state mapping and first-order optimality conditions

Within this subsection we investigate the differentiability of the control-to-state mapping $q \mapsto u(q)$. In order to show this we will use the Implicit Function Theorem, the following version can be found in [3], Theorem 2.3.

Theorem 2.1. *Let $B \in \mathrm{C}^k\left(X^{ad} \times Y^{ad}, Z\right)$, $k \geq 1$, where Z is a Banach space and X^{ad}, Y^{ad} are open subsets of Banach spaces X and Y, respectively. Suppose $B(x^*, y^*) = 0$ and that $B'_y(x^*, y^*)$ is continuously invertible. Then there exist neighborhoods Θ of x^* in X and Φ of y^* in Y and a map $g \in \mathrm{C}^k(\Theta, Y)$ such that*

- *$B(x, g(x)) = 0$ for all $x \in \Theta$,*
- *$B(x,y) = 0$, $(x,y) \in \Theta \times \Phi$, implies $y = g(x)$,*
- *$g'(x) = -\left(B_y(x, g(x))\right)^{-1} \circ B_x(x, g(x))$ for $x \in \Theta$.*

Lemma 2.2. *The mapping $Q \ni q \mapsto F(q) \in \mathcal{F}$ is twice continuously Fréchet differentiable.*

Proof. As the mapping $q \mapsto F(q)$ is linear, the result follows with Corollary 1.8. □

Lemma 2.3. *The mapping $\operatorname{int}\left(Q^{\mathrm{ad}}\right) \ni q \mapsto u(q) \in \mathrm{H}^1_0(\Omega_0)$ is twice continuously Fréchet differentiable.*

Proof. We set $X = Q$, $X^{\mathrm{ad}} = \operatorname{int}\left(Q^{\mathrm{ad}}\right)$, $Y = Y^{\mathrm{ad}} = \mathrm{H}^1_0(\Omega_0)$ and $Z = \mathrm{H}^{-1}(\Omega_0)$. Furthermore, let

$$\begin{aligned} &B\colon Q \times \mathrm{H}^1_0(\Omega_0) \to \mathrm{H}^{-1}(\Omega_0),\\ &B(q,u) = a(F(q))(u,\cdot) - l(F(q))(\cdot). \end{aligned}$$

Then B is affine linear in u and twice continuously differentiable with respect to q, as follows from Lemma 3.4, Lemma 2.2 and (6). The result now follows with Theorem 2.1. □

In order to be able to use Lemma 2.3 we make the following assumption.

Assumption 2.4. We assume that the optimal control $\overline{q}$ under consideration is an element of the interior of the admissible set, $\overline{q} \in \operatorname{int}(Q^{\mathrm{ad}})$.

We also recall the definition of the operator S and its derivatives, which follow by a direct calculation.

(1) $u = S(q) \in \mathrm{H}^1_0(\Omega_0)$ is the solution of

$$a(F)(u,z) = l(F)(z) \qquad \forall z \in \mathrm{H}^1_0(\Omega_0), \tag{27}$$

where $F = F(q)$.

(2) $\delta u = S'(q)(\delta q) \in \mathrm{H}^1_0(\Omega_0)$ is the solution of

$$\begin{aligned} a(F)(\delta u, z) = \left(f \circ T_F, z \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) + \left(\left(\nabla f \circ T_F\right)^T \cdot \delta F, z\gamma_F\right) \\ - \left(\nabla u, A'_{F,\delta F} \cdot \nabla z\right) - \left(u, z \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) \qquad \forall z \in \mathrm{H}^1_0(\Omega_0), \end{aligned} \tag{28}$$

where $\delta F = F'(q)(\delta q) = F(\delta q)$.

(3) $\delta\tau u = S''(q)(\delta q, \tau q) \in \mathrm{H}^1_0(\Omega_0)$ is the solution of

$$
\begin{aligned}
a(F)(\delta\tau u, z) = {} & (f \circ T_F, z\,(\mathrm{tr}(\mathrm{D}\delta F)\,\mathrm{tr}(\mathrm{D}\tau F) - \mathrm{tr}(\mathrm{D}\delta F \cdot \mathrm{D}\tau F))) \\
& + \left(\tau F^T \cdot \nabla^2 f \circ T_F \cdot \delta F, z\gamma_F\right) - \left(\nabla u, A''_{F,\delta F,\tau F} \cdot \nabla z\right) \\
& + \left((\nabla f \circ T_F)^T \cdot \delta F, z \,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \tau F\right)\right) \\
& + \left((\nabla f \circ T_F)^T \cdot \tau F, z \,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) \\
& - \left(\nabla \tau u, A'_{F,\delta F} \cdot \nabla z\right) - \left(\nabla \delta u, A'_{F,\tau F} \cdot \nabla z\right) \\
& - \left(\tau u, z \,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) - \left(\delta u, z \,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \tau F\right)\right) \\
& - (uz, \mathrm{tr}(\mathrm{D}\delta F)\,\mathrm{tr}(\mathrm{D}\tau F) - \mathrm{tr}(\mathrm{D}\delta F \cdot \mathrm{D}\tau F)) \qquad \forall z \in \mathrm{H}^1_0(\Omega_0),
\end{aligned}
\tag{29}
$$

where $\tau u = S'(q)(\tau q)$ and $\tau F = F'(q)(\tau q) = F(\tau q)$.

Furthermore we also state the definitions of the reduced cost functional j and its derivatives, which follow by a direct calculation. The fact that j is at least twice continuously differentiable follows from Lemma 2.3.

$$
j(q) = \frac{1}{2}\left(S(q) - u_d \circ T_F, (S(q) - u_d \circ T_F)\,\gamma_F\right) + \frac{\alpha}{2}\,(q, q)_{\mathrm{H}^2(I)}\,, \tag{30}
$$

$$
\begin{aligned}
j'(q)(\delta q) = {} & \frac{1}{2}\left(S(q) - u_d \circ T_F, (S(q) - u_d \circ T_F)\,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) \\
& + \left(S'(q)(\delta q) - (\nabla u_d \circ T_F)^T \cdot \delta F, (S(q) - u_d \circ T_F)\,\gamma_F\right) + \alpha\,(q, \delta q)_{\mathrm{H}^2(I)}\,,
\end{aligned}
\tag{31}
$$

$$
\begin{aligned}
j''(q)(\delta q, \tau q) = {} & \frac{1}{2}\left(S(q) - u_d \circ T_F, (S(q) - u_d \circ T_F)\,(\mathrm{tr}(\mathrm{D}\delta F)\,\mathrm{tr}(\mathrm{D}\tau F) - \mathrm{tr}(\mathrm{D}\delta F \cdot \mathrm{D}\tau F))\right) \\
& + \left(S'(q)(\delta q) - (\nabla u_d \circ T_F)^T \cdot \delta F, \left(S'(q)(\tau q) - (\nabla u_d \circ T_F)^T \cdot \tau F\right)\gamma_F\right) \\
& + \left(S(q) - u_d \circ T_F, \left(S'(q)(\delta q) - (\nabla u_d \circ T_F)^T \cdot \delta F\right)\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \tau F\right)\right) \\
& + \left(S(q) - u_d \circ T_F, \left(S'(q)(\tau q) - (\nabla u_d \circ T_F)^T \cdot \tau F\right)\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\right) \\
& + \left(S(q) - u_d \circ T_F, \left(S''(q)(\delta q, \tau q) - \tau F^T \cdot \nabla^2 u_d \circ T_F \cdot \delta F\right)\gamma_F\right) + \alpha\,(\delta q, \tau q)_{\mathrm{H}^2(I)}
\end{aligned}
\tag{32}
$$

Remark 2.5. The representations (29) as well as (32) show that the second derivatives are symmetric with respect to the directions.

For stability results concerning these operators and functionals, which will be needed in the context of second-order calculus in Subsection 2.5, we again refer to the Annex, Section 3.

Due to Assumption 2.4 and the differentiability of j, the first-order optimality condition in $\overline{q}$ is just

$$
j'(\overline{q})(\delta q) = 0 \qquad \forall \delta q \in Q. \tag{33}
$$

Our goal is to use the first-order optimality condition (33) to show higher regularity of the optimal control $\overline{q}$. As we are using a control-theoretic approach, we first need to introduce the very weak formulation for the transformation equation and the Lagrangian.

2.2. The very weak formulation

As the control q enters the equation for the transformation F on the boundary, (7) is kind of a Dirichlet control problem which is known not to be of variational type. In [28] the authors present various possibilities on how to deal with such problems. They propose the use of the so-called very weak formulation, which is also used in [9] and [11]. We will also stick to that formulation, therefore we are having a closer look at the solution u to the problem

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ \quad u = g & \text{on } \Gamma. \end{cases} \tag{34}$$

If $f \in \mathrm{H}^{-1}(\Omega)$ and $g \in \mathrm{H}^{1/2}(\Gamma)$, then one can proceed in a standard way as follows. Let $B\colon \mathrm{H}^{1/2}(\Gamma) \to \mathrm{H}^1(\Omega)$ be an arbitrary right inverse to the trace operator. The existence of such a B is ensured by Theorem 1.6. Now set $u = u_\Omega + u_\Gamma$, where $u_\Gamma = B(g)$ and $u_\Omega \in \mathrm{H}_0^1(\Omega)$ solves

$$(\nabla u_\Omega, \nabla v) = -(\nabla u_\Gamma, \nabla v) + (f, v) \qquad \forall v \in \mathrm{H}_0^1(\Omega). \tag{35}$$

The drawback of formulation (35) is the fact that one has to split u into the sum of the two functions u_Γ and u_Ω. This makes it more difficult to take the derivative of u with respect to g, which is crucial in order to derive an optimality system, where we have to take the derivative of (7) with respect to q. One possibility to overcome this difficulty is the use of the very weak formulation, which can be obtained from the weak formulation of (34) by partial integration,

$$-(u, \Delta v) + \langle g, \partial_n v \rangle = (f, v) \qquad \forall v \in \mathrm{H}_0^1(\Omega) \cap \mathrm{H}^2(\Omega), \tag{36}$$

which also allows for solutions $u \in \mathrm{L}^2(\Omega)$ of the boundary value problem. For an overview see [4,14,15,31].

In what follows we always assume that the domain Ω is sufficiently smooth in the sense that problem (34) is H^2-regular, i.e. for arbitrary $f \in \mathrm{L}^2(\Omega)$ and $g \in \mathrm{H}^{3/2}(\Gamma)$ it holds that the weak solution u possesses the regularity $u \in \mathrm{H}^2(\Omega)$. In [16], Theorem 9.1.20, it is shown that this assumption is satisfied if Ω has a C^2-boundary. If $\mathrm{H}_*^{-2}(\Omega)$ denotes the dual space of $\mathrm{H}_0^1(\Omega) \cap \mathrm{H}^2(\Omega)$, then the following lemma can be shown, cf. [31].

Lemma 2.6. *For any given $f \in \mathrm{H}_*^{-2}(\Omega)$ and $g \in \mathrm{H}^{-1/2}(\Gamma)$, the very weak formulation* (36) *possesses a unique solution $u \in \mathrm{L}^2(\Omega)$. There holds the a-priori estimate*

$$\|u\|_{\mathrm{L}^2(\Omega)} \le c\left(\|f\|_{\mathrm{H}_*^{-2}(\Omega)} + \|g\|_{\mathrm{H}^{-1/2}(\Gamma)}\right).$$

Corollary 2.7. *Any weak solution u to* (34) *is also a very weak solution. Vice versa, if the very weak solution possesses the additional regularity $u \in \mathrm{H}^1(\Omega)$, then it is also a weak solution.*

Proof. It follows from the definition that every weak solution also fulfills the very weak formulation (36), uniqueness has already been shown in Lemma 2.6. If the very weak solution is more regular, then one can perform partial integration and the result follows. □

2.3. **The Lagrangian**

The aim of this subsection is to introduce the Lagrangian for problem (23). Let

$$\begin{aligned} &\mathcal{L}\colon Q \times \mathrm{H}_0^1(\Omega_0) \times \mathrm{H}_0^1(\Omega_0) \times \mathrm{H}^{5/2}(\Omega_0) \times \mathrm{H}_0^1(\Omega_0) \cap \mathrm{H}^2(\Omega_0) \to \mathbb{R}, \\ &\mathcal{L}(q,u,z,F,G) = J(q,u,F) + l(F)(z) - a(F)(u,z) + (F, \Delta G) - \langle q\, n, \partial_n G \rangle. \end{aligned} \tag{37}$$

Furthermore, define

$$\mathcal{G} = \mathrm{H}_0^1(\Omega_0) \cap \mathrm{H}^2(\Omega_0), \tag{38}$$

with norm $\|\cdot\|_{\mathcal{G}}^2 = \|\cdot\|_{\mathrm{H}_0^1(\Omega_0)}^2 + |\cdot|_{\mathrm{H}^2(\Omega_0)}^2$.

Lemma 2.8. *In $\mathcal{G}$, the norms $\|\Delta \cdot\|_{\mathrm{L}^2(\Omega_0)}$ and $\|\cdot\|_{\mathcal{G}}$ are equivalent.*

Proof. Let $v \in \mathcal{G}$ be arbitrary. First, we have

$$\|\Delta v\|_{\mathrm{L}^2(\Omega_0)}^2 = \int_{\Omega_0} v_{xx}^2 + v_{yy}^2 + 2 v_{xx} v_{yy} \,\mathrm{d}x \le 2 \int_{\Omega_0} v_{xx}^2 + v_{yy}^2 \,\mathrm{d}x \le 2\, |v|_{\mathrm{H}^2(\Omega_0)}^2 .$$

As $v \in \mathrm{H}_0^1(\Omega_0)$, we know that there exists $c_{\Omega_0} > 0$ such that

$$\|v\|_{\mathrm{L}^2(\Omega_0)} \leq c_{\Omega_0} \|v\|_{\mathrm{H}_0^1(\Omega_0)},$$

and hence

$$\begin{aligned}\|v\|^2_{\mathrm{H}_0^1(\Omega_0)} &= \int_{\Omega_0} \nabla v^T \cdot \nabla v \,\mathrm{d}x = -\int_{\Omega_0} v \Delta v \,\mathrm{d}x \leq \|v\|_{\mathrm{L}^2(\Omega_0)} \|\Delta v\|_{\mathrm{L}^2(\Omega_0)} \\ &\leq c_{\Omega_0} \|v\|_{\mathrm{H}_0^1(\Omega_0)} \|\Delta v\|_{\mathrm{L}^2(\Omega_0)},\end{aligned}$$

so we arrive at

$$\|v\|_{\mathrm{H}_0^1(\Omega_0)} \leq c_{\Omega_0} \|\Delta v\|_{\mathrm{L}^2(\Omega_0)}.$$

In [16], Zusatz 9.1.27, it is proven that for convex Ω_0 it holds that

$$|v|_{\mathrm{H}^2(\Omega_0)} \leq \|\Delta v\|_{\mathrm{L}^2(\Omega_0)},$$

which finishes the proof. □

If $u = u(q)$ and $F = F(q)$, then $\mathcal{L}(q, u, z, F, G) = j(q)$ for all $z \in \mathrm{H}_0^1(\Omega_0)$ and $G \in \mathcal{G}$. This fact is well known and exploited in order to receive an optimality system. In general, one is looking for a stationary point of $\mathcal{L}$, but in order to ensure that every local minima of (23) is also a stationary point of $\mathcal{L}$, one needs some additional regularity which does not hold in general in our case.

Lemma 2.9. *Let $q \in Q^{\mathrm{ad}}$. Then $F(q) \in \mathcal{F}^{\mathrm{ad}}$ is the unique solution to*

$$\mathcal{L}'_G(q, u, z, F, G)(\delta G) = 0 \qquad \forall \delta G \in \mathcal{G}. \tag{39}$$

Proof. As $\mathcal{L}$ is linear in G, it follows that (39) just reads as

$$(F, \Delta\delta G) - \langle q\, n, \partial_n \delta G\rangle = 0 \qquad \forall \delta G \in \mathcal{G}.$$

which is just the very weak formulation. The result follows with Lemma 2.6 and Corollary 2.7. □

Lemma 2.10. *Let $q \in Q^{\mathrm{ad}}$ and $F = F(q)$. Then it holds that $u(q) \in \mathrm{H}_0^1(\Omega_0)$ is the unique solution to*

$$\mathcal{L}'_z(q, u, z, F, G)(\delta z) = 0 \qquad \forall \delta z \in \mathrm{H}_0^1(\Omega_0). \tag{40}$$

Proof. As $l(F)(\cdot)$ as well as $a(F)(u, \cdot)$ are linear it immediately follows that $\mathcal{L}'_z$ exists. As (40) just reads as

$$l(F)(\delta z) = a(F)(u, \delta z) \qquad \forall \delta z \in \mathrm{H}_0^1(\Omega),$$

the result follows with Lemma 1.18. □

Lemma 2.11. *Let $q \in Q^{\mathrm{ad}}$, $F = F(q)$ and $u = u(q)$. Then there exists a unique $z \in \mathrm{H}_0^1(\Omega_0)$ such that*

$$\mathcal{L}'_u(q, u, z, F, G)(\delta u) = 0 \qquad \forall \delta u \in \mathrm{H}_0^1(\Omega_0). \tag{41}$$

Proof. First, equation (41) can be rewritten as

$$a(F)(\delta u, z) = J'_u(q, u, F)(\delta u) \qquad \forall \delta u \in \mathrm{H}_0^1(\Omega_0),$$

which reads as

$$a(F)(\delta u, z) = ((u - u_d \circ T_F)\gamma_F, \delta u) \qquad \forall \delta u \in \mathrm{H}_0^1(\Omega_0). \tag{42}$$

As the right hand side in (42) is a continuous functional on $\mathrm{L}^2(\Omega_0)$, existence and uniqueness follow with standard arguments. □

Remark 2.12. With $z(q)$, $z(F)$ or $z(u)$ we will denote the adjoint state z as the solution to (41) for given q, F or u, cf. Remark 1.19.

To follow the standard procedure, we are now going to compute the derivative of $\mathcal{L}$ with respect to F, which exists due to Lemma 3.4. The goal is to show the existence of an adjoint transformation $G \in \mathcal{G}$ such that $\mathcal{L}'_F(q, u, z, F, G)(\delta F) = 0$ for all $\delta F \in \mathcal{F}$. As the transformation F enters $\mathcal{L}$ in a highly nonlinear way, we split the computation. First, it holds that

$$\begin{aligned} J'_F(q,u,F)(\delta F) &= \frac{1}{2}\int_{\Omega_0} (u - u_d \circ T_F)^2 \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right) \mathrm{d}x \\ &\quad - \int_{\Omega_0} (u - u_d \circ T_F)\left(\nabla u_d \circ T_F\right)^T \cdot \delta F \gamma_F \,\mathrm{d}x \\ &= \int_{\Gamma_0} \frac{1}{2}(u - u_d \circ T_F)^2 \gamma_F \delta F^T \cdot \mathrm{D}T_F^{-T} \cdot n \,\mathrm{d}s - \int_{\Omega_0} (u - u_d \circ T_F)\nabla u^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F \,\mathrm{d}x, \end{aligned} \tag{43}$$

$$\begin{aligned} l'_F(F)(\delta F, z) &= \int_{\Omega_0} f \circ T_F \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right) z + \left(\nabla f \circ T_F\right)^T \cdot \delta F \gamma_F z \,\mathrm{d}x \\ &= -\int_{\Omega_0} f \circ T_F \gamma_F \nabla z^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \,\mathrm{d}x, \end{aligned} \tag{44}$$

$$\begin{aligned} a'_F(F)(\delta F, u, z) &= \int_{\Omega_0} \nabla u^T \cdot A'_{F,\delta F} \cdot \nabla z + uz \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right) \mathrm{d}x \\ &= \int_{\Omega_0} \nabla u^T \cdot A'_{F,\delta F} \cdot \nabla z - \left(u\nabla z + z\nabla u\right)^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F \,\mathrm{d}x, \end{aligned} \tag{45}$$

where we used the Divergence Theorem, $\nabla f \circ T_F = \mathrm{D}T_F^{-T} \cdot \nabla\left(f \circ T_F\right)$ as well as the analog formula for u_d and $uz \in \mathrm{W}_0^{1,p}(\Omega_0)$ for $p < 2$ due to Lemma 1.11. By combinig (43), (44) and (45) with the definition of the Lagrangian, (37), we get

$$\begin{aligned} \mathcal{L}'_F(q,u,z,F,G)(\delta F) = &\int_{\Gamma_0} \frac{1}{2}\left(u - u_d \circ T_F\right)^2 \gamma_F \delta F^T \cdot \mathrm{D}T_F^{-T} \cdot n \,\mathrm{d}s - \int_{\Omega_0} \left(u - u_d \circ T_F\right)\nabla u^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F \,\mathrm{d}x \\ &- \int_{\Omega_0} f \circ T_F \gamma_F \nabla z^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \,\mathrm{d}x \\ &- \int_{\Omega_0} \nabla u^T \cdot A'_{F,\delta F} \cdot \nabla z \,\mathrm{d}x + \int_{\Omega_0} \left(u\nabla z + z\nabla u\right)^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F \,\mathrm{d}x \\ &+ \int_{\Omega_0} \delta F \Delta G \,\mathrm{d}x. \end{aligned} \tag{46}$$

Lemma 2.13. *For $q \in Q^{\mathrm{ad}}$, $u = u(q)$, $z = z(q)$, $F = F(q)$ and $G \in \mathcal{G}$ there exists $d \in \mathrm{H}^1(\Omega_0)$ such that*

$$\mathcal{L}'_F(q,u,z,F,G)(\delta F) = (-d, \delta F)_{\mathrm{H}^1(\Omega_0)} + (\delta F, \Delta G) \qquad \forall \delta F \in \mathrm{H}^1(\Omega_0).$$

i.e. the derivative $\mathcal{L}'_F(q,u,z,F,G)$ is a continuous linear functional on $\mathrm{H}^1(\Omega_0)$.

Proof. Linearity of $\mathcal{L}'_F(q,u,z,F,G)$ follows from (46) and Lemma 3.4. Boundedness in $\mathrm{H}^1(\Omega_0)$ with respect to δF follows with Lemma 3.6, Lemma 3.7 and Theorem 1.6. We also have to make use of the improved regularity $u(q), z(q) \in \mathrm{W}^{1,4}_0(\Omega_0)$, which follows from [32], Theorem 1. The Riesz Representation Theorem (cf. [2], Theorem 4.1) now ensures the existence of such an element $d \in \mathrm{H}^1(\Omega_0)$. □

Remark 2.14. As $u, z \in \mathrm{H}^{3/2-\varepsilon}(\Omega_0)$ due to Theorem 1.4 and the definition of $A'_{F,\delta F}$, Lemma 3.4, it follows that $\mathcal{L}'_F(q,u,z,F,G)$ is in general not a continuous linear functional on $\mathrm{L}^2(\Omega_0)$. As $\Delta\colon \mathcal{G} \to \mathrm{L}^2(\Omega_0)$ is an isomorphism, it follows that the equation

$$\mathcal{L}'_F(q,u(q),z(q),F(q),G)(\delta F) = 0 \qquad \forall \delta F \in \mathrm{H}^1(\Omega_0),$$

need not have a solution $G \in \mathcal{G}$ for general $q \in Q^{\mathrm{ad}}$.

With Remark 2.14 it follows that, in order to show the existence of an adjoint transformation G, it is necessary that the (adjoint) state as well as the transformation have a higher regularity. This is the case if the corresponding control is more regular.

2.4. Higher regularity of the optimal solution

This subsection is devoted to proof Theorem 1.3 regarding the improved regularity of the optimal control $\overline{q}$. In order to do so, we exploit the first-order optimality condition (33), which relies on Assumption 2.4. First,

$$\begin{aligned} j'(\overline{q})(\delta q) &= \frac{\mathrm{d}}{\mathrm{d}t} J\left(\overline{q} + t\ \delta q, u(\overline{q} + t\ \delta q), F(\overline{q} + t\ \delta q)\right)\Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{L}\left(\overline{q} + t\ \delta q, u(\overline{q} + t\ \delta q), z, F(\overline{q} + t\ \delta q), G\right)\Big|_{t=0} \qquad \forall z \in \mathrm{H}^1_0(\Omega_0), G \in \mathcal{G}. \end{aligned}$$

We now choose $z = z(\overline{q})$, $G = 0$. With (33), (28) and Lemma 2.11 we get

$$\begin{aligned} j'(\overline{q})(\delta q) &= \mathcal{L}'_q(\overline{q}, u(\overline{q}), z(\overline{q}), F(\overline{q}), 0)(\delta q) \\ &\quad + \mathcal{L}'_F(\overline{q}, u(\overline{q}), z(\overline{q}), F(\overline{q}), 0)(\delta F) = 0 \qquad \forall \delta q \in Q, \delta F = F'(\overline{q})(\delta q) \in \mathcal{F} \end{aligned} \tag{47}$$

With Lemma 2.13 we can rewrite (47) as

$$\alpha(\overline{q}, \delta q)_{\mathrm{H}^2(I)} - (d, \delta F)_{\mathrm{H}^1(\Omega)} = 0 \qquad \forall \delta q \in Q, \delta F = F'(\overline{q})(\delta q) \in \mathcal{F}, \tag{48}$$

with some $d \in \mathrm{H}^1(\Omega_0)$. With Cauchy-Schwarz it holds that

$$\left|(d, \delta F)_{\mathrm{H}^1(\Omega)}\right| \le \|d\|_{\mathrm{H}^1(\Omega_0)} \|\delta F\|_{\mathrm{H}^1(\Omega_0)}.$$

Furthermore $\delta q \mapsto \delta F$ is linear and $\|\delta F\|_{\mathrm{H}^1(\Omega_0)} \le c\, \|\delta q\|_{\mathrm{H}^1(I)}$, which proofs the existence of $d_1 \in \mathrm{H}^1(I)$ such that

$$(d, \delta F)_{\mathrm{H}^1(\Omega)} = (d_1, \delta q)_{\mathrm{H}^1(I)} \qquad \forall \delta q \in Q. \tag{49}$$

Inserting (49) into (48), we get

$$\alpha(\overline{q}, \delta q)_{\mathrm{H}^2(I)} = (d_1, \delta q)_{\mathrm{H}^1(I)} \qquad \forall \delta q \in Q. \tag{50}$$

To proceed, we need the following lemma.

Lemma 2.15. *Let $\lambda \in \mathrm{H}^2_{\mathrm{per}}(I)$, $\psi \in \mathrm{H}^1_{\mathrm{per}}(I)$ such that*

$$(\lambda, \varphi)_{\mathrm{H}^2(I)} = (\psi, \varphi)_{\mathrm{H}^1(I)} \qquad \forall \varphi \in \mathrm{C}^\infty_{\mathrm{per}}(I), \tag{51}$$

Then it holds that $\lambda \in \mathrm{H}^3_{\mathrm{per}}(I)$.

Proof. Equation (51) just reads as

$$\int_0^{2\pi} \lambda''\varphi'' + \lambda'\varphi' + \lambda\varphi \,\mathrm{d}x = \int_0^{2\pi} \psi'\varphi' + \psi\varphi \,\mathrm{d}x \qquad \forall \varphi \in \mathrm{C}^\infty_{\mathrm{per}}(I).$$

Partial integration yields

$$\int_0^{2\pi} \left(\lambda'' - \lambda + \psi\right)\varphi'' \,\mathrm{d}x = \int_0^{2\pi} \left(-\lambda + \psi\right)\varphi \,\mathrm{d}x \qquad \forall \varphi \in \mathrm{C}^\infty_{\mathrm{per}}(I). \tag{52}$$

As (52) is just the definition of the second weak derivative, and $-\lambda + \psi \in \mathrm{H}^1_{\mathrm{per}}(I)$, this yields

$$\lambda'' - \lambda + \psi \in \mathrm{H}^3_{\mathrm{per}}(I) \subset \mathrm{H}^1_{\mathrm{per}}(I),$$

and because of $\lambda, \psi \in \mathrm{H}^1_{\mathrm{per}}(I)$ we end up with $\lambda'' \in \mathrm{H}^1_{\mathrm{per}}(I)$, hence $\lambda \in \mathrm{H}^3_{\mathrm{per}}(I)$. □

By applying Lemma 2.15 to (50) we get $\overline{q} \in \mathrm{H}^3(I)$. This improved regularity then yields $\overline{F} \in \mathrm{H}^{7/2}(\Omega_0)$, $\mathrm{D}\overline{F} \in \mathrm{H}^{5/2}(\Omega_0) \hookrightarrow \mathrm{C}^{1,1/2}(\overline{\Omega_0})$. Hence, $A_{\overline{F}}, \gamma_{\overline{F}} \in \mathrm{C}^{1,1/2}(\overline{\Omega_0})$, and Theorem 1.4 yields $\overline{u}, \overline{z} \in \mathrm{W}^{2,p}(\Omega_0)$ for $p < \infty$. Theorem 1.6 now implies $\nabla u|_{\Gamma_0}, \nabla z|_{\Gamma_0} \in \mathrm{W}^{1-1/p,p}(\Gamma_0)$. Due to this improved regularity we can further simplify some of the expressions in (46). First, we recall that

$$A'_{F,\delta F} = \mathrm{tr}\big(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\big)\, A_F - \mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F \cdot A_F - A_F \cdot \mathrm{D}\delta F^T \cdot \mathrm{D}T_F^{-T},$$

hence

$$\begin{aligned} -\int_{\Omega_0} \nabla u^T \cdot A_F \cdot \nabla z \,\mathrm{tr}\big(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\big)\,\mathrm{d}x &= -\int_{\Omega_0} \nabla u^T \cdot \mathrm{D}T_F^{-1} \cdot \mathrm{D}T_F^{-T} \cdot \nabla z \,\mathrm{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)\,\mathrm{d}x \\ &= -\int_{\Gamma_0} \left(\mathrm{D}T_F^{-T} \cdot \nabla u\right)^T \cdot \left(\mathrm{D}T_F^{-T} \cdot \nabla z\right) \gamma_F \delta F^T \cdot \mathrm{D}T_F^{-T} \cdot n \,\mathrm{d}s \\ &\quad + \int_{\Omega_0} \nabla \left(\left(\mathrm{D}T_F^{-T} \cdot \nabla u\right)^T \cdot \left(\mathrm{D}T_F^{-T} \cdot \nabla z\right)\right)^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F \,\mathrm{d}x. \end{aligned} \tag{53}$$

It also holds that

$$\begin{aligned} &\int_{\Omega_0} \nabla \left(\left(\mathrm{D}T_F^{-T} \cdot \nabla u\right)^T \cdot \left(\mathrm{D}T_F^{-T} \cdot \nabla z\right)\right)^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \gamma_F + \nabla u^T \cdot \left(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F \cdot A_F + A_F \cdot \mathrm{D}\delta F^T \cdot \mathrm{D}T_F^{-1}\right) \cdot \nabla z \,\mathrm{d}x \\ &= \int_{\Omega_0} \nabla u^T \cdot A_F \cdot \nabla \left(\nabla z^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F\right) + \nabla z^T \cdot A_F \cdot \nabla \left(\nabla u^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F\right)\,\mathrm{d}x \\ &= \int_{\Omega_0} -\mathrm{div}\left(A_F \cdot \nabla u\right) \nabla z^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F - \mathrm{div}\left(A_F \cdot \nabla z\right) \nabla u^T \cdot \mathrm{D}T_F^{-1} \cdot \delta F \,\mathrm{d}x \\ &\quad + 2\int_{\Gamma_0} \left(\mathrm{D}T_F^{-T} \cdot \nabla u\right)^T \cdot \left(\mathrm{D}T_F^{-T} \cdot \nabla z\right) \gamma_F \delta F^T \cdot \mathrm{D}T_F^{-T} \cdot n \,\mathrm{d}s. \end{aligned} \tag{54}$$

So, if we insert (53) and (54) into (46), we finally arrive at

$$
\begin{aligned}
\mathcal{L}'_F(q,u,z,F,G)(\delta F) &= \int_{\Gamma_0} \frac{1}{2}(u-u_d\circ T_F)^2\gamma_F \delta F^T\cdot \mathrm{D}T_F^{-1}\cdot n\,\mathrm{d}s \\
&+\int_{\Gamma_0} \left(\mathrm{D}T_F^{-T}\cdot\nabla u\right)^T\cdot\left(\mathrm{D}T_F^{-T}\cdot\nabla z\right)\gamma_F\delta F^T\cdot \mathrm{D}T_F^{-1}\cdot n\,\mathrm{d}s \\
&+\int_{\Omega_0} \underbrace{\left(-\operatorname{div}(A_F\cdot\nabla u)+u\gamma_F - f\circ T_F\gamma_f\right)}_{=0}\left(\nabla z^T\cdot \mathrm{D}T_F^{-1}\cdot\delta F\right)\,\mathrm{d}x \\
&+\int_{\Omega_0} \underbrace{\left(-\operatorname{div}(A_F\cdot\nabla z)+z\gamma_F-(u-u_d\circ T_F)\gamma_F\right)}_{=0}\left(\nabla u^T\cdot \mathrm{D}T_F^{-1}\cdot\delta F\right)\,\mathrm{d}x \qquad (55)\\
&+\int_{\Omega_0}\delta F\Delta G\,\mathrm{d}x \\
&=\int_{\Gamma_0}\left(\frac{1}{2}(u-u_d\circ T_F)^2+\left(\mathrm{D}T_F^{-T}\cdot\nabla u\right)^T\cdot\left(\mathrm{D}T_F^{-T}\cdot\nabla z\right)\right)\gamma_F\delta F^T\cdot\mathrm{D}T_F^{-1}\cdot n\,\mathrm{d}s \\
&+\int_{\Omega_0}\delta F\Delta G\,\mathrm{d}x,
\end{aligned}
$$

where we made use of the strong formulations of the (adjoint) state equation, (40) and (41), which hold due to the improved regularity of u and z.

Remark 2.16. One may note that (55) looks similar to shape derivatives obtained by different methods as done for example in [26] and [36]. The fact that we end up with a boundary integral is due to the well-known Hadamard-Zolesio Theorem (cf. [36], Theorem 2.27), which holds if all the involved functions are sufficiently smooth.

As in the proof of Lemma 2.13 it is now possible to show that there exists $d_2 \in \mathrm{H}^{1/2}(\Gamma_0)$ such that

$$
\mathcal{L}'_F(\overline{q},\overline{u},\overline{z},\overline{F},G)(\delta F) = -\langle d_2,\delta F\rangle + (\delta F,\Delta G) \qquad \forall \delta F\in\mathcal{F}. \qquad (56)
$$

If we want to choose $G \in \mathcal{G}$ such that (56) vanishes, then this G has to fulfill certain boundary conditions.

Lemma 2.17. *The normal derivative* $\partial_n\colon \mathrm{H}^1_0(\Omega_0)\cap\mathrm{H}^2(\Omega_0)\to\mathrm{H}^{1/2}(\Gamma_0)$ *is continuous and surjective.*

Proof. Continuity follows from Theorem 1.6. Furthermore, this theorem ensures that the mapping $v \mapsto \left(v|_{\Gamma_0}, \partial_n v|_{\Gamma_0}\right)$ from $\mathrm{H}^2(\Omega_0)$ to $\mathrm{H}^{3/2}(\Gamma_0)\times\mathrm{H}^{1/2}(\Gamma_0)$ is surjective and the result follows, cf. [37], page 70. □

This proves the existence of $\overline{G}\in\mathcal{G}$ with $\partial_n\overline{G} = d_2$. It now holds that

$$
\left(\delta F,\Delta\overline{G}\right) = -\left(\nabla\delta F,\nabla\overline{G}\right)+\langle\partial_n\overline{G},\delta F\rangle = \langle\partial_n\overline{G},\delta F\rangle, \qquad (57)
$$

where the first term vanishes due to the fact that δF is harmonic and $\overline{G}\in\mathcal{G}\subset\mathrm{H}^1_0(\Omega_0)$. Inserting (57) into (56) yields

$$
\mathcal{L}'_F(\overline{q},\overline{u},\overline{z},\overline{F},\overline{G})(\delta F) = 0 \qquad \forall\delta F\in\mathcal{F},
$$

and we arrive at

$$
\begin{aligned}
j'(\overline{q})(\delta q) &= \mathcal{L}'_q(\overline{q},\overline{u},\overline{z},\overline{F},\overline{G})(\delta q)\\
&= \alpha\,(\overline{q},\delta q)_{\mathrm{H}^2(I)} - \langle \delta q\, n, \partial_n\overline{G}\rangle \qquad \forall\delta q\in Q.
\end{aligned}
$$

Remark 2.18. One may notice that $\overline{G} \in \mathcal{G}$ is not uniquely defined as $\mathrm{H}_0^2(\Omega_0)$ is in the kernel of the operator ∂_n, as presented in Lemma 2.17. As easily follows from (57), all computed values just depend on $\partial_n \overline{G}$, which is indeed unique.

The following lemma can be proven similar to Lemma 2.15.

Lemma 2.19. *Let $\lambda \in \mathrm{H}^3_{\mathrm{per}}(I)$, $\psi \in \mathrm{H}^{1/2}_{\mathrm{per}}(I)$ such that*

$$(\lambda, \varphi)_{\mathrm{H}^2(I)} = (\psi, \varphi)_{\mathrm{L}^2(I)} \qquad \forall \varphi \in \mathrm{C}^\infty_{\mathrm{per}}(I).$$

Then it holds that $\lambda \in \mathrm{H}^{9/2}_{\mathrm{per}}(I)$.

With the help of Lemma 2.19 it easily follows that $\overline{q} \in \mathrm{H}^{9/2}(I)$ which finally proves Theorem 1.3. □

Remark 2.20. By using a bootstrap argument it is possible to show an even higher regularity of $\overline{q}$. With [16], Theorem 9.1.20, one can show that $\overline{q} \in \mathrm{H}^7(I)$, $\overline{F} \in \mathrm{H}^{15/2}(\Omega_0)$, $\overline{u}, \overline{z} \in \mathrm{H}^5(\Omega_0)$ and $\overline{G} \in \mathrm{H}^{9/2-\varepsilon}(\Omega_0)$. A further improvement is not possible in general due to the regularity of f and u_d, cf. (6). Any further improvement in the regularity of f and u_d would result in a further improved regularity of $\overline{q}, \overline{u}, \overline{z}, \overline{F}, \overline{G}$. For $f, u_d \in \mathrm{C}^\infty(\hat{\Omega})$ we get $\overline{q} \in \mathrm{C}^\infty_{\mathrm{per}}(I)$ and $\overline{u}, \overline{z}, \overline{F}, \overline{G} \in \mathrm{C}^\infty(\Omega_0)$.

2.5. Second order optimality conditions

Within this subsection we are going to state a sufficient second-order optimality condition, which is necessary due to the nonlinearity of the problem. The following lemmas and proofs have been inspired by [10].

Lemma 2.21. *Let $q \in Q^{\mathrm{ad}}$, $\delta q \in Q$ and $(\delta q_n)_{n\in\mathbb{N}} \subset Q$. If $\delta q_n \to \delta q$ in $\mathrm{H}^{3/2+\varepsilon}(I)$, then it holds that*

(1) $S'(q)(\delta q_n) \to S'(q)(\delta q)$ in $\mathrm{H}^1_0(\Omega_0)$,
(2) $S''(q)(\delta q_n, \delta q_n) \to S''(q)(\delta q, \delta q)$ in $\mathrm{H}^1_0(\Omega_0)$.

Proof. (1) Let $\delta F = F'(q)(\delta q) = F(\delta q)$ and $\delta F_n = F'(q)(\delta q_n) = F(\delta q_n)$. With Corollary 1.8 it follows that $\delta F_n \to \delta F$ in $\mathrm{H}^{2+\varepsilon}(\Omega_0)$, and with Lemma 1.11 it follows that $A'_{F,\delta F_n} \to A'_{F,\delta F}$ and $\operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F_n\right) \to \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right)$ in $\mathrm{H}^{1+\varepsilon}(\Omega_0) \hookrightarrow C(\overline{\Omega_0})$. As a result, the right hand side in (28) converges in $\mathrm{H}^{-1}(\Omega_0)$, and the result follows with the standard H^1-stability result.

(2) The second part is proven analogously to the first part. In order to show that the right hand side in (29) converges in $\mathrm{H}^{-1}(\Omega_0)$ one has to make use of the first part, Lemma 3.4 and the fact that the trace of a matrix: $X^{2\times 2} \to X$ is continuous in every Banach space X. □

Lemma 2.22. *Let $q \in Q^{\mathrm{ad}}$, $\delta q \in Q$ and $(\delta q_n)_{n\in\mathbb{N}} \subset Q$ with $\delta q_n \to \delta q$ in $\mathrm{H}^{3/2+\varepsilon}(I)$. Let $m\colon Q^{\mathrm{ad}} \times Q \to \mathbb{R}$ and $n\colon Q^{\mathrm{ad}} \times Q \to \mathbb{R}$ be defined by*

$$\begin{aligned} m(q)(\delta q) &= j'(q)(\delta q) - \alpha(q, \delta q)_{\mathrm{H}^2(I)}, \\ n(q)(\delta q) &= j''(q)(\delta q, \delta q) - \alpha(\delta q, \delta q)_{\mathrm{H}^2(I)}. \end{aligned}$$

Then it holds that

$$\begin{aligned} m(q)(\delta q_n) &\to m(q)(\delta q), \\ n(q)(\delta q_n) &\to n(q)(\delta q), \qquad \text{for } n \to \infty. \end{aligned}$$

Proof. This lemma follows directly from the representations (31) and (32) in combination with Lemma 2.21. □

Lemma 2.23. *Let $q \in Q^{\mathrm{ad}}$, $\delta q \in Q$ and $(\delta q_n)_{n\in\mathbb{N}} \subset Q$. If $\delta q_n \rightharpoonup \delta q$ in $\mathrm{H}^2(I)$ then*

(1) $j'(q)(\delta q_n) \to j'(q)(\delta q)$,
(2) $j''(q)(\delta q, \delta q) \le \liminf_{n\to\infty} j''(q)(\delta q_n, \delta q_n)$

Proof. As $\mathrm{H}^2(I)$ is compactly embedded into $\mathrm{H}^{3/2+\varepsilon}(I)$ for $\varepsilon < 1/2$, we get $\delta q_n \to \delta q$ in $\mathrm{H}^{3/2+\varepsilon}(I)$.

(1) As $(q, \delta q_n)_{\mathrm{H}^2(I)} \to (q, \delta q)_{\mathrm{H}^2(I)}$, this part follows from the first part of Lemma 2.22.
(2) The squared H^2-norm is a continuous and convex functional on $\mathrm{H}^2(I)$ and therefore weakly lower semicontinuous, hence $(\delta q, \delta q)_{\mathrm{H}^2(I)} \leq \liminf_{n\to\infty}(\delta q_n, \delta q_n)_{\mathrm{H}^2(I)}$, and this part follows from the second part of Lemma 2.22. □

Lemma 2.24. *Let $q \in Q^{\mathrm{ad}}$, $\delta q \in Q$, $(\delta q_n)_{n\in\mathbb{N}} \subset Q$ and $\delta q_n \rightharpoonup \delta q$ in $\mathrm{H}^2(I)$. If*

$$\lim_{n\to\infty} j''(q)(\delta q_n, \delta q_n) = j''(q)(\delta q, \delta q),$$

then

$$\delta q_n \to \delta q \qquad \text{in } \mathrm{H}^2(I).$$

Proof. Again we get $\delta q_n \to \delta q$ in $\mathrm{H}^{3/2+\varepsilon}(I)$ for $\varepsilon < 1/2$. With the second part of Lemma 2.22 it follows that $\|\delta q_n\|_{\mathrm{H}^2(I)} \to \|\delta q\|_{\mathrm{H}^2(I)}$. The result follows from the fact that strong convergence is equivalent to weak convergence plus convergence of the norm. □

Theorem 2.25. *Let $\overline{q} \in Q^{\mathrm{ad}}$ be a solution of (23). If*

$$j''(\overline{q})(\delta q, \delta q) > 0 \qquad \forall \delta q \in Q\backslash\{0\}, \tag{58}$$

then there exists $\beta > 0$ such that

$$j''(\overline{q})(\delta q, \delta q) \geq \beta \|\delta q\|^2_{\mathrm{H}^2(I)} \qquad \forall \delta q \in Q. \tag{59}$$

Proof. Assume that (59) does not hold. Then there exists a sequence $(\delta q_n)_{n\in\mathbb{N}} \subset Q$ with $\|\delta q_n\|_{\mathrm{H}^2(I)} = 1$ and

$$j''(\overline{q})(\delta q_n, \delta q_n) < \frac{1}{n}.$$

Possibly after extracting a subsequence we get the existence of an element $\overline{\delta q} \in Q$ with $\delta q_n \rightharpoonup \overline{\delta q}$ in $\mathrm{H}^2(I)$. We get

$$0 \leq j''(\overline{q})(\overline{\delta q}, \overline{\delta q}) \leq \liminf_{n\to\infty} j''(\overline{q})(\delta q_n, \delta q_n) \leq \limsup_{n\to\infty} j''(\overline{q})(\delta q_n, \delta q_n) \leq \limsup_{n\to\infty} \frac{1}{n} = 0. \tag{60}$$

The first inequality is just the necessary optimality condition of second order, and the second inequality is due to Lemma 2.23. Equation (60) now yields

$$j''(\overline{q})(\delta q_n, \delta q_n) \to j''(\overline{q})(\overline{\delta q}, \overline{\delta q}) = 0.$$

As a result, (58) implies $\overline{\delta q} = 0$, whereas Lemma 2.24 implies $\delta q_n \to \overline{\delta q}$ in $\mathrm{H}^2(I)$, which contradicts $\|\delta q_n\|_{\mathrm{H}^2(I)} = 1$. □

Lemma 2.26. *Let $q \in Q^{\mathrm{ad}}$ and $\beta > 0$ such that*

$$j''(q)(\delta q, \delta q) \geq \beta \|\delta q\|^2_{\mathrm{H}^2(I)} \qquad \forall \delta q \in Q.$$

Then there exists $\delta > 0$ such that for all $p \in Q^{\mathrm{ad}}$ with $\|q - p\|_{\mathrm{H}^2(I)} \leq \delta$ it holds that

$$j''(p)(\delta q, \delta q) \geq \frac{\beta}{2} \|\delta q\|^2_{\mathrm{H}^2(I)} \qquad \forall \delta q \in Q.$$

Proof. With Lemma 3.14 one gets

$$\begin{aligned} j''(p)(\delta q,\delta q) &= j''(q)(\delta q,\delta q) + j''(p)(\delta q,\delta q) - j''(q)(\delta q,\delta q) \\ &\geq j''(q)(\delta q,\delta q) - |j''(p)(\delta q,\delta q) - j''(q)(\delta q,\delta q)| \\ &\geq \beta \|\delta q\|^2_{\mathrm{H}^2(I)} - c\,\|q-p\|_{\mathrm{H}^2(I)} \|\delta q\|^2_{\mathrm{H}^2(I)} \\ &= \left(\beta - c\,\|q-p\|_{\mathrm{H}^2(I)}\right) \|\delta q\|^2_{\mathrm{H}^2(I)}, \end{aligned}$$

and the result follows for $\delta \leq \frac{\beta}{2c}$. □

Lemma 2.27. *Let $\overline{q} \in Q^{\mathrm{ad}}$ be a solution of (23). Then the following two statements are equivalent*

(1) There exists $\beta_1 > 0$ such that

$$j''(\overline{q})(\delta q,\delta q) \geq \beta_1 \|\delta q\|^2_{\mathrm{H}^2(I)} \qquad \forall \delta q \in Q,$$

(2) There exist $\beta_2, \delta > 0$ such that

$$j(p) \geq j(\overline{q}) + \beta_2 \|p-\overline{q}\|^2_{\mathrm{H}^2(I)} \qquad \forall p \in Q^{\mathrm{ad}}\colon\ \|p-\overline{q}\|_{\mathrm{H}^2(I)} \leq \delta.$$

Proof. (1) If the first statement holds, then we have for some $t \in [0,1]$:

$$\begin{aligned} j(p) &= j(\overline{q}) + j'(\overline{q})(p-\overline{q}) + \frac{1}{2} j''(\overline{q} + t(p-\overline{q}))(p-\overline{q}, p-\overline{q}) \\ &= j(\overline{q}) + \frac{1}{2} j''(\overline{q} + t(p-\overline{q}))(p-\overline{q}, p-\overline{q}) \\ &\geq j(\overline{q}) + \frac{\beta_1}{4} \|p-\overline{q}\|^2_{\mathrm{H}^2(I)}, \end{aligned}$$

whereas in the second step we used the first-order optimality condition (33), in the third step we used Lemma 2.26.

(2) If the second condition holds, then $\overline{q}$ is a local solution to

$$\min_{q \in Q^{\mathrm{ad}}} j(q) - \beta_2 \|q-\overline{q}\|^2_{\mathrm{H}^2(I)},$$

and the necessary optimality conditions of second order yield

$$j''(\overline{q})(\delta q,\delta q) - 2\beta_2 \|\delta q\|^2_{\mathrm{H}^2(I)} \geq 0 \qquad \forall \delta q \in Q.$$ □

3. Annex

Within this section we are going to collect various regularity as well as stability results related to the transformation T_F, the (bi)linear forms $a(F)(\cdot,\cdot)$ and $l(F)(\cdot)$, the solution operator S and the reduced cost functional j.

Lemma 3.1. *If $s > 3/2$ and $q \in \mathrm{H}^s(I)$, then it holds that $\gamma_{F(q)}, A_{F(q)} \in \mathrm{H}^{s-1/2}(\Omega_0)$.*

Proof. The regularity result for $\gamma_{F(q)}$ follows from (12), Corollary 1.8 and Lemma 1.11. Because of

$$\mathrm{D}T^{-1}_{F(q)} = \frac{1}{\gamma_{F(q)}} \begin{pmatrix} 1 + \partial_y F_2(q) & -\partial_y F_1(q) \\ -\partial_x F_2(q) & 1 + \partial_x F_1(q) \end{pmatrix}, \tag{61}$$

and $\mathrm{D}F \in \mathrm{H}^{s-1/2}(\Omega_0)$, Lemma 1.13 yields $\mathrm{D}T_{F(q)}^{-1} \in \mathrm{H}^{s-1/2}(\Omega_0)$, and the regularity for $A_{F(q)}$ follows with (15) and the first part of this lemma. □

Lemma 3.2. *For $\|q\|_{\mathrm{H}^2(I)} \to 0$ it holds that*

(1) $T_{F(q)} \to \mathrm{Id}$ *in* $\mathrm{H}^{5/2}(\Omega_0) \hookrightarrow \mathrm{C}^{1,1/2}(\overline{\Omega_0})$.
(2) $\gamma_{F(q)} \to 1$ *in* $\mathrm{H}^{3/2}(\Omega_0) \hookrightarrow \mathrm{C}^{0,1/2}(\overline{\Omega_0})$.
(3) $\mathrm{D}T_{F(q)}^{-1} \to \mathrm{I}$ *in* $\mathrm{H}^{3/2}(\Omega_0)$.
(4) $A_{F(q)} \to \mathrm{I}$ *in* $\mathrm{H}^{3/2}(\Omega_0)$.

Proof. (1) This statement follows from (10) and Corollary 1.8.
(2) This part follows from (12), Lemma 3.1 and the first part of this lemma.
(3) This part follows from (61), Lemma 1.11 and the first two parts of this lemma.
(4) The last part follows from (15), the parts (2) and (3) and again Lemma 1.11. □

With these explicit definitions at hand, one can easily derive some stability results which follow by a direct calculation and the boundedness of $\mathcal{F}^{\mathrm{ad}}$ in $\mathrm{H}^{5/2}(\Omega_0)$, as well as the fact that $u_d, f \in \mathrm{C}^{2,1}(\hat{\Omega})$.

Lemma 3.3. *For $F, E \in \mathcal{F}^{\mathrm{ad}}$, $s \in (1, 3/2]$, we have*

- $\|\gamma_F - \gamma_E\|_{\mathrm{H}^s(\Omega_0)} \le c_s \|F - E\|_{\mathrm{H}^{s+1}(\Omega_0)}$,
- $\|T_F - T_E\|_{\mathrm{H}^{s+1}(\Omega_0)} \le c_s \|F - E\|_{\mathrm{H}^{s+1}(\Omega_0)}$,
- $\|\mathrm{D}T_F - \mathrm{D}T_E\|_{\mathrm{H}^s(\Omega_0)} \le c_s \|F - E\|_{\mathrm{H}^{s+1}(\Omega_0)}$,
- $\left\|\mathrm{D}T_F^{-1} - \mathrm{D}T_E^{-1}\right\|_{\mathrm{H}^s(\Omega_0)} \le c_s \|F - E\|_{\mathrm{H}^{s+1}(\Omega_0)}$,
- $\|A_F - A_E\|_{\mathrm{H}^s(\Omega_0)} \le c_s \|F - E\|_{\mathrm{H}^{s+1}(\Omega_0)}$,
- $\|f \circ T_F - f \circ T_E\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,
- $\|\nabla f \circ T_F - \nabla f \circ T_E\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,
- $\left\|\nabla^2 f \circ T_F - \nabla^2 f \circ T_E\right\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,
- $\|u_d \circ T_F - u_d \circ T_E\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,
- $\|\nabla u_d \circ T_F - \nabla u_d \circ T_E\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,
- $\left\|\nabla^2 u_d \circ T_F - \nabla^2 u_d \circ T_E\right\|_{\mathrm{L}^\infty(\Omega_0)} \le c \|F - E\|_{\mathrm{L}^\infty(\Omega_0)}$,

Furthermore, the expressions T_F, $f \circ T_F$, $\nabla f \circ T_F$, $\nabla^2 \circ T_F$, $u_d \circ T_F$, $\nabla u_d \circ T_F$ and $\nabla^2 u_d \circ T_F$ are bounded in $\mathrm{H}^{5/2}(\Omega_0)$, γ_F and $\mathrm{D}T_F$ are bounded in $\mathrm{H}^{3/2}(\Omega_0)$.

Lemma 3.4. *Let $F \in \mathcal{F}^{\mathrm{ad}}$, $\delta F, \tau F \in \mathrm{H}^{5/2}(\Omega_0)$. Then the following operators are Fréchet differentiable.*

(1) $\gamma_F \colon \mathrm{H}^{5/2}(\Omega_0) \to \mathrm{H}^{3/2}(\Omega_0)$ *with derivative*

$$\gamma'_{F,\delta F} = \gamma_F \operatorname{tr}\bigl(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\bigr) = \operatorname{div}\left(\gamma_F \mathrm{D}T_F^{-1} \cdot \delta F\right).$$

(2) $\mathrm{D}T_F^{-1} \colon \mathrm{H}^{5/2}(\Omega_0) \to \mathrm{H}^{3/2}(\Omega_0)$ *with derivative*

$$\left(\mathrm{D}T_F^{-1}\right)'_{\delta F} = -\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F \cdot \mathrm{D}T_F^{-1}.$$

(3) $\gamma'_{F,\delta F} \colon \mathrm{H}^{5/2}(\Omega_0) \times \mathrm{H}^{5/2}(\Omega_0) \to \mathrm{H}^{3/2}(\Omega_0)$ *with derivative*

$$\begin{aligned}\gamma''_{F,\delta F,\tau F} &= \gamma_F \operatorname{tr}\bigl(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\bigr) \operatorname{tr}\bigl(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\tau F\bigr) - \gamma_F \operatorname{tr}\bigl(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\tau F \cdot \mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\bigr)\\ &= \operatorname{tr}(\mathrm{D}\delta F) \operatorname{tr}(\mathrm{D}\tau F) - \operatorname{tr}(\mathrm{D}\delta F \cdot \mathrm{D}\tau F).\end{aligned}$$

(4) $A_F \colon \mathrm{H}^{5/2}(\Omega_0) \to \mathrm{H}^{3/2}(\Omega_0)$ *with derivative*

$$A'_{F,\delta F} = \operatorname{tr}\bigl(\mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F\bigr) A_F - \mathrm{D}T_F^{-1} \cdot \mathrm{D}\delta F \cdot A_F - A_F \cdot \mathrm{D}\delta F^T \cdot \mathrm{D}T_F^{-T}.$$

(5) $A'_{F,\delta F}\colon \mathrm{H}^{5/2}(\Omega_0)\times \mathrm{H}^{5/2}(\Omega_0)\to \mathrm{H}^{3/2}(\Omega_0)$ *with derivative*

$$\begin{aligned}A''_{F,\delta F,\tau F} =& -\operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\cdot \mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\, A_F + \operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\big)\, A_F\\ &- \operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\,\mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\cdot A_F - \operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\big)\,\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\cdot A_F\\ &- \operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\, A_F\cdot \mathrm{D}\tau F^T\cdot \mathrm{D}T_F^{-T} - \operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\big)\, A_F\cdot \mathrm{D}\delta F^T\cdot \mathrm{D}T_F^{-T}\\ &+ \mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\cdot \mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\cdot A_F + \mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\cdot \mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\cdot A_F\\ &+ \mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\cdot A_F\cdot \mathrm{D}\tau F^T\cdot \mathrm{D}T_F^{-T} + \mathrm{D}T_F^{-1}\cdot \mathrm{D}\tau F\cdot A_F\cdot \mathrm{D}\delta F^T\cdot \mathrm{D}T_F^{-T}\\ &+ A_F\cdot \mathrm{D}\delta F^T\cdot \mathrm{D}T_F^{-T}\cdot \mathrm{D}\tau F^T\cdot \mathrm{D}T_F^{-T} + A_F\cdot \mathrm{D}\tau F^T\cdot \mathrm{D}T_F^{-T}\cdot \mathrm{D}\delta F^T\cdot \mathrm{D}T_F^{-T}\end{aligned}$$

Proof. (1) By a direct calculation it follows that

$$\begin{aligned}&\lim_{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}\to 0}\frac{\big\|\gamma_{F+\delta F}-\gamma_F-\gamma_F\operatorname{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\big\|_{\mathrm{H}^{3/2}(\Omega_0)}}{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}}\\ =&\lim_{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}\to 0}\frac{\|\partial_x\delta F_1\,\partial_y\delta F_2-\partial_y\delta F_1\,\partial_x\delta F_2\|_{\mathrm{H}^{3/2}(\Omega_0)}}{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}}\\ \le&\lim_{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}\to 0}\frac{c\,\|\delta F\|^2_{\mathrm{H}^{5/2}(\Omega_0)}}{\|\delta F\|_{\mathrm{H}^{5/2}(\Omega_0)}}=0,\end{aligned}$$

where in the second step we made use of Lemma 1.11.

(2) This part follows from a direct calculation.

(3) This part follows from the fact that the trace is linear, the product rule as well as the first two parts of this lemma.

(4) The fourth part follows from the previous two parts, the product rule and Lemma 1.11.

(5) The last part follows from a direct calculation and the previous parts. □

Remark 3.5. For $A,B\in\mathbb{R}^{n\times n}$ it holds that $\operatorname{tr}(A\cdot B)=\operatorname{tr}(B\cdot A)$, hence the second derivatives $A''_{F,\delta F,\tau F}$ and $\gamma''_{F,\delta F,\tau F}$ which are computed in Lemma 3.4 are symmetric with respect to the directions.

Lemma 3.6. *For $F\in\mathcal{F}^{\mathrm{ad}}$, $\delta F,\tau F\in\mathcal{F}$, $s\in(1,3/2]$, we have*

(1) $\|\gamma_F\|_{\mathrm{H}^{3/2}(\Omega_0)}\le c$,

(2) $\left\|\gamma'_{F,\delta F}\right\|_{\mathrm{H}^s(\Omega_0)}\le c_s\,\|\delta F\|_{\mathrm{H}^{s+1}(\Omega_0)}$.

(3) $\left\|\gamma''_{F,\delta F,\tau F}\right\|_{\mathrm{H}^s(\Omega_0)}\le c_s\,\|\delta F\|_{\mathrm{H}^{s+1}(\Omega_0)}\,\|\tau F\|_{\mathrm{H}^{s+1}(\Omega_0)}$.

Proof. The first part follows from the definition of $\mathcal{F}^{\mathrm{ad}}$ and the comment afterward, the second and the third part follow from the representations obtained in Lemma 3.4. □

Lemma 3.7. *For $F\in\mathcal{F}^{\mathrm{ad}}$, $\delta F,\tau F\in\mathcal{F}$, $s\in(1,3/2]$, we have*

(1) $\|A_F\|_{\mathrm{H}^{3/2}(\Omega_0)}\le c$,

(2) $\left\|A'_{F,\delta F}\right\|_{\mathrm{H}^s(\Omega_0)}\le c_s\,\|\delta F\|_{\mathrm{H}^{s+1}(\Omega_0)}$.

(3) $\left\|A''_{F,\delta F,\tau F}\right\|_{\mathrm{H}^s(\Omega_0)}\le c_s\,\|\delta F\|_{\mathrm{H}^{s+1}(\Omega_0)}\,\|\tau F\|_{\mathrm{H}^{s+1}(\Omega_0)}$.

Proof. (1) Due to (15) it holds that

$$\|A_F\|_{\mathrm{H}^{3/2}(\Omega_0)}=\big\|\gamma_F\mathrm{D}T_F^{-1}\cdot \mathrm{D}T_F^{-T}\big\|_{\mathrm{H}^{3/2}(\Omega_0)}\le c\left\|\frac{1}{\gamma_F}\right\|_{\mathrm{H}^{3/2}(\Omega_0)}\|\mathrm{D}T_F\|^2_{\mathrm{H}^{3/2}(\Omega_0)}\le c,$$

where we made use of Lemma 1.13 and Lemma 1.11.

(2) In order to proof the second assertion we use Lemma 3.4 and get

$$\begin{aligned}\left\|A'_{F,\delta F}\right\|_{\mathrm{H}^s(\Omega_0)} &= \left\|\mathrm{tr}\big(\mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\big)\, A_F - \mathrm{D}T_F^{-1}\cdot \mathrm{D}\delta F\cdot A_F - A_F\cdot \mathrm{D}\delta F^T\cdot \mathrm{D}T_F^{-T}\right\|_{\mathrm{H}^s(\Omega_0)}\\ &\le c\,\|\delta F\|_{\mathrm{H}^{s+1}(\Omega_0)}\,,\end{aligned}$$

where we again made use of Lemma 1.11 and the first part of this lemma.

(3) This last part can be proven in the same way as the previous part. □

The following three lemmas are direct consequences of the definitions (18), (19), Lemma 3.3, Lemma 3.6 and Lemma 3.7.

Lemma 3.8. *The bilinear form $a(F)(\cdot,\cdot)$ is continuous and coercive in $\mathrm{H}^1(\Omega_0)$, i.e. there exist $c_1, c_2 > 0$, independent of $F\in\mathcal{F}^{\mathrm{ad}}$, such that for all $u, z\in \mathrm{H}^1(\Omega_0)$ it holds that*

$$\begin{aligned}|a(F)(u,z)| &\le c_1\,\|u\|_{\mathrm{H}^1(\Omega_0)}\,\|z\|_{\mathrm{H}^1(\Omega_0)}\,,\\ a(F)(u,u) &\ge c_2\,\|u\|^2_{\mathrm{H}^1(\Omega_0)}\,.\end{aligned}$$

Furthermore, there exists $c_3 > 0$, independent of $F\in\mathcal{F}^{\mathrm{ad}}$ and $p\in[1,\infty]$, such that for $u\in \mathrm{W}^{1,p}(\Omega_0)$ and $z\in \mathrm{W}^{1,p'}(\Omega_0)$ with $\frac{1}{p}+\frac{1}{p'}=1$ the following Hölder-like inequality holds

$$|a(F)(u,z)| \le c_3\,\|u\|_{\mathrm{W}^{1,p}(\Omega_0)}\,\|z\|_{\mathrm{W}^{1,p'}(\Omega_0)}\,.$$

Lemma 3.9. *For $F, E\in\mathcal{F}^{\mathrm{ad}}$ and $u, z\in \mathrm{H}^1(\Omega_0)$ it holds that*

$$|a(F)(u,z) - a(E)(u,z)| \le c_\varepsilon\,\|F-E\|_{\mathrm{H}^{2+\varepsilon}(\Omega_0)}\,\|u\|_{\mathrm{H}^1(\Omega_0)}\,\|z\|_{\mathrm{H}^1(\Omega_0)}\,.$$

Lemma 3.10. *For $F, E\in\mathcal{F}^{\mathrm{ad}}$ and $z\in \mathrm{L}^2(\Omega_0)$ it holds that*

$$|l(F)(z) - l(E)(z)| \le c\,\|F-E\|_{\mathrm{H}^1(\Omega_0)}\,\|z\|_{\mathrm{L}^2(\Omega_0)}\,.$$

Lemma 3.11. *For $F, E\in\mathcal{F}^{\mathrm{ad}}$ it holds that*

$$\|u(F)-u(E)\|_{\mathrm{H}^1(\Omega_0)} \le c_\varepsilon\,\|F-E\|_{\mathrm{H}^{2+\varepsilon}(\Omega_0)}\,.$$

Proof. Let $e = u(F)-u(E)$. With Lemma 3.9, Lemma 3.10 and Lemma 3.12 we have

$$\begin{aligned}c\,\|e\|^2_{\mathrm{H}^1(\Omega_0)} &\le a(F)(e,e) = a(F)(u(F),e) - a(F)(u(E),e)\\ &= a(F)(u(F),e) - a(E)(u(E),e) + a(E)(u(E),e) - a(F)(u(e),e)\\ &\le |l(F)(e) - l(E)(e)| + |a(E)(u(E),e) - a(F)(u(E),e)|\\ &\le c_\varepsilon\,\|e\|_{\mathrm{H}^1(\Omega_0)}\,\|F-E\|_{\mathrm{H}^{2+\varepsilon}(\Omega_0)}\,.\end{aligned}$$ □

Lemma 3.12. *For $q\in Q^{\mathrm{ad}}$, $\delta q\in Q$, it holds with q-independent constants that*

(1) $\|S(q)\|_{\mathrm{H}^1_0(\Omega_0)} \le c$,
(2) $\|S'(q)(\delta q)\|_{\mathrm{H}^1_0(\Omega_0)} \le c\,\|\delta q\|_{\mathrm{H}^2(I)}$,
(3) $\|S''(q)(\delta q,\delta q)\|_{\mathrm{H}^1_0(\Omega_0)} \le c\,\|\delta q\|^2_{\mathrm{H}^2(I)}$.

Proof. (1) As $a(F)(\cdot,\cdot)$ is uniformly coercive we have

$$\begin{aligned} c\left\|u(F)\right\|^2_{\mathrm{H}^1_0(\Omega_0)} &\leq a(F)(u(F),u(F)) = l(F)(u(F)) \\ &\leq c\left\|f\circ T_F\right\|_{\mathrm{L}^2(\Omega_0)}\left\|u(F)\right\|_{\mathrm{H}^1_0(\Omega_0)}\left\|\gamma_F\right\|_{\mathrm{L}^\infty(\Omega_0)}. \end{aligned}$$

(2) and (3) are proven in the same way, one additionally has to make use of Lemma 3.6, Lemma 3.7, Corollary 1.8 and the embedding $\mathrm{H}^{3/2}(\Omega_0)\hookrightarrow\mathrm{L}^\infty(\Omega_0)$. □

Lemma 3.13. *For $q,p\in Q^{\mathrm{ad}}$, $\delta q\in Q$, it holds that*

(1) $\left\|S(q)-S(p)\right\|_{\mathrm{H}^1_0(\Omega_0)}\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}$,
(2) $\left\|S'(q)(\delta q)-S'(p)(\delta q)\right\|_{\mathrm{H}^1_0(\Omega_0)}\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}\left\|\delta q\right\|_{\mathrm{H}^2(I)}$,
(3) $\left\|S''(q)(\delta q,\delta q)-S''(p)(\delta q,\delta q)\right\|_{\mathrm{H}^1_0(\Omega_0)}\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}\left\|\delta q\right\|^2_{\mathrm{H}^2(I)}$.

Proof. (1) Let $e=S(q)-S(p)$, $F_q=F(q)$ and $F_p=F(p)$. With Lemma 3.9 we get

$$\begin{aligned} c\left\|e\right\|^2_{\mathrm{H}^1_0(\Omega_0)} &\leq a(F_q)(e,e) = a(F_q)(S(q),e)-a(F_q)(S(p),e) \\ &\leq a(F_q)(S(q),e)-a(F_p)(S(p),e)+c_\varepsilon\left\|F_q-F_p\right\|_{\mathrm{H}^{2+\varepsilon}(\Omega_0)}\left\|S(p)\right\|_{\mathrm{H}^1_0(\Omega_0)}\left\|e\right\|_{\mathrm{H}^1_0(\Omega_0)}. \end{aligned}$$

Now we use the definition of $S(q)$, $S(p)$ and Lemma 3.10 and get

$$a(F_q)(S(q),e)-a(F_p)(S(p),e) = l(F_q)(e)-l(F_p)(e)\leq c\left\|F_q-F_p\right\|_{\mathrm{H}^1(\Omega_0)}\left\|e\right\|_{\mathrm{H}^1_0(\Omega_0)}.$$

The proof is finished with Corollary 1.8 and Lemma 3.12.

(2) and (3) are proven in the same way. □

The following lemma can be proven in essentially the same way as Lemma 3.13.

Lemma 3.14. *For $q,p\in Q^{\mathrm{ad}}$, $\delta q\in Q$, it holds that*

(1) $|j(q)-j(p)|\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}$,
(2) $|j'(q)(\delta q)-j'(p)(\delta q)|\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}\left\|\delta q\right\|_{\mathrm{H}^2(I)}$,
(3) $|j''(q)(\delta q,\delta q)-j''(p)(\delta q,\delta q)|\leq c\left\|q-p\right\|_{\mathrm{H}^2(I)}\left\|\delta q\right\|^2_{\mathrm{H}^2(I)}$.

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