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Theoretical and Numerical Aspects of Shape Optimization with Navier-Stokes Flows

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Abstract

In this work, shape optimization problems in flows governed by the stationary and instationary Navier-Stokes equations are discussed. Building on the 'perturbation of identity' ansatz by Murat and Simon, a suitable framework for 2D and 3D optimal design problems is developed. In particular, for the instationary case, the Fréchet differentiability of the design-to-state operator for $W^{2,\infty}$ domain transformations is proved. An adjoint-based calculation of first and second order material derivatives is developed and the correlation to common parametrizations is discussed. Finally numerical results are presented.

Zusammenfassung

In dieser Arbeit werden Formoptimierungsprobleme in Strömungen, welche durch die stationären und instationären Navier-Stokes-Gleichungen beschrieben werden, untersucht. Aufbauend auf dem von Murat und Simon entwickelten "perturbation of identity"-Ansatz wird ein passender Rahmen zur Formulierung des Formoptimierungsproblems in 2D und 3D angegeben. Insbesondere wird für den instationären Fall die Fréchet-Differenzierbarkeit des Design-zu-Zustand-Operators für $W^{2,\infty}$-Gebietstransformationen gezeigt. Es wird eine adjungierten-basierte Berechnung der ersten und zweiten Formableitungen entwickelt und die Beziehung zu allgemeinen Parametrisierungen diskutiert. Schließlich werden numerische Resultate präsentiert.

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1 Introduction

Shape optimization is an important research topic with many interesting applications in various engineering fields. The typical problem is to find the optimal design of an object with respect to an objective function while satisfying some constraints, e.g. constraints on the geometry of the object. Of particular interest are PDE constrained shape optimization problems where the objective function depends on the solution of a partial differential equation on the design object. In abstract formulation this problem can be stated as

$$\min_{(y,\Omega)} J(y,\Omega) \quad \text{s.t. } E(y,\Omega) = 0,\ \Omega \in \mathcal{O}_{\text{ad}} \tag{1.1}$$

where the state y is the solution of a PDE E on the domain Ω. J denotes the objective function and $\mathcal{O}_{\text{ad}}$ describes the set of admissible domains including some geometric constraints for example.

A rigorous discussion about fundamental aspects of shape optimization problems can be found in the book of Delfour and Zolésio [14], in particular how topologies on sets of domains can be established and how continuity and differentiation of domain variations can be introduced. Sokolowski and Zolésio discussed in [58] special aspects of shape optimization problems under a state constraint like (1.1). Various applications of shape optimization in structural mechanics can be found in the books of Choi and Kim [11] and [12] including theoretical and numerical aspects. Shape optimization in fluid mechanics or aerodynamics are discussed in, e.g., [41] and next to other applications also in [25].

In this work we will focus on shape optimization in Navier-Stokes flows where one or more objects are exposed to a flow governed by the stationary or instationary Navier-Stokes equations.

We describe the admissible domains by transformations of a reference object Ω_{ref}, following the ansatz introduced by Murat and Simon ([44], [45]). Based on this approach, we can formulate the shape optimization problem on a fixed reference domain obtaining an optimal control problem. In this framework we can use methods of optimal control for calculating derivatives of an objective function with respect to domain variations represented by transformations.

The work presented covers theoretical and numerical aspects and the structure of this thesis is the following. After introducing some notations in Section 2, in Section 3.1 we will describe the transformation setting and how shape derivatives with respect to transformations can be calculated via the adjoint ansatz for shape optimization problems of the type (1.1). We describe how the evaluation of shape derivatives on the actual domain is possible and how second derivatives can be calculated. Finally we link this approach to shape optimization problems where the design of the object is parametrized via a shape parameter and show how derivatives with respect to shape parameters can be obtained.

The framework of Section 3.1 is then applied to shape optimization problems governed by the Navier-Stokes equations where we mainly discuss the instationary setting. In Section 3.2 we start with some basic results about the regularity of solutions for the instationary Navier-Stokes equations with homogeneous boundary conditions. After defining the concrete setting we show how the shape optimization problem defined on the reference domain can be obtained. We describe how first order shape derivatives for an objective function can be calculated on a formal level using the adjoint approach. For the derivative we use a domain integral representation which can be transformed into a boundary integral in Hadamard form as shown in Appendix A. Furthermore we illustrate how second order shape derivatives can be obtained. Finally first order shape derivatives are given for problems governed by the inhomogeneous instationary or stationary Navier-Stokes equations.

In Section 4 we intensify the discussion of Section 3.2 to determine the concrete setting for shape optimization problems governed by the Navier-Stokes equations. In this context we introduce the design-to-state operator $v(\tau)$ that maps a transformation τ (identified with a domain $\Omega(\tau) = \tau(\Omega_{\text{ref}})$) to the velocity field $v(\tau)$ as the solution of the Navier-Stokes equations on $\Omega(\tau)$. For a rigorous setting we like to show the differentiability of this map in suitable function spaces for τ and $v(\tau)$. The analysis of the Navier-Stokes equations

$$\begin{aligned} \boldsymbol{v}_t - \nu\Delta\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} + \nabla p &= \boldsymbol{f} \text{ on } \Omega\times I, \\ \operatorname{div}\,\boldsymbol{v} &= 0 \text{ on } \Omega\times I, \\ \boldsymbol{v} &= \boldsymbol{0} \text{ on } \partial\Omega\times I, \\ \boldsymbol{v}(\cdot,0) &= \boldsymbol{v}_0 \text{ on } \Omega, \end{aligned}$$

is ususally based on the weak formulation

$$\begin{aligned} \langle \boldsymbol{v}_t(\cdot,t), \boldsymbol{w}\rangle_{V(\Omega)^*,V(\Omega)} &+ \int_\Omega \boldsymbol{v}(x,t)^T\nabla\boldsymbol{v}(x,t)\boldsymbol{w}(x)\,dx + \int_\Omega \nu\nabla\boldsymbol{v}(x,t) : \nabla\boldsymbol{w}(x)\,dx \\ &= \int_\Omega \boldsymbol{f}(x,t)^T\boldsymbol{w}(x)\,dx \quad \forall\,\boldsymbol{w}\in V(\Omega) \;\text{ for a.a. } t\in I, \\ \boldsymbol{v}(\cdot,0) &= \boldsymbol{v}_0, \end{aligned}$$

where the solenoidality of $\boldsymbol{v}$ is included in the test and trial spaces. In particular the pressure term ∇p drops out in the weak formulation since the test function $\boldsymbol{w}$ is divergence-free. However, if the state equation is transformed to the reference domain the solenoidality of the functions is not preserved. This causes additional difficulties.

There are different possibilities to overcome these. For stationary Stokes flow Simon [55] uses a variant of the implicit function theorem to show differentiability of the design-to-state operator. Bello et al. ([7], [6]) introduced a family of isomorphisms to rewrite the equation $\operatorname{div}\,\boldsymbol{v}(\tau) = 0$ appropriately and showed differentiability of the drag in the case of stationary Navier-Stokes equations for $W^{2,\infty}$ domains. In [5] Bello et al. extended this result to $W^{1,\infty}$ transformations by stating the incompressibility equation explicitly introducing a weak velocity-pressure formulation.

In this work, we derive differentiability results of the design-to-state map also for the instationary Navier-Stokes equations. As done in [5] the incompressibility equation is stated explicitly. However, for the instationary problem significant additional complications occur. They are caused by the fact that in the standard setting the time regularity of the pressure is very low. Furthermore the skew symmetry of the trilinear convection term cannot be used since it only holds if the first argument is solenoidal. Therefore we impose more regularity on the solution of the Navier-Stokes equations and need the requirement $\tau \in \mathbf{W}^{2,\infty}$ to maintain these regularities under transformations. Under these assumptions we can show Fréchet differentiability of the design-to-state map

$$\mathbf{W}^{2,\infty} \ni \tau \mapsto \boldsymbol{v}(\tau) \in W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) + W(I; V(\Omega_{\text{ref}}))$$

which leads up in Theorem 4.5 as one of the main results of this thesis.

In Section 5 we start with the discussion of numerical aspects. In various applications the shape of the boundary object is given through a boundary parametrization. We describe how parametrizations of the boundary like B-Splines, Bezier curves and NURBS or the parametrization via the so-called pseudo-solid approach can be linked to the transformation approach. Many parametrizations describe a boundary curve (in 2D) or surface (in 3D) and we use an elasticity equation to transport the boundary displacements into the domain. This process is considered in an efficient adjoint approach for calculating the shape derivatives with respect to shape parameters. Furthermore details about the discretization of the state equation and the updating of the meshes are described.

Finally in Section 6 numerical results for problems governed by the stationary and instationary Navier-Stokes equations are presented. The implementation was done in C++ resulting in a new software package `FlowOpt` using various third party codes. In particular `Sundance` [37] is used for the implementation of the finite element discretization. The numerical tests are based on a DFG benchmark problem in 2D that desribes the flow around an object in a channel. The design of the object exposed to the flow is optimized for different viscosities resulting in different optimal designs. For our numerical tests we used B-splines and the pseudo-solid approach to parametrize the design object.

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2 Notations, Definitions, and Basic Theorems

In this chapter we introduce some basic notations and definitions that we will use throughout this thesis. For the sake of completeness we also describe some terms of the shape optimization ansatz that will be introduced in detail in chapter 3. Finally we state some basic theorems that we will use repeatedly.

2.1 Notations and Definitions

2.1.1 Basic Notations

$\mathbb{N}$	the set of natural numbers
$\mathbb{N}_0$	the set of natural numbers with zero, $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$
$\mathbb{R}$	the set of real numbers
d	the space dimension $d \in \{2, 3\}$
$\mathbb{R}^d$	the d-dimensional space of real numbers
$\mathbb{R}^{d \times d}$	the space of $d \times d$ matrices with real entries
$\mathcal{P}(A)$	the power set of a set $A \subset \mathbb{R}^d$, i.e. $\mathcal{P}(A) := \{B \mid B \subset A\}$
Ω	a bounded domain $\Omega \subset \mathbb{R}^d$, i.e. a nonempty, bounded, open connected set
$\partial\Omega$	the boundary of Ω
B	the design object(s) $B \subset \mathbb{R}^d$ to be shape optimized
Γ_B	the design boundary $\Gamma_B \subset \partial\Omega$ of B
Γ_{ext}	the boundary without the design boundary $\Gamma_{\text{ext}} = \partial\Omega \backslash \Gamma_B$
$\Gamma_{D_{\text{ext}}}$	a part of the exterior Dirichlet boundary, that does not contain any points of the design boundary, i.e. $\Gamma_B \cap \Gamma_{D_{ext}} = \emptyset$
Γ_D	a part of the Dirichlet boundary, $\Gamma_D \subset \partial\Omega$
Γ_N	a part of the Neumann boundary, $\Gamma_N \subset \partial\Omega$, in our applications even $\Gamma_N \subset \Gamma_{\text{ext}}$
$\bar{\Omega}$	the closure of Ω, i.e. $\bar{\Omega} = \Omega \cup \partial\Omega$
n	the dimension of the design space
U	the design space $U \subset \mathbb{R}^n$
I	the identity matrix of dimension d
A^T	the transpose of a vector or matrix A
$\det A$	the determinant of a square matrix A
$\operatorname{tr} A$	the trace of a square matrix $A \in \mathbb{R}^{m \times m}$, i.e. $\operatorname{tr} A := \sum_{i=1}^m A_{ii}$
$A : B$	the Frobenius inner product of matrices $A, B \in \mathbb{R}^{m \times m}$, i.e. $(A : B) := \sum_{i,j=1}^m A_{ij} B_{ij} \in \mathbb{R}$

In context of vector spaces we use

$\|\|v\|\|_p$	p-norm of a vector $v \in \mathbb{R}^d$ for $p \in \mathbb{N}$, i.e. $\|\|v\|\|_p := \sqrt[p]{\sum_{i=1}^d \|v_i\|^p}$
$\|\|v\|\|$	euclidian norm of a vector $v \in \mathbb{R}^d$, i.e. $\|\|v\|\| := \|\|v\|\|_2$
$\|\|v\|\|_X$	the standard norm of a vector $v \in X$, where X is a vector space
$B_{\|\|\cdot\|\|_X}(x;r)$	the open ball around x with radius r, i.e. $B_{\|\|\cdot\|\|_X}(x;r) := \{y \in X \mid \|\|y-x\|\|_X < r\}$
$B(x;r)$	the euclidian open ball around x with radius r, i.e. $B(x;r) := \{y \in \mathbb{R}^d \mid \|\|y-x\|\|_2 < r\}$
$X+Y$	the sum of two subspaces $X, Y \subset W$, where W is a vector space, i.e. $X+Y := \{x+y \mid x \in X, y \in Y\}$
$L(X,Y)$	the vector space of continuous linear functions $f : X \to Y$
X^*	the dual space of a vector space X, i.e. $X^* = L(X, \mathbb{R})$
$\langle \cdot, \cdot \rangle_{X^*,X}$	the dual pairing, i.e. $\langle y, x \rangle_{X^*,X} := y(x) \in \mathbb{R}$
$(\cdot,\cdot)$	the L^2 scalar product
A^*	the dual operator of a bounded linear operator $A \in L(X,Y)$, i.e. $A^* \in L(Y^*, X^*)$ with $\langle A^*y, x\rangle_{X^*,X} := \langle y, Ax \rangle_{Y^*,Y}$
$X \hookrightarrow Y$	the space X is continuously embedded into the space Y
$X \hookrightarrow\hookrightarrow Y$	the space X is compactly embedded into the space Y
$\mathrm{cl}_{\|\|\cdot\|\|_X} Y$	the closure of a vector space Y with respect to the $\|\|\cdot\|\|_X$-norm

2.1.2 Functions

id	the identity function, i.e. $\mathrm{id}(x) := x$ on a suitable domain
$\boldsymbol{f}$	a vector-valued function (bold print)
$\boldsymbol{f}'$	the Jacobian $D\boldsymbol{f}$ of a vector-valued function
$\nabla \boldsymbol{f}$	the gradient of a vector-valued function; i.e. for a function $\boldsymbol{f} : \mathbb{R}^d \to \mathbb{R}^m$ we have $\nabla \boldsymbol{f} := (\boldsymbol{f}')^T = \left(\frac{\partial \boldsymbol{f}_j}{\partial x_i}\right)_{\substack{i=1,\ldots,d \\ j=1,\ldots,m}} = \begin{pmatrix} \frac{\partial \boldsymbol{f}_1}{\partial x_1} & \cdots & \frac{\partial \boldsymbol{f}_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{f}_1}{\partial x_d} & \cdots & \frac{\partial \boldsymbol{f}_m}{\partial x_d} \end{pmatrix}$
$\det F$	the determinant of a function $F : \mathbb{R}^d \to \mathbb{R}^{m \times m}$; $(\det F)(x) := \det F(x)$
$\mathrm{tr}\ F$	the trace of a function $F : \mathbb{R}^d \to \mathbb{R}^{m\times m}$; $(\mathrm{tr}\ F)(x) :=\ \mathrm{tr}\ F(x)$
$\mathrm{div}\ \boldsymbol{f}$	the divergence of a vector field $\boldsymbol{f} : \mathbb{R}^d \to \mathbb{R}^d$; $\mathrm{div}\ (\boldsymbol{f}) := \nabla \cdot \boldsymbol{f} := \sum_{i=1}^d \frac{\partial \boldsymbol{f}_i}{\partial x_i} \in \mathbb{R}$
Δf	the Laplace operator applied to a function $f : \mathbb{R}^d \to \mathbb{R}$; $\Delta f :=\ \mathrm{div}\ (\nabla f)$
$\Delta \boldsymbol{f}$	the vector Laplacian for $\boldsymbol{f} : \mathbb{R}^d \to \mathbb{R}^d$; $\Delta \boldsymbol{f} := (\mathrm{div}\ (\nabla f_1) \ldots\ \mathrm{div}\ (\nabla f_d))^T$
$\boldsymbol{f}_t$	the time derivative of $\boldsymbol{f}$; $\boldsymbol{f}_t := \frac{\partial \boldsymbol{f}}{\partial t}$
$\boldsymbol{f}_{x_i}$	the spacial derivative in the i-th unit direction, i.e. $\boldsymbol{f}_{x_i} := \frac{\partial \boldsymbol{f}}{\partial x_i}$
$\partial_i \boldsymbol{f}$	the spacial derivative in the i-th unit direction, i.e. $\partial_i \boldsymbol{f} := \boldsymbol{f}_{x_i}$
$\partial_n \boldsymbol{f}$	the spacial derivative in the normal direction $n(x) \in \mathbb{R}^d$ (on a Lipschitz boundary)
$(\boldsymbol{w} \cdot \nabla)\boldsymbol{v}$	the convection term; $(\boldsymbol{w} \cdot \nabla)\boldsymbol{v} := \left(\sum_{j=1}^d \boldsymbol{w}_j \frac{\partial v_i}{\partial x_j}\right)_{i=1,\ldots,d}$
$\mathrm{supp}(f)$	the support of f, i.e. $\mathrm{supp}(f) := \overline{\{x \in \Omega \mid f(x) \neq 0\}}$

2.1.3 Functions and Function Spaces in context of Shape Optimization with Transformations

The following expressions will be introduced in detail in Section 3.2. For the sake of completeness we tabulate them also here:

Ω_{ref}	the reference domain
τ	a transformation function $\tau : \Omega_{\text{ref}} \to \mathbb{R}^d$ to transform Ω_{ref} to a domain $\Omega(\tau) = \tau(\Omega_{\text{ref}})$
$\Omega(\tau)$	the domain that belongs to a transformation τ, i.e. $\Omega(\tau) := \tau(\Omega_{\text{ref}})$
$\tilde{\tau}$	a transformation function defined on the actual domain $\tau(\Omega_{\text{ref}})$ to transform $\tau(\Omega_{\text{ref}})$ to a domain $\tilde{\tau}(\tau(\Omega_{\text{ref}}))$
T_{ref}	an affine space of transformations $\tau : \Omega_{\text{ref}} \to \mathbb{R}^d$
$T(\Omega)$	an affine space of transformations $\tau : \Omega \to \mathbb{R}^d$
Y_{ref}	a state space with functions defined on the domain Ω_{ref}
$Y(\Omega)$	a state space with functions defined on the domain Ω
$Y(\tau)$	a state space with functions defined on the domain $\tau(\Omega_{\text{ref}})$
Z_{ref}	a function space with functions defined on the domain Ω_{ref}, usually the image space of the state equation
$Z(\Omega)$	a function space with functions defined on the domain Ω, usually the image space of the state equation
$Z(\tau)$	a function space with functions defined on the domain $\tau(\Omega_{\text{ref}})$, usually the image space of the state equation

2.1.4 Classical Differentiability and Regular Domains

In this part we follow [31]. There are many books describing the basic concepts of this subsection. For a more detailed description within optimal control see e.g. [31], [61] or [18].
In this work $\Omega \subset \mathbb{R}^d$ will always be a bounded domain, i.e. a nonempty, bounded, open, connected set. Some of the following definitions are also reasonable if Ω is only an open set or an open, bounded set. However for a clear arrangement we will always use that Ω is a bounded domain and not discuss generalizations of the concepts.
For a *multiindex* $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ the *order* of the multiindex is defined by $|\alpha| := \sum_{i=1}^d \alpha_i$. The $|\alpha|$-th order partial derivative of a function $f : \Omega \to \mathbb{R}$ in $x \in \Omega$ is defined by

$$D^\alpha f(x) := \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots x_d^{\alpha_d}}(x).$$

First we define basic spaces of continuous and differentiable functions. We define for $k \in \mathbb{N}_0$ and $\beta \in (0,1]$:

$$\begin{aligned}
C(\Omega) &:= \{f : \Omega \to \mathbb{R} \mid f \text{ is continuous}\},\\
C(\bar{\Omega}) &:= \{f : \bar{\Omega} \to \mathbb{R} \mid f \text{ is continuous}\},\\
C^k(\Omega) &:= \{f \in C(\Omega) \mid D^\alpha f \in C(\Omega) \text{ for } |\alpha| \le k\},\\
C^k(\bar{\Omega}) &:= \{f \in C^k(\Omega) \mid D^\alpha f \text{ has a continuous extension to } \bar{\Omega} \text{ for } |\alpha| \le k\},\\
C^{k,\beta}(\bar{\Omega}) &:= \{f \in C^k(\bar{\Omega}) \mid D^\alpha f \text{ is } \beta\text{-Hölder continuous for } |\alpha| \le k\},\\
C^\infty(\Omega) &:= \{f \in C(\Omega) \mid D^\alpha f \in C(\Omega)\ \forall \alpha \in \mathbb{N}_0^d\},\\
C^\infty(\bar{\Omega}) &:= \{f \in C^\infty(\Omega) \mid D^\alpha f \text{ has a continuous extension to } \bar{\Omega}\ \forall \alpha \in \mathbb{N}_0^d\},\\
C_c^\infty(\Omega) &:= \{f \in C^\infty(\bar{\Omega}) \mid \operatorname{supp}(f) \subset \Omega \text{ compact}\}.
\end{aligned}$$

Here, a function $f : \bar{\Omega} \to \mathbb{R}$ is *β-Hölder continuous* if there exists a constant $c > 0$ with

$$|f(x) - f(y)| \le c||x - y||^\beta \qquad \forall x, y \in \bar{\Omega}.$$

It is common to set $C^{k,0}(\bar{\Omega}) := C^k(\bar{\Omega})$. 1-Hölder continuity is also known as *Lipschitz continuity.*
The following spaces are Banach spaces with the indicated norms:

$$\begin{aligned}
&\Big(C(\bar{\Omega}),\ ||f||_{C(\bar{\Omega})} := \sup_{x \in \Omega} |f(x)|\Big),\\
&\Big(C^k(\bar{\Omega}),\ ||f||_{C^k(\bar{\Omega})} := \sum_{|\alpha| \le k} ||D^\alpha f||_{C(\Omega)}\Big),\\
&\Big(C^{k,\beta}(\bar{\Omega}),\ ||f||_{C^{k,\beta}(\bar{\Omega})} := ||f||_{C^k(\bar{\Omega})} + \sum_{|\alpha| = k} \sup_{x,y \in \bar{\Omega}, x \ne y} \frac{|D^\alpha f(x) - D^\alpha f(y)|}{||x - y||^\beta}\Big).
\end{aligned}$$

With this basis we can define a classification of the boundary of Ω and define normal derivatives.
For $k \in \mathbb{N}_0 \cup \{\infty\}$ and $\beta \in [0,1]$ we say that Ω *has a $C^{k,\beta}$-boundary*, if for all $x \in \partial\Omega$ there exists $r > 0, l \in \{1, \dots, d\}, \sigma \in \{-1, +1\}$, and a function $\gamma \in C^{k,\beta}(\mathbb{R}^{d-1})$ such that

$$\Omega \cap B(x; r) = \{y \in B(x; r) \mid \sigma y_l < \gamma(y_1, \dots, y_{l-1}, y_{l+1}, \dots, y_d)\}.$$

Instead of $C^{0,1}$-boundary we say also *Lipschitz boundary.* A domain Ω with Lipschitz boundary is called a *Lipschitz domain.* In the same fashion we can speak of domains with $W^{k,p}$-boundaries.
If $\partial\Omega$ is a Lipschitz boundary the outward pointing unit normal $n(x)$ exists for a.a. $x \in \partial\Omega$. Thus we can define the *unit outer normal field* $n : \partial\Omega \to \mathbb{R}^d$ where $||n(x)|| = 1$. Furthermore let $f \in C^1(\bar{\Omega})$. If $\partial\Omega$ is a Lipschitz boundary we can define the *normal derivative*

$$\frac{\partial f}{\partial n}(x) := \sum_{i=1}^d n_i(x) \frac{\partial f}{\partial x_i}(x) \in \mathbb{R}, \qquad x \in \partial\Omega.$$

This definition can be extended to vector-valued functions $\boldsymbol{f}$ in a canonical way. For introducing weak derivatives we state here the well-known integration by parts formula.

Lemma 2.1. ***(Gauß-Green theorem, integration by parts formula)*** *Let Ω be a Lipschitz domain and $u, v \in C^1(\bar{\Omega})$. Then*

$$\int_\Omega u_{x_i}(x)v(x)\ dx = -\int_\Omega u(x)v_{x_i}(x)\ dx + \int_{\partial\Omega} u(x)v(x)n_i(x)\ dS(x).$$

2.1.5 Lebesgue and Sobolev Spaces

We recall the definition of the Lebesgue spaces. For $1 \leq p \leq \infty$ we have

$$\mathcal{L}^p(\Omega) := \{f : \Omega \to \mathbb{R} \mid f \text{ Lebesgue measurable}, ||f||_{L^p(\Omega)} < \infty\},$$

where for $p \in [1, \infty)$

$$||f||_{L^p(\Omega)} := \left(\int_\Omega |f(x)|^p\ dx\right)^{1/p}$$

and

$$||f||_{L^\infty(\Omega)} := \operatorname*{ess\,sup}_{x\in\Omega} |f(x)| := \inf_{\mu(\omega)=0} (\sup_{x\in\Omega\setminus\omega} |f(x)|).$$

Here, μ is the d-dimensional Lebesgue measure. Let $\sim_p$ be the equivalence relation defined by $f \sim_p g :\Leftrightarrow ||f - g||_{L^p(\Omega)} = 0$. Then with

$$L^p(\Omega) := \mathcal{L}^p(\Omega)/\sim_p$$

the space $(L^p(\Omega),\ ||\cdot||_{L^p(\Omega)})$ is a Banach space for $p \in [1, \infty]$. For $p \in (1, \infty)$ this space is also reflexive. Furthermore for $p \in [1, \infty)$ the dual space $(L^p(\Omega))^*$ can be identified with $L^q(\Omega)$ where $\frac{1}{p} + \frac{1}{q} = 1$. In fact, the map $f \in L^q(\Omega) \mapsto g^* \in (L^p(\Omega))^*$, where $\langle g^*, g\rangle_{L^p(\Omega)^*, L^p(\Omega)} := \int_\Omega f(x)g(x)\ dx$ is an isometric isomorphism.
Furthermore we define

$$\mathcal{L}^p_{loc}(\Omega) := \{f : \Omega \to \mathbb{R} \mid f \text{ Lesbesgue measureable}, f \in \mathcal{L}^p(K)\ \forall K \subset \Omega \text{ compact}\}$$

and $L^p_{loc}(\Omega) := \mathcal{L}^p_{loc}(\Omega)/\sim_p$.
To define the Sobolev spaces we introduce the well-known weak differentiability concept. Let $f \in L^1_{loc}(\Omega)$ and $\alpha \in \mathbb{N}_0^d$ be a multiindex. If there exists a function $g \in L^1_{loc}(\Omega)$ such that

$$\int_\Omega g(x)\phi(x)\ dx = (-1)^{|\alpha|} \int_\Omega f(x)D^\alpha\phi(x)\ dx, \qquad \forall\phi \in C_c^\infty(\Omega)$$

then we call $D^\alpha f := g$ the *α-th weak partial derivative* of f.
For $k \in \mathbb{N}_0$ and $p \in [1, \infty]$ we define the *Sobolev space*

$$W^{k,p}(\Omega) := \{f \in L^p(\Omega) \mid f \text{ has weak derivatives } D^\alpha f \in L^p(\Omega)\ \forall|\alpha| \leq k\},$$

which is a Banach space with the norm

$$||f||_{W^{k,p}(\Omega)} := \left(\sum_{|\alpha|\leq 1} ||D^\alpha f||^p_{L^p(\Omega)} \right)^{1/p} \qquad \forall k \in \mathbb{N}_0, \forall p \in [1,\infty),$$

$$||f||_{W^{k,\infty}(\Omega)} := \sum_{|\alpha|\leq 1} ||D^\alpha f||_{L^\infty(\Omega)} \qquad \forall k \in \mathbb{N}_0.$$

Let $k \in \mathbb{N}_0$ and $p \in [1,\infty]$. Based on $W^{k,p}(\Omega)$ we will use the following spaces:

$$\begin{aligned} W_0^{k,p}(\Omega) &:= \mathrm{cl}_{||\cdot||_{W^{k,p}(\Omega)}} \left(C_c^\infty(\Omega)\right), \\ H^k(\Omega) &:= W^{k,2}(\Omega), \\ H_0^k(\Omega) &:= W_0^{k,2}(\Omega), \\ H^{-k}(\Omega) &:= (H_0^k(\Omega))^*, \\ H_0^{-k}(\Omega) &:= (H^k(\Omega))^*. \end{aligned}$$

We also have a Gauß-Green theorem for Sobolev spaces

Lemma 2.2. ***(Weak Gauß-Green theorem, integration by parts formula)*** *Let Ω be a Lipschitz domain and $u \in W^{1,p}(\Omega), v \in W^{1,q}(\Omega)$ with $\frac{1}{p} + \frac{1}{q} = 1$. Then for $i = 1, \dots, d$*

$$\int_\Omega u_{x_i}(x)v(x)\ dx = -\int_\Omega u(x)v_{x_i}(x)\ dx + \int_{\partial\Omega} u(x)v(x)n_i(x)\ dS(x).$$

The proof can be found in, e.g. [4, Theorem A6.8].

2.1.6 Banach Space-valued Spaces

Now we need to introduce spaces that also include a time component. For a separable Banach space $(X,\ ||\cdot||_X)$ and a time interval $I = [0,T]$ with $T > 0$, we introduce the *Bochner spaces*

$$L^p(I;X) := \{f : I \to X \text{ str. measurable} \mid ||f||_{L^p(I;X)} := (\int_I ||f(t)||_X^p\ dt)^{\frac{1}{p}} < \infty\}$$

and

$$L^\infty(I;X) := \{f : I \to X \text{ str. measurable} \mid ||f||_{L^\infty(I;X)} := \operatorname*{ess\,sup}_{t\in I} ||f(t)||_X < \infty\}.$$

For the concept of strongly measurable functions in context of Banach space-valued functions see e.g. [18, Appendix E] or in more detail [69].
If X is a function space, $X \subset \{f : \Omega \to \mathbb{R}\}$, an element $g \in L^p(I;X)$ can also be considered as a real-valued function $g = g(\cdot,t) = g(x,t)$, with $x \in \Omega$ and $t \in I$. Then for a.a. $t \in I$ we have $g(\cdot,t) \in X$ with respect to the spacial variable x.

For a Banach space X the corresponding Bochner space $L^p(I;X)$ is also a Banach space for $p \in [1,\infty]$. Furthermore for $1 \le p < \infty$ the dual space of $L^p(I;X)$ can isometrically be identified with $L^q(I;X^*)$, where $\frac{1}{p}+\frac{1}{q}=1$, via

$$\langle f, g\rangle_{L^q(I;X^*),L^p(I;X)} := \int_0^T \langle f(t), g(t)\rangle_{X^*,X} \; dt.$$

Furthermore we introduce the spaces

$$\begin{aligned} W_{p,q}(I;X) &:= \{f \in L^p(I;X) \mid f_t \in L^q(I;X^*)\}, \\ W(I;X) &:= W_{2,2}(I;X). \end{aligned}$$

We consider a Gelfand triple $V \hookrightarrow W = W^* \hookrightarrow V^*$ where V, W are Hilbert spaces with the continuous and dense embedding $V \hookrightarrow W$. Then $W(I;V)$ is a Banach space with the norm

$$||f||_{W(I;V)} := \sqrt{||f||^2_{L^2(I;V)} + ||f_t||^2_{L^2(I;V^*)}}.$$

For a Gelfand triple we have the following nice embedding theorem for the time-dependent spaces:

Lemma 2.3. *Let $V \hookrightarrow W \hookrightarrow V^*$ be a Gelfand triple. Then $W(I;V)$ is a Hilbert space and we have the continuous embedding*

$$W(I;V) \hookrightarrow C(I;W).$$

2.1.7 Product Spaces

The d-dimensional product space of a space X is denoted by a bold letter $\boldsymbol{X}$. In detail we have $\boldsymbol{X} := \{\boldsymbol{v} \in X^d\}$. If X is a Banach space, $\boldsymbol{X}$ is also a Banach space equipped with the norm

$$||\boldsymbol{v}||_{\boldsymbol{X}} := \left(\sum_{i=1}^d ||v_i||^2_X\right)^{1/2}.$$

2.2 Basic Theorems

We will use the following theorems in the remainder of this work. A well-known tool in the analysis of parabolic partial differential equations is Gronwall's inequality. There are various versions of this inequality. For a variant in differential or integral form, see e.g. [18, Appendix B].

Lemma 2.4. ***(Gronwall's inequality in differential form)*** *Let $\eta : [0,T] \to \mathbb{R}$ be a continuously differentiable function, which satisfies for a.a. $t \in [0,T]$ the differential inequality*

$$\eta'(t) \le \phi(t)\eta(t) + \psi(t)$$

where $\phi : [0,T] \to \mathbb{R}$ and $\psi : [0,T] \to \mathbb{R}$ are continuous functions. Then for all $t \in [0,T]$

$$\eta(t) \le \eta(0)e^{\int_0^t \phi(u)\; du} + \int_0^t \psi(s) e^{\int_s^t \phi(u)\; du}\; ds. \tag{2.1}$$

Proof. Because there are different versions of Gronwall's inequality, we state a short proof for this version. Let $\alpha(t) := e^{-\int_0^t \phi(u)du}$. Then

$$(\alpha\eta)' = -\phi\alpha\eta + \alpha\eta' \leq -\phi\alpha\eta + \alpha\psi + \alpha\phi\eta = \alpha\psi.$$

Using the fundamental theorem of calculus and $\alpha(0) = 1$ we arrive at

$$\alpha(t)\eta(t) - \eta(0) \leq \int_0^t \psi(s)\alpha(s)\ ds.$$

Multiplying with $\frac{1}{\alpha(t)} = e^{\int_0^t \phi(u)du}$ we finally arrive at (2.1). □

Another very helpful elementary lemma is Young's inequality.

Lemma 2.5. ***(Young's inequality)*** *Let $p, q \in [1, \infty)$ with $\frac{1}{p} + \frac{1}{q} = 1$. Then for all $a, b > 0$*

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q}. \tag{2.2}$$

For the simple proof see e.g. [18, Appendix B]. We will especially use the following direct consequence.

Lemma 2.6. ***(Young's inequality with ϵ)*** *Let $p, q \in (1, \infty)$ with $\frac{1}{p} + \frac{1}{q} = 1$. Then for all $a, b > 0$ and $\epsilon > 0$*

$$ab \leq \epsilon a^p + C(\epsilon, p, q)b^q \tag{2.3}$$

where $C(\epsilon, p, q) := \frac{(\epsilon p)^{-q/p}}{q}$ is independent of a and b.

Furthermore we will use Hölder's inequality:

Lemma 2.7. ***(Hölder's inequality)*** *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain.*

1. *Let $1 \leq p, q \leq \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$ and $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$. Then $fg \in L^1(\Omega)$ and*

   $$||fg||_{L^1(\Omega)} \leq ||f||_{L^p(\Omega)}||g||_{L^q(\Omega)}.$$

   The above inequality is known as Hölder's inequality.

2. *Let $m \geq 3$ and $1 \leq p_i \leq \infty$ for $i \in \{1, \ldots, m\}$ with $\sum_{i=1}^m \frac{1}{p_i} = 1$. Furthermore let $f_i \in L^{p_i}(\Omega)$. Then $\prod_{i=1}^m f_i \in L^1(\Omega)$ and*

   $$||\prod_{i=1}^m f_i||_{L^1(\Omega)} \leq \prod_{i=1}^m ||f_i||_{L^{p_i}(\Omega)}.$$

Proof. The proof of the well-known first assertion can be found in, e.g., [67, Theorem I.1.6]. The second part follows by successive application of the first part. □

We will now state some embedding results. Using Hölder's inequality we can show a simple embedding for the Lebesgue spaces:

Lemma 2.8. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and $1 \le p \le q \le \infty$. Then $L^q(\Omega) \hookrightarrow L^p(\Omega)$. In detail we have*

$$||f||_{L^p(\Omega)} \le \mu(\Omega)^{1/p-1/q}||f||_{L^q(\Omega)}.$$

For the Sobolev spaces we use the following compact embeddings:

Lemma 2.9. ***(Sobolev embeddings)*** *Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz domain, $p \in [1, \infty]$ and $m \in \mathbb{N}_0$. Then we have the follwoing embeddings:*

1. *Let $m < \frac{d}{p}$ and $\frac{1}{p^*} = \frac{1}{p} - \frac{m}{d}$. Then*

$$W^{m,p}(\Omega) \hookrightarrow\hookrightarrow L^{p^*}(\Omega).$$

2. *Let $m = \frac{d}{p}$ and $1 \le p \le q \le \infty$. Then*

$$W^{m,p}(\Omega) \hookrightarrow\hookrightarrow L^q(\Omega).$$

3. *Let $m > \frac{d}{p}$. Then*

$$W^{m,p}(\Omega) \hookrightarrow\hookrightarrow C^0(\bar{\Omega}).$$

The proof can be found in [2, Theorem 5.4] where also further imbedding theorems are given.

3 Shape Optimization with Navier-Stokes Equations

In this chapter we will describe our approach to shape optimization with the Navier-Stokes equations. To this end we will first introduce a shape optimization setting that is based on the *perturbation of the identity* method, introduced by Murat and Simon, c.f. [44], [45]. This ansatz provides a clean framework based on function spaces which makes techniques of optimal control applicable. Furthermore we state results about existence theory of optimal solutions and show how shape derivatives can be calculated in this setting.
We will then apply these techniques to shape optimization problems in Navier-Stokes flow and describe how first and second shape derivatives can be calculated efficiently.

3.1 Shape Optimization in the Abstract Setting

We consider the following shape optimization problem: Find a domain $\Omega \subset \mathbb{R}^d$ that minimizes an objective function $\bar{J}$, where Ω is restricted to a set of admissible domains $\mathcal{O}_{\text{ad}}$ which may model geometric constraints. Here, $\bar{J}$ depends on a domain Ω and a state $\tilde{y}$, where $\tilde{y}$ is the solution of a partial or ordinary differential equation that lives on the domain Ω. Usually, $\tilde{y}$ is contained in a Banach space of functions $Y(\Omega)$ and the fact that $\tilde{y}$ solves a differential equation can be expressed as $\bar{E}(\tilde{y}, \Omega) = 0$ with an operator $\bar{E}$ including initial and boundary conditions. Formally we have:

Problem 3.1. *Let $d \in \{2, 3\}$ and $\mathcal{O}_{ad} \subset \{\Omega \subset \mathbb{R}^d \mid \Omega \text{ is a bounded domain}\}$ be a set of admissible domains. Furthermore for each $\Omega \in \mathcal{O}_{ad}$ let $Y(\Omega)$ and $Z(\Omega)$ be Banach spaces of functions defined on Ω. Let $\bar{J}$ be the objective function*

$$\bar{J} : \{(\tilde{y}, \Omega) \mid \tilde{y} \in Y(\Omega), \Omega \in \mathcal{O}_{ad}\} \to \mathbb{R},$$

and $\bar{E}$ be an operator between the sets of admissible function spaces

$$\bar{E} : \{(\tilde{y}, \Omega) \mid \tilde{y} \in Y(\Omega), \Omega \in \mathcal{O}_{ad}\} \to \{\tilde{z} \mid \tilde{z} \in Z(\Omega)\}.$$

Then we call

$$\min \bar{J}(\tilde{y}, \Omega) \quad s.t.\ \bar{E}(\tilde{y}, \Omega) = 0,\ \Omega \in \mathcal{O}_{ad} \tag{3.1}$$

the ***shape optimization problem****.*

It is also possible to consider shape optimization problems even more general than problem (3.1), c.f. [14]. However, even the framework of problem (3.1) is not suitable for an analytical investigation of topics like shape continuity, shape differentiability, existence and uniqueness theory of optimal solutions, and optimality conditions for optimal solutions.
To overcome this difficulty there a different approaches in the literature. First of all we may want to define a suitable topology on the set of admissible domains $\mathcal{O}_{\text{ad}} \subset \mathcal{P}(\mathbb{R}^d)$. Unfortunately, there is no straight forward way to do this. To get control of the variation of subsets of $\mathbb{R}^d$ many authors represent domains in different ways. One way is to represent domains as level sets of a function or local epigraphs. Another way is to represent domains as the image of a

transformation of a *reference domain*. Depending on the representation of the domain different topology concepts have been introduced, e.g. the *Courant metric*, topologies generated by distance functions (*characteristic functions*, *(complementary) Hausdorff metric*, $W^{1,p}$*-topology*) and *algebraic and signed distance functions*.
Usually the 'set of admissible domains belongs to some shape space which is generally nonlinear and nonconvex' ([14, p.8]). To use well known methods of differential calculus some linear space structure has to be introduced if one wants to analyze the continuity and differentiability of shapes. Historically, Hadamard [24] was one of the first contributors to shape optimization in this context. Two common frameworks to define *shape derivatives* in context of transformations are

- the *velocity method* (also known as *speed method*), introduced by Zolésio [71], [72] and
- the *method of perturbation of the identity*, introduced by Murat and Simon [45], [44], [43].

For some families of transformations both methods can shown to be equivalent in a certain sense, c.f. [14].
Another concept is the *topological derivative*, introduced by Sokolowski and Zochowski [57]. This derivative incorporates sensitivity of a shape function to the presence of holes. This is important for optimization problems where the optimal topology of the domain is not known a priori (e.g. the number of holes).
Also second order shape derivatives can be studied. Early works of second-order methods in context of shape optimization include Fujii [19], [39], Simon [54] and Guillaume and Masmoudi [23].
We will now introduce the shape optimization problem using transformations in the velocity method setting and will link this approach to the method of perturbations by Murat and Simon that we will use. We will then state the shape optimization problem and show how first and second derivatives can be derived in this setting.

3.1.1 Shape Optimization with Domains Represented by Transformations

In 1972 Micheletti [40] introduced the *Courant metric* on a family of C^k-domains which are images of a reference domain of class C^k through a family of C^k-diffeomorphisms of $\mathbb{R}^d$. For the metric, the underlying algebraic structure is not a vector space structure but a group structure w.r.t. the compositions of transformations. In general for a Banach space Θ of transformations from a fixed open set $D \subset \mathbb{R}^d$ into $\mathbb{R}^d$ Micheletti considers the group of diffeomorphisms

$$\mathcal{F}(\Theta) := \{F : D \to D \mid F - \mathrm{id} \in \Theta, F^{-1} - \mathrm{id} \in \Theta\}.$$

Then for a reference domain $\Omega_{\mathrm{ref}} \subset D$ the set of admissible domains $\mathcal{O}_{\mathrm{ad}}$ can be represented by a subset of

$$T(\Omega_{\mathrm{ref}}) := \{F(\Omega_{\mathrm{ref}}) \mid F \in \mathcal{F}(\Theta)\}.$$

For specific choices of D, Θ and Ω_{ref} the quotient group $\mathcal{F}(\Theta)/\mathcal{G}(\Omega_{\text{ref}})$ with

$$\mathcal{G}(\Omega_{\text{ref}}) := \{F \in \mathcal{F}(\Theta) \mid F(\Omega_{\text{ref}}) = \Omega_{\text{ref}}\}$$

can be endowed with the so-called Courant metric to make it a complete metric space. For $D = \mathbb{R}^d$ transformations of the form $\text{id} + \theta$ belong to $\mathcal{F}(\Theta)$ if $||\theta||_\Theta$ is small enough. Hence perturbations of the identity, i.e. Ω_{ref}, can be chosen in the vector space Θ. This makes it possible to define directional derivatives and speak of Gâteaux and Fréchet differentiability in the classical Banach space setting. Details about this approach and about the construction of metrics for the shapes can be found in [14, Chapter 2]. Unfortunately, this approach does not directly extend for domains D that are constrained in a certain way.
However, the basic ideas can be used to derive a similar framework as the *velocity method* or the *method of perturbation of the identity* mentioned above. For the recent ansatz Murat and Simon [45], [44], [43] use $W^{k,\infty}$-transformations of a reference domain to represent domains. Here, the vector space topology of function spaces is used. They introduced a systematic foundation of shape calculus and this will be the setting that we will use, first for defining a general shape optimization problem and later for the case of instationary Navier-Stokes shape optimization. However, it cannot cover design topology changes like the insertion of holes.
We describe now the shape calculus based on transformations as introduced by Zolésio [71] resulting in the 'speed method' or 'velocity method'. We follow here the descriptions in [11, Section 6.1], [14, Chapter 8] and [17, Section 2.2]. Then we will link this approach to the ansatz of Murat and Simon.
Consider a domain $\Omega \in \mathcal{O}_{\text{ad}}$. A shape perturbation can be considered as a map T from Ω to Ω_t where t denotes a scalar design parametrization that measures the shape change where $\Omega = \Omega_0$. The mapping $T : \Omega \times [0, \tau] \to \Omega_t$ with $T : (x, t) \mapsto x_t(x)$ describes the change

$$\begin{aligned} x_t &= T(x, t), \\ \Omega_t &= T(\Omega, t). \end{aligned}$$

This pertubation of Ω to Ω_t can be viewed as a dynamic deforming process where t plays the role of time. With the introduction of T we can interpret domains as a transformation and furthermore a smooth design change for $t \to 0$ can be defined. The name 'speed method' or 'velocity method' comes from interpreting t as time and introducing a design velocity as

$$V(x_t, t) := \frac{dx_t}{dt} = \frac{dT(x,t)}{dt}. \tag{3.2}$$

The design trajectory that was at x at $t = 0$ is then given as the solution of the differential equation

$$\dot{x}_t = V(x_t, t), x_0 = x. \tag{3.3}$$

Thus, if T is given, the design velocity V can be obtained via (3.2). On the other hand for a given velocity V we can construct T with (3.3) and $T(x, t) := x_t$.

Murat and Simon [45] introduced a perturbation of the identity of the actual domain Ω. This approach can be interpreted as the introduction of a transformation of the form

$$T_t(x) := T(x,t) := x + tW(x)$$

where $W(x)$ is a vector field in a suitable Banach space. We can construct the time dependent velocity field $V(x,t)$ associated with the perturbation of the identity. The appropriate choice of V that solves (3.3) is

$$V(x,t) := W(T_t^{-1}(x)) \qquad \forall x \in \mathbb{R}^d, \forall t \geq 0. \tag{3.4}$$

3.1.2 Shape Derivatives

We will now introduce shape derivatives where we use the velocity method concept of the last section to describe perturbations of domains. The same results can be obtained for the perturbation of identity ansatz as these transformations can be recovered with nonautonomous velocity fields via (3.4). We will follow the rather general approach decribed in [14, Section 8.3]. First of all we define shape functions.

Definition 3.1. *Let $\emptyset \neq D \subset \mathbb{R}^d$ and $\mathcal{A} \subset \mathcal{P}(D) = \{\Omega \mid \Omega \subset D\}$. Furthermore let E be a topological space. A shape function is a map*

$$J : \mathcal{A} \to E$$

such that for any homeomorphism T of $\bar{D}$ we have

$$T(\Omega) = \Omega \Rightarrow J(\Omega) = J(T(\Omega)) \quad \forall \Omega \in \mathcal{A}.$$

For the velocity field V we assume, c.f. [14, Assumption (3.1)],

$$(V) \quad \begin{cases} \exists \tau > 0 : \forall x \in \mathbb{R}^d : \ V(x,\cdot) \in C([0,\tau],\mathbb{R}^d), \\ \exists c > 0 : \forall x,y \in \mathbb{R}^d : \ ||V(y,\cdot) - V(x,\cdot)||_{C([0,\tau],\mathbb{R}^d)} \leq c||y-x||. \end{cases}$$

We can now define some differentiability concepts for shape functions, based on [14, Definition 3.1].

Definition 3.2. *Let Θ be a topological vector subspace of Lipschitz continuous functions from $\mathbb{R}^d$ to $\mathbb{R}^d$ and J be a real-valued shape function.*

1. *Let a velocity field V satisfying (V) be given. J is said to have an Eulerian semiderivative at Ω in the direction V if*

   $$dJ(\Omega, V) := \lim_{t \to 0, t > 0} \frac{J(\Omega_t(V)) - J(\Omega)}{t}$$

   exists where $\Omega_t(V) = T(\Omega, t)$ with T given through the design velocity V.

2. *For a time independent Lipschitz continuous function $\theta : \mathbb{R}^d \to \mathbb{R}^d$ we define the autonomous velocity field*

   $$V_\theta(x,t) := \theta(x) \quad \forall t \in [0,\tau]$$

   and use the notation $dJ(\Omega, \theta) := dJ(\Omega, V_\theta)$.

3. *Let $\theta \in \Theta$. Then J is said to have a Hadamard semiderivative at Ω in the direction θ with respect to Θ if for all V satisfying (V) with $V(t) \in \Theta$ and $V(0) = \theta$ we have that $dJ(\Omega, V)$ exists and only depends on $V(0) = \theta$. The Hadamard semiderivative is denoted by*

$$d_H J(\Omega, \theta) := dJ(\Omega, V(0)).$$

4. *J is said to be differentiable at Ω in Θ^* if it has an Eulerian semiderivative at Ω in all direction $\theta \in \Theta$ and if the map*

$$G(\Omega) : \theta \mapsto dJ(\Omega, \theta) \tag{3.5}$$

is linear and bounded. $G(\Omega)$ is called the gradient of J in the dual space Θ^* of Θ.

We obviously have that if J has a Hadamard semiderivative, then it also has an Eulerian semiderivative and $d_H J(\Omega, \theta) = dJ(\Omega, \theta)$. The choice of a shape gradient depends on the choice of the space Θ. In the following we will choose $\Theta := \mathcal{D}(\mathbb{R}^d, \mathbb{R}^d)$ where $\mathcal{D}(\mathbb{R}^d, \mathbb{R}^d)$ is the space of all infinitely differentiable transformations θ of $\mathbb{R}^d$ with compact support. It can be shown that all $V \in \mathcal{D}(\mathbb{R}^d, \mathbb{R}^d)$ satisfy the assumption (V). We define shape differentiability as follows, see also [14, Definition 3.3].

Definition 3.3. *Let J be a real-valued shape function and $\Omega \subset \mathbb{R}^d$.*

1. *The function J is said to be shape differentiable at Ω if it is differentiable at Ω for all $\theta \in \mathcal{D}(\mathbb{R}^d, \mathbb{R}^d)$.*

2. *The map (3.5) defines a vector distribution $G(\Omega) \in \mathcal{D}(\mathbb{R}^d, \mathbb{R}^d)^*$ which is called shape gradient of J at Ω.*

3. *When for $k \geq 0$, $G(\Omega)$ is continuous for the $\mathcal{D}^k(\mathbb{R}^d, \mathbb{R}^d)$ topology, we say that the shape gradient $G(\Omega)$ is of order k.*

The structure theorem [14, Theorem 3.5 + Corollary 1] gives us a nice representation of the shape derivatives that results in the so called *Hadamard formula* (3.6):

Theorem 3.1. *Let J be a real-valued shape function and assume that J has a shape gradient $G(\Omega)$ of order $k \geq 0$ for an open domain $\Omega \subset \mathbb{R}^d$. Furthermore let the boundary Γ of Ω be of class C^{k+1}. Then for all $x \in \Gamma$ the tangent space $L_\Omega(x)$ is a $(d-1)$-dimensional hyperplane to Ω at x and there exists a unique outward unit normal $n(x)$ which belongs to $C^k(\Gamma, \mathbb{R}^d)$. Furthermore there exists a scalar distribution $g(\Gamma)$ in $\mathbb{R}^d$ with support in Γ such that $g(\Gamma) \in C^k(\Gamma)^*$ and for all $V \in \mathcal{D}^k(\mathbb{R}^d, \mathbb{R}^d)$*

$$dJ(\Omega, V) = \langle g(\Gamma), V_{|\Gamma} \cdot n \rangle_{C^k(\Gamma)^*, C^k(\Gamma)}$$

where $V_{|\Gamma}$ denotes the trace operator on Γ. Finally if $g(\Gamma) \in L^1(\Gamma)$ we have

$$dJ(\Omega, V) = \int_\Gamma g V \cdot n d\Gamma \tag{3.6}$$

For the Hadamard formula there are also other versions, e.g. for constrained domains (c.f. [13]).
We now give some basic shape calculus results for calculating shape derivatives for shape functions being a domain or boundary integral. We follow here [17] but other good depictions can be found in [14], [58], [11] or [29]. For domain integrals we have, c.f., e.g. [17, Lemma 2.2.7]:

Theorem 3.2. *Let $\tau > 0$ and V be given such that for $t \in [0, \tau]$ $V(t)$ satisfies (V). Furthermore let $V \in C^0([0, \tau], C^1(\mathbb{R}^d, \mathbb{R}^d))$. Given a function $\phi \in W^{1,1}(\mathbb{R}^d)$ and a bounded measurable domain Ω with boundary Γ, the shape derivative of the function*

$$J_1(\Omega_t) = \int_{\Omega_t} \phi(x)\ dx$$

at $t = 0$ is given by

$$dJ_1(\Omega, V) = \left(\frac{d}{dt} J_1(\Omega_t)\right)_{|t=0} = \int_\Omega div\ (\phi V(0))\ dx$$

where $\Omega_t = T(\Omega, t)$ with T given through the design velocity V. If Ω is an open domain with Lipschitz boundary Γ we have

$$dJ_1(\Omega, V) = \int_\Gamma \phi V(0)^T n\ dx.$$

A more general version can be found in [14, Theorem 4.2]. We exemplarily show how Theorem 3.2 can be proofed via the transformation ansatz:
For $\Omega_t = T(\Omega, t)$ we can use the transformation rule for integrals to rewrite

$$\int_{\Omega_t} \phi(x)\ dx = \int_\Omega \phi(T(x,t)) \det T'(x,t)\ dx.$$

Recalling that $V(x, 0) = \frac{dT(x,0)}{dt}$ we have

$$\begin{aligned}
dJ_1(\Omega, V) &= \frac{d}{dt}\left(\int_\Omega \phi(T(x,t)) \det T'(x,t)\ dx\right)_{|t=0} \\
&= \int_\Omega \left(\phi'(T(x,0))\frac{dT(x,0)}{dt} \det T'(x,0) + \phi(T(x,0))\ \text{tr}\ (\frac{dT'(x,0)}{dt})\right)\ dx \\
&= \int_\Omega \left(\phi'(x)V(x,0) + \phi(x)\ \text{div}\ (V(x,0))\right)\ dx \\
&= \int_\Omega \text{div}\ (\phi V(0))\ dx \\
&= \int_\Gamma \phi V(0)^T n\ dx
\end{aligned}$$

where we used that $\frac{d}{dt}\det(M(t)) = \text{tr}\ (\frac{d}{dt}M(t))$ if $M(t) = I$ and that $x = T(x, 0)$ and $T'(x, 0) = I$.
For boundary integrals we obtain, c.f., e.g. [17, Lemma 2.2.7]:

Theorem 3.3. *Let $\tau > 0$ and for $t \in [0, \tau]$ the velocity field $V(t)$ satisfying (V). Furthermore let $V \in C^0([0,\tau], C^1(\mathbb{R}^d, \mathbb{R}^d))$. Given a function $\psi \in W^{2,1}(\mathbb{R}^d)$ and a bounded measurable domain Ω with C^k boundary Γ, the shape derivative of the function*

$$J_2(\Omega_t) = \int_{\Gamma_t} \psi(x)\ dS$$

at $t = 0$ is given by

$$dJ_2(\Omega, V) = \int_\Gamma D\psi V(0) + \psi[\ div\ (V(0)) - n^T V'(0) n]\ dS$$

where Γ_t is the boundary of $\Omega_t = T(\Omega, t)$ with T given through the design velocity V. Using tangential calculus we can represent $dJ_2(\Omega, V)$ in Hadamard form

$$dJ_2(\Omega, V) = \int_\Gamma (\frac{\partial \psi}{\partial n} + \kappa \psi) V(0)^T n$$

where κ denotes the curvature of Γ in $\mathbb{R}^2$ and twice the number of mean curvature of Γ in $\mathbb{R}^3$. κ is the tangential divergence of n and defined as

$$\kappa := div\ {}_\Gamma n = div\ n - n^T \nabla n n.$$

The proof can be found in a more general version in [14, Theorem 4.3].

3.1.3 Material Derivatives

In context of shape optimization with a state equation as a constraint, objective functions appear that also depend on the solution of the differential equation. In this context we have to use the chain rule to obtain so called *material derivatives.*

We will demonstrate this concept for the material derivative of a state variable, see also [11, Section 6.1.1]. Let $z_t(x_t)$ be a smooth classical solution of an operator state equation

$$\begin{aligned} Az_t &= f \quad \text{for } x \in \Omega_t, \\ z_t &= 0 \quad \text{for } x \in \Gamma_t, \end{aligned}$$

where A is a differential operator. Then $z_t(x_t) = z_t(T(x,t))$ is defined on Ω and $z_t(x_t)$ depends on t in two ways. First of all it is the solution of the state equation on Ω_t and second it is evaluated at $x_t = T(x,t)$. Therefore the *pointwise material derivative* is defined as

$$\dot{z} = \frac{d}{dt} z_t(T(x,t))_{|t=0} = \lim_{t \to 0} \frac{z_t(T(x,t)) - z(x)}{t} \tag{3.7}$$

where $z(x) = z_0(x_0)$. If z_t has a regular extension into a neighbourhood of $\bar{\Omega}_t$, then the material derivative can be seperated into two parts

$$\begin{aligned} \dot{z}(x) &= \lim_{t \to 0} \frac{z_t(T(x,t)) - z(x)}{t} \\ &= \lim_{t \to 0} \frac{z_t(x) - z(x)}{t} + \lim_{t \to 0} \frac{z_t(T(x,t)) - z_t(x)}{t} \\ &= z'(x) + \nabla z \frac{dT(x,t)}{dt}_{|t=0} \end{aligned}$$

where $z'(x)$ is the shape derivative $z'(x) = \lim_{t\to 0} \frac{z_t(x)-z(x)}{t}$. Note that for perturbations of the identity we have $T(x,t) = x + tW(x)$ and therefore

$$\dot{z}(x) = z'(x) + \nabla z W(x).$$

The pointwise material derivative is only defined for classical solutions of a differential equation. However, for variational problems a similar *material derivative* for state variables in Sobolev spaces can be defined, see e.g. [11, Section 6.1.1] and [17, Section 2.2.4] or in more detail [58]. We will discuss this in the next section for the perturbation of identity method.
In the following we will call derivatives of terms that depend on a domain variable (like the solution of a PDE) material derivative. However, derivatives of terms that depend only implicit on such terms (like domain or boundary integrals depending on the solution of a PDE) will be called shape derivative - we follow here the usual notation as for example done in [17, Section 2.2.4] and [58].

3.1.4 The Perturbation of the Identity Method

In this section we present the perturbation of the identity method as introduced by Murat and Simon [45], [44], [43]. In a first step we fix a bounded domain $\Omega_{\text{ref}} \in \mathcal{O}_{\text{ad}}$, called *reference domain*. We assume that an admissible domain $\Omega \subset \mathcal{O}_{\text{ad}}$ can be characterized by a suitable, associated transformation $\tau \in T_{\text{ad}} \subset T(\Omega_{\text{ref}})$, such that $\tau(\Omega_{\text{ref}}) = \Omega$. Here

$$T(\Omega_{\text{ref}}) = \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in S\}$$

is an affine space of transformations defined on Ω_{ref} and S is a suitable Banach space. Furthermore we will restrict the transformations $\tau \in T(\Omega_{\text{ref}})$ to a set T_{ad} of bi-Lipschitz functions where $(\tau - \text{id}) \in D \subset S$ and D is open in S. To link this approach to the set of admissible domains, we assume

$$T_{\text{ad}} = \{\tau \in T(\Omega_{\text{ref}}) \mid \tau(\Omega_{\text{ref}}) \in \mathcal{O}_{\text{ad}}\}.$$

Using this approach the optimization problem (3.1) takes form

Problem 3.2. *Let $d \in \{2,3\}$ and $T_{ad} \subset T(\Omega_{ref})$ be a set of admissible transformations of a reference domain $\Omega_{ref} \in \mathcal{O}_{ad}$. Furthermore for each $\tau \in T_{ad}$ let $Y(\tau)$ and $Z(\tau)$ be Banach spaces of functions defined on $\tau(\Omega_{ref})$. Let $\tilde{J}$ be the objective function*

$$\tilde{J} : \{(\tilde{y}, \tau) \mid \tilde{y} \in Y(\tau), \tau \in T_{ad}\} \to \mathbb{R},$$

and $\tilde{E}$ be an operator between the sets of admissible function spaces

$$\tilde{E} : \{(\tilde{y}, \tau) \mid \tilde{y} \in Y(\tau), \tau \in T_{ad}\} \to \{\tilde{z} \mid \tilde{z} \in Z(\tau)\}.$$

Then we call

$$\min \tilde{J}(\tilde{y}, \tau) \quad s.t.\ \tilde{E}(\tilde{y}, \tau) = 0,\ \tau \in T_{ad} \tag{3.8}$$

*the **shape optimization problem with transformations**.*

To make this approach well defined we require

$$\text{Let } \tau_1,\tau_2 \in T_{\text{ad}} \text{ with } \tau_1(\Omega_{\text{ref}}) = \tau_2(\Omega_{\text{ref}}) =: \hat{\Omega}. \text{ Then for the solutions } y_1 \text{ and } y_2 \text{ of } \tilde{E}(y_1,\tau_1) = 0 \text{ and } \tilde{E}(y_2,\tau_2) \text{ we have } y_1 \circ \tau_1^{-1} = y_2 \circ \tau_2^{-1} =: \hat{y}. \tag{O1}$$

This assumption is needed because different transformations describing the same domain $\hat{\Omega}$ should imply the same state $\hat{y}$ such that $\bar{E}(\hat{y},\hat{\Omega}) = 0$ is guaranteed. However, usually this assumption can be easily fulfilled.
In this setting τ lives in an affine space, but $\tilde{y}$ lives in the set $\bigcup_{\tau\in T_{\text{ad}}} Y(\tau)$ which we have not equipped with a topology yet. The idea is now to transport the spaces $Y(\tau)$ into the space $Y(\text{id})$ whose functions are defined on the reference domain Ω_{ref}. In fact, a function $\tilde{y} \in Y(\tau)$ can be transformed into a function $y = \tilde{y} \circ \tau$ defined on Ω_{ref} using the transformation τ. To achieve that $y = \tilde{y} \circ \tau$ lies in the Banach space $Y(\text{id})$ the affine space of transformations $T(\Omega_{\text{ref}})$ and the Banach spaces $Y(\tau)$ have to be chosen carefully. For this end the transformations are usually chosen to conserve a certain degree of boundary smoothness and the regularity of a function. Usually the set of admissible transformations T_{ad} has also to be chosen small to attain this goal, i.e. only small perturbations of the identity are allowed.
In order to define a suitable space of transformations $T(\Omega_{\text{ref}})$ we consider for the Banach space S the Sobolev space $\mathbf{W}^{k,\infty}(\mathbb{R}^d) = W^{k,\infty}(\mathbb{R}^d)^d$ as defined in Section 2.1.5. Using $S = \mathbf{W}^{k,\infty}(\mathbb{R}^d)$, $T(\Omega_{\text{ref}})$ takes the form of the space $\mathcal{V}^{k,\infty}$ as introduced by Murat and Simon (see Section 2.1 in [45]) via

$$\mathcal{V}^{k,\infty} := \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in \mathbf{W}^{k,\infty}(\mathbb{R}^d)\}$$

with $k \geq 1$. In this context for each transformation $\tau \in \mathcal{V}^{k,\infty}$ we associate a *displacement* $(\tau - \text{id}) \in \mathbf{W}^{k,\infty}(\mathbb{R}^d)$. Note that $\text{id} \in \mathcal{V}^{1,\infty}$ since the displacement $\text{id} - \text{id} \in \mathbf{W}^{1,\infty}(\mathbb{R}^d)$ but $\text{id} \notin \mathbf{L}^{\infty}(\mathbb{R}^d) \supset \mathbf{W}^{1,\infty}(\mathbb{R}^d)$. We obviously have

$$\mathcal{V}^{k,\infty} = \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in \mathbf{L}^{\infty}(\mathbb{R}^d), \\ D^{\alpha}\tau \in \mathbf{L}^{\infty}(\mathbb{R}^d)\ \forall \alpha \in \mathbb{N}_0^d \text{ with } 1 \leq |\alpha| \leq k\}$$

Furthermore $\mathcal{V}^{k,\infty}$ can be characterized by (c.f. [45, Remark 2.1], [46, Theorem 2.2.2] or [15]):

$$\mathcal{V}^{k,\infty} = \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in \mathbf{L}^{\infty}(\mathbb{R}^d), D^{\alpha}\tau \in \mathbf{C}(\mathbb{R}^d), \\ \sup_{x,y\in\mathbb{R}^d, x\neq y} \frac{||D^{\alpha}\tau(y) - D^{\alpha}\tau(x)||}{||y-x||} < \infty\ \forall \alpha \in \mathbb{N}_0^d \text{ with } 0 \leq |\alpha| \leq k-1\}$$

As a certain minimum requirement for the transformations we suppose from now on that T_{ad} is a subset of

$$\mathcal{T}^{k,\infty} := \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid \tau \text{ invertible with } \tau \in \mathcal{V}^{k,\infty}, \tau^{-1} \in \mathcal{V}^{k,\infty}\}$$

for $k \geq 1$. We thus have the relation

$$T_{\text{ad}} \subset \mathcal{T}^{k,\infty} \subset \mathcal{V}^{k,\infty} = T(\Omega_{\text{ref}}) = \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in S\}$$

with the Banach space $S = \mathbf{W}^{k,\infty}(\mathbb{R}^d)$. Note that the affine space $T(\Omega_{\text{ref}})$ - and therefore T_{ad} - can be equipped with the topology induced by the displacement space S.
Regarding the conservation of boundary smoothness and regularity of transformed functions Murat and Simon showed in [45] some basic results that we state for completeness in the next section.

3.1.5 Transforming Domains, Boundaries and Functions

For a bounded domain Ω_{ref} and $\tau \in \mathcal{T}^{k,\infty}$ the set $\tau(\Omega_{\text{ref}})$ is again a bounded domain. Furthermore for the regularity of boundaries we have the following result (c.f. Assertion (2.52) in [45]):

Lemma 3.1. *Let Ω_{ref} be a bounded domain with $W^{k,\infty}$-boundary with $k \geq 1$ and let $\tau \in \mathcal{T}^{k,\infty}$. Then $\tau(\Omega_{ref})$ is a domain with $W^{k,\infty}$-boundary.*

Also Lipschitz domains can be conserved if the $\mathbf{W}^{1,\infty}(\mathbb{R}^d)$-transformations are small enough [5, Lemma 3]:

Lemma 3.2. *Let Ω_{ref} be a bounded domain with Lipschitz boundary. Then there exists a constant $c(\Omega_{ref})$ with $0 < c(\Omega_{ref}) < 1$ such that for all $\tau \in \mathbf{W}^{1,\infty}(\mathbb{R}^d)$*

$$||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\mathbb{R}^d)} < c(\Omega_{ref}) \Rightarrow$$
$$\tau(\Omega_{ref}) \textit{ is a bounded domain with Lipschitz boundary.}$$

Now we analyze the transformation of functions to a reference domain. Let $\tilde{f} : \Omega \to \mathbb{R}^m$ be a function with domain $\Omega = \tau(\Omega_{\text{ref}})$ and $\tilde{f} \in L^1(\tau(\Omega_{\text{ref}}))$. Given a map $\tau \in \mathcal{T}^{k,\infty}$ we define the associated transformed function

$$f : \Omega_{\text{ref}} \to \mathbb{R}^m, \quad f(x) := (\tilde{f} \circ \tau)(x) = \tilde{f}(\tau(x)).$$

We call f the *pullback of $\tilde{f}$ onto Ω_{ref} via τ*. If f is differentiable we obtain for the derivatives

$$D_{\tilde{x}}\tilde{f}(\tau(x)) = D_x f(x)\tau'(x)^{-1}, \qquad \nabla_{\tilde{x}}\tilde{f}(\tau(x)) = \tau'(x)^{-T}\nabla_x f(x).$$

where $\tilde{x} = \tau(x)$ is the space variable on $\tau(\Omega_{\text{ref}})$. Murat and Simon discussed how a transformation affects the regularity of a function. They showed [45, Lemma 4.1]:

Lemma 3.3. *Let Ω be an open domain, $\tau \in \mathcal{T}^{1,\infty}$ and $1 \leq p \leq \infty$. Then*

1. *$f \in L^p(\tau(\Omega)) \Leftrightarrow f \circ \tau \in L^p(\Omega)$.*
2. *$f \in W^{1,p}(\tau(\Omega)) \Leftrightarrow f \circ \tau \in W^{1,p}(\Omega)$.*
3. *If $p \in (1, \infty)$ then $f \in W_0^{1,p}(\tau(\Omega)) \Leftrightarrow f \circ \tau \in W_0^{1,p}(\Omega)$.*

This lemma caps common applications because in many shape optimization problems the state of the underlying PDE belongs to an L^p- or Sobolev space. In Chapter 4, in context of the instationary Navier-Stokes equations, we will analyze the continuity of the map $f \mapsto f \circ \tau$ in detail, in particular also for time dependent spaces.

3.1.6 Reformulating the PDE on a Fixed Domain

We can now define the whole optimization problem on a fixed domain Ω_{ref} by transforming the underlying PDE onto the domain Ω_{ref}. In the setting of problem (3.8) the operator $\tilde{E}$ is defined between spaces

$$\tilde{E} : \{(\tilde{y}, \tau) \mid \tilde{y} \in Y(\tau), \tau \in T_{\text{ad}}\} \to \{\tilde{z} \mid \tilde{z} \in Z(\tau)\}.$$

In the following, we will write T_{ref} for $T(\Omega_{\text{ref}})$. The idea is to transform the spaces $Y(\tau)$ and $Z(\tau)$ to fixed spaces Y_{ref} and Z_{ref} and define an operator $E : Y_{\text{ref}} \times T_{\text{ref}} \to Z_{\text{ref}}$ such that for all $\tau \in T_{\text{ad}}$ and all $\tilde{y} \in Y(\tau)$, it holds that

$$E(y, \tau) = 0 \Leftrightarrow \tilde{E}(\tilde{y}, \tau) = 0.$$

In a similar way an objective function $J : Y_{\text{ref}} \times T_{\text{ref}} \to \mathbb{R}$ is defined with $J(y, \tau) = \tilde{J}(\tilde{y}, \tau)$ for $y = \tilde{y} \circ \tau \in Y_{\text{ref}}$ and $\tau \in T_{\text{ad}}$.
We assume that

$$\left.\begin{aligned} Y(\text{id}) = \{\tilde{y} \circ \tau : \tilde{y} \in Y(\tau)\}, \\ \tilde{y} \in Y(\tau) \mapsto y := \tilde{y} \circ \tau \in Y(\text{id}) \text{ is a homeomorphism} \end{aligned}\right\} \quad \forall \tau \in T_{\text{ad}} \tag{A0}$$

Furthermore we assume that $Z(\tau)$ can be transformed in a similar way. Then with $Y_{\text{ref}} := Y(\text{id})$ and $Z_{\text{ref}} := Z(\text{id})$ we can rewrite problem (3.8) as

Problem 3.3. *We call*

$$\min J(y, \tau) \quad s.t. \; E(y, \tau) = 0, \;\; \tau \in T_{ad}, \tag{3.9}$$

where $J : Y_{ref} \times T_{ref} \to \mathbb{R}$ and $E : Y_{ref} \times T_{ref} \to Z_{ref}$, the ***shape optimization problem with transformations on a fixed domain****.*

In this formulation we have an optimal control problem on fixed function spaces where τ is the control. Hence, we can apply techniques from optimal control to derive optimality conditions and use optimization algorithms to solve the problem.

Remark 3.1. *Note that in contrast to the other range and image spaces of J and E the affine space T_{ref} is no vector space. In fact, we only have*

$$\begin{aligned} T_{ref} &= \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in S\} \\ &= \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid \tau = \text{id} + \hat{\tau}, \hat{\tau} \in S\} =: \text{id} + S \end{aligned}$$

where S is a Banach space. However, since we have an one-to-one map between the transformation $\tau \in T_{ref}$ and the corresponding displacement $\hat{\tau} = \tau - \text{id}$, we can identify T_{ref} with the Banach space S. Since we will use optimal control methods to analyze the shape optimization problem, we can use the fact that for E and J directional derivatives with respect to τ can be calculated in all directions of the Banach space S. Therefore we will use the dual pairings based on S for derivatives with respect to τ, e.g.

$$\langle J_\tau(y, \tau), V \rangle_{S^*, S}$$

for $y \in Y_{ref}, \tau \in T_{ad}$ and $V \in S$.

We will now demonstrate how such an operator E can be obtained if the state equation is given in a variational form

$$\langle \tilde{E}(\tilde{y}, \tau), \tilde{\phi} \rangle_{Z(\tau), Z(\tau)^*} = 0 \quad \forall \tilde{\phi} \in Z(\tau)^* \tag{3.10}$$

where $Z(\tau)^*$ is a suitable space of test functions defined on $\Omega = \tau(\Omega_{\text{ref}})$ for $\tau \in T_{\text{ad}}$. We show how the state equation can be transformed in this setting to obtain a variational formulation with state and test functions defined on a fixed domain.
As for the state we transport the test function in the variational formulation from Ω to Ω_{ref} via defining the pullback $\phi(x) := (\tilde{\phi} \circ \tau)(x)$ for $x \in \Omega_{\text{ref}}$ and $\tilde{\phi}$ being the test function for the problem defined on $\Omega = \tau(\Omega_{\text{ref}})$. Next, we define $E(y, \tau)$ via

$$\begin{aligned} \langle E(\tilde{y} \circ \tau, \tau), \tilde{\phi} \circ \tau \rangle_{Z_{\text{ref}}, Z_{\text{ref}}^*} := \langle \tilde{E}(\tilde{y}, \tau), \tilde{\phi} \rangle_{Z(\tau), Z(\tau)^*} \quad & \forall \tilde{y} \in Y(\tau), \\ & \forall \tilde{\phi} \in Z(\tau)^*, \ \forall \tau \in T_{\text{ad}}. \end{aligned}$$

Suppose that

- We can choose a Banach space Y_{ref} such that for all $\tau \in T_{\text{ad}}$ we have $Y_{\text{ref}} \subset \{\tilde{y} \circ \tau \mid \tilde{y} \in Y(\tau)\}$.
- We can choose a Banach space Z_{ref} such that for all $\tau \in T_{\text{ad}}$ we have ${Z_{\text{ref}}}^* = \{\tilde{\phi} \circ \tau \mid \tilde{\phi} \in Z(\tau)^*\}$.
- The solution $\tilde{y}(\tau)$ of
$$\tilde{E}(\tilde{y}(\tau), \tau) = 0 \tag{3.11}$$
satisfies $\tilde{y}(\tau) \circ \tau \in Y_{\text{ref}}$ for all $\tau \in T_{\text{ad}}$.

Let $\tau \in T_{\text{ad}}$. Then the transformed state equation in variational form reads

$$\langle E(y, \tau), \phi \rangle_{Z_{\text{ref}}, Z_{\text{ref}}^*} = 0 \quad \forall \phi \in {Z_{\text{ref}}}^*. \tag{3.12}$$

In this setting (3.12) is equivalent to (3.10) in the sense that $\tilde{y}(\tau)$ solves (3.12) if and only if $y(\tau) := \tilde{y}(\tau) \circ \tau \in Y_{\text{ref}}$ solves (3.10). Conversely, $y(\tau) \in Y_{\text{ref}}$ solves (3.11) if and only if $\tilde{y}(\tau) := y(\tau) \circ \tau^{-1}$ solves (3.12).

3.1.7 Transforming the Variational Form of the State Equation

Usually, the concrete variational form of the state equation after transformation to the reference domain is obtained by using the transformation rule for integrals and for derivatives. Therefore, in this section we take a look at common transformations in this context.
Let $\tau \in \mathcal{T}^{1,\infty}$ and $\tilde{f} \in L^1(\tau(\Omega_{\text{ref}}))$. Then, using the transformation rule for integrals, $f = (\tilde{f} \circ \tau)|\det \tau'|$ is integrable over Ω_{ref} and

$$\int_{\tau(\Omega_{\text{ref}})} \tilde{f}(x)\ dx = \int_{\Omega_{\text{ref}}} (\tilde{f} \circ \tau)(x) |\det \tau'(x)|\ dx.$$

On the other hand

$$\int_{\Omega_{\text{ref}}} (\tilde{f} \circ \tau)(x)\; dx = \int_{\tau(\Omega_{\text{ref}})} \tilde{f}(x) |\det(\tau^{-1})'(x)|\; dx.$$

In context of analyzing differentiability properties of the optimization problem (3.9) it is interesting whether $E(y, \tau)$ is differentiable with respect to y and τ. As mentioned in the last section the transformation rule for integrals is usually used to transport the variational formulation of the state equation from $\tau(\Omega_{\text{ref}})$ to Ω_{ref}. In this case the differentiability of the mappings $\tau \mapsto |\det \tau'|$ and $\tau \mapsto \tau'^{-1}$ is of special interest.
We then have the following lemma:

Lemma 3.4. *1. Let $\tau \in \mathcal{T}^{1,\infty}$. Then there exists $\delta > 0$ such that*

$$|\det \tau'(x)| \geq \delta \text{ for a.a. } x \in \mathbb{R}^d.$$

2. *Let $k \geq 1$. The mapping $g_1(\tau) := |\det \tau'|$ is differentiable from $\mathcal{V}^{k,\infty}$ to $W^{k-1,\infty}(\mathbb{R}^d)$ for all $\tau \in \mathcal{T}^{k,\infty}$. Furthermore for all $\psi \in W^{k,\infty}(\mathbb{R}^d)^d$ we have*
$$g_1'(\tau)\psi = \text{ tr } (\tau'^{-1}\psi')|\det \tau'|. \tag{3.13}$$

3. *Let $k \geq 1$. The mapping $g_2(\tau) := \tau'^{-1}$ is differentiable from $\mathcal{V}^{k,\infty}$ to $W^{k-1,\infty}(\mathbb{R}^d)^{d\times d}$ for all $\tau \in \mathcal{T}^{k,\infty}$. Furthermore for all $\psi \in W^{k,\infty}(\mathbb{R}^d)^d$ we have*
$$g_2'(\tau)\psi = -\tau'^{-1}\psi'\tau'^{-1}. \tag{3.14}$$

Proof. The first part follows from part ii) in the proof of Lemma 4.2 in [45]. The Fréchet differentiability in the second and third part also follows from Lemma 4.2 and 4.3 in [45]. □

If the transformation τ represents an object that is near the reference object, then $\det \tau' \geq \delta > 0$ and we can omit the absolute value in (3.13).

3.1.8 Reduced Problem, Existence of Solutions, Optimality Conditions

Let Y_{ref}, S and Z_{ref} be Banach spaces and $T_{\text{ref}} = \text{id}+S$. Then problem (3.9) is an optimal control problem with control τ and state $y(\tau)$ and we can use optimal control theory to analyze existence of solutions and optimality conditions.
As usual we introduce feasible sets, optimal solutions and the well-known control-to-state operator, which is called design-to-state operator in this context.

Definition 3.4. *The set*

$$\mathcal{F} := \{(y, \tau) \in Y_{ref} \times T_{ref} \mid E(y, \tau) = 0, \tau \in T_{ad}\}$$

is called ***feasible set*** *of problem* (3.9)*. Furthermore, we call $(\bar{y}, \bar{\tau}) \in \mathcal{F}$ a* ***global optimal solution*** *if*

$$J(\bar{y}, \bar{\tau}) \leq J(y, \tau) \qquad \forall (y, \tau) \in \mathcal{F}.$$

$(\bar{y}, \bar{\tau}) \in \mathcal{F}$ *is called a* ***local optimal solution*** *if there exists* $\epsilon > 0$ *such that*

$$J(\bar{y}, \bar{\tau}) \leq J(y, \tau) \qquad \forall (y, \tau) \in \mathcal{F} \cap (Y_{ref} \times B_{||\cdot||_S}(\bar{\tau}; \epsilon)).$$

If for every $\tau \in T_{ad}$ *there exists a unique* $y(\tau) \in Y_{ref}$ *such that* $E(y(\tau), \tau) = 0$, *then we introduce the* ***design-to-state operator***

$$S_y : T_{ad} \to Y_{ref}, \quad \tau \mapsto y(\tau).$$

Furthermore in this case we can define the ***reduced shape optimization problem*** *(associated with problem* (3.3)*)*

$$\min j(\tau) := J(S_y(\tau), \tau) \quad s.t.\ \tau \in T_{ad}. \tag{3.15}$$

Brandenburg [8] introduced a setting in which the existence of a solution for problem (3.9) can be shown, which we state here for completeness:

Lemma 3.5. *We assume that* S *is a Banach space,* $T_{ref} = \mathrm{id} + S$, T_{ad} *is nonempty, closed and bounded, and* Y_{ref} *is a reflexive Banach space. Furthermore let the state equation* $E : Y_{ref} \times T_{ref} \to Z_{ref}$, *the objective function* $J : Y_{ref} \times T_{ref} \to Z_{ref}$ *and the solution operator* $S_y : T_{ad} \to Y_{ref}$ *be continuous functions. In addition let* $\bar{S}$ *be a reflexive Banach space with compact embedding* $\bar{S} \hookrightarrow\hookrightarrow S$ *and* $\bar{T}_{ad} \subset \mathrm{id} + \bar{S}$ *be nonempty, closed, bounded and convex such that* $\bar{T}_{ad} \cap T_{ad} \neq \emptyset$. *Then, the shape optimization problem* (3.9) *has a global optimal solution in* $\bar{T}_{ad} \cap T_{ad}$.

The proof is shown in [8, Theorem 4.12] and uses standard techniques of optimal control.
In order to derive optimality conditions we use:

Assumption 3.1.

(A1) $T_{ad} \subset T_{ref}$ *is nonempty, convex and closed.*

(A2) $J : Y_{ref} \times T_{ref} \to \mathbb{R}$ *and* $E : Y_{ref} \times T_{ref} \to Z_{ref}$ *are continuously differentiable.*

(A3) There exists an open neighbourhood $\tilde{T}_{ref}$ *of* T_{ad} *with* $T_{ad} \subset \tilde{T}_{ref} \subset T_{ref}$ *such that the design-to-state operator* $S_y : \tilde{T}_{ref} \to Y_{ref}$ *exists and* S_y *is continuously differentiable.*

(A4) The derivative $E_y(y(\tau), \tau)$ *is injective for all* $\tau \in T_{ad}$ *and* $y(\tau) = S_y(\tau)$.

Remark 3.2. *Assumption (A3) is satisfied if* $E_y(y(\tau), \tau) \in L(Y_{ref}, Z_{ref})$ *is continuously invertible for all* $\tau \in \tilde{T}_{ref}$, *by the implicit function theorem for Fréchet differentiable functions [70]. If* E *corresponds to the Navier-Stokes equations additional difficulties arise such that the continuous invertibility of* $E_y(y(\tau), \tau)$ *is delicate to show. We will analyse this problem in Section 4.2 in detail.*

In order to derive optimality conditions we introduce the **Lagrangian function** $\mathcal{L} : Y_{\mathrm{ref}} \times T_{\mathrm{ref}} \times {Z_{\mathrm{ref}}}^* \to \mathbb{R}$,

$$\mathcal{L}(y, \tau, \lambda) := J(y, \tau) + \langle \lambda, E(y, \tau) \rangle_{{Z_{\mathrm{ref}}}^*, Z_{\mathrm{ref}}}.$$

Under assumptions (A1)-(A4), a local optimal solution $(\bar{y}, \bar{\tau}) \in Y_{\text{ref}} \times T_{\text{ad}}$ of problem (3.9) satisfies with an appropriate adjoint state $\bar{\lambda} \in {Z_{\text{ref}}}^*$ the following first order necessary optimality conditions, also called *Karush-Kuhn-Tucker conditions*:

$$
\begin{aligned}
\mathcal{L}_\lambda(\bar{y}, \bar{\tau}, \bar{\lambda}) &= E(\bar{y}, \bar{\tau}) = 0, \\
\mathcal{L}_y(\bar{y}, \bar{\tau}, \bar{\lambda}) &= J_y(\bar{y}, \bar{\tau}) + E_y(\bar{y}, \bar{\tau})^* \bar{\lambda} = 0, \\
\langle \mathcal{L}_\tau(\bar{y}, \bar{\tau}, \bar{\lambda}), \hat{\tau} - \bar{\tau} \rangle_{S^*, S} &= \langle J_\tau(\bar{y}, \bar{\tau}) + E_\tau(\bar{y}, \bar{\tau})^* \bar{\lambda}, \hat{\tau} - \bar{\tau} \rangle_{S^*, S} \geq 0 \ \forall \hat{\tau} \in T_{\text{ad}}.
\end{aligned}
$$

The first equation is the *state equation* and the second one is the *adjoint equation.* Furthermore we have a variational inequality that can take form of a so called *design equation* for nice structured S and T_{ad}.

3.1.9 Calculation of Shape Derivatives

Under the assumptions (A1)-(A4) the derivatives of the reduced objective function $j(\tau) := J(y(\tau), \tau)$ can formally be computed via the chain rule, where we write $y(\tau) = S_y(\tau)$ as an alternative notation of the design-to-state operator. In fact, for the derivative of j in $\tau \in T_{\text{ad}}$ in direction $V \in S$ we have

$$
\begin{aligned}
\langle j'(\tau), V \rangle_{S^*, S} &= \langle J_y(y(\tau), \tau), y'(\tau) V \rangle_{{Y_{\text{ref}}}^*, Y_{\text{ref}}} + \langle J_\tau(y(\tau), \tau), V \rangle_{S^*, S} \\
&= \langle y'(\tau)^* J_y(y(\tau), \tau), V \rangle_{S^*, S} + \langle J_\tau(y(\tau), \tau), V \rangle_{S^*, S} \\
&= \langle y'(\tau)^* J_y(y(\tau), \tau) + J_\tau(y(\tau), \tau), V \rangle_{S^*, S}.
\end{aligned}
$$

Here, $y'(\tau)^* \in L({Y_{\text{ref}}}^*, S^*)$ is the adjoint operator of $y'(\tau) \in L(S, Y_{\text{ref}})$. Therefore the reduced derivative $j'(\tau) \in S^*$ is given by

$$
j'(\tau) = y'(\tau)^* J_y(y(\tau), \tau) + J_\tau(y(\tau), \tau). \tag{3.16}
$$

Usually in many applications an efficient evaluation of the second term is available. For the first term we use the so called *adjoint approach* to avoid the calculation of $y'(\tau)$. The adjoint approach is a common approach in optimal control and is based on the following considerations:
The total derivative of the state equation $E(y(\tau), \tau) = 0$ yields

$$
E_y(y(\tau), \tau) y'(\tau) = -E_\tau(y(\tau), \tau), \tag{3.17}
$$

and hence

$$
y'(\tau)^* E_y(y(\tau), \tau)^* = -E_\tau(y(\tau), \tau)^*.
$$

Now we introduce the adjoint equation

$$
E_y(y(\tau), \tau)^* \lambda = -J_y(y(\tau), \tau).
$$

Because of (A4) the operator $E_y(y(\tau), \tau)^*$ is surjective. Hence, the adjoint equation has a solution $\lambda \in {Z_{\text{ref}}}^*$. We obtain for the first term of (3.16)

$$
\begin{aligned}
y'(\tau)^* J_y(y(\tau), \tau) &= y'(\tau)^* (-E_y(y(\tau), \tau)^* \lambda) \\
&= E_\tau(y(\tau), \tau)^* \lambda.
\end{aligned}
$$

Thus we arrive at the following compact formula for calculating the reduced derivative:

$$j'(\tau) = E_\tau(y(\tau),\tau)^*\lambda + J_\tau(y(\tau),\tau). \tag{3.18}$$

In context of shape optimization problems $j'(\tau)$ is also called *shape derivative*. Using this characterization of the derivative we have the following procedure for calculating shape derivatives:

Algorithm 3.1. ***(Calculation of Shape Derivatives)*** *Let $\tau \in T_{ad}$ be given.*

1. *Find $y(\tau) \in Y_{ref}$ by solving the state equation*

$$E(y(\tau),\tau) = 0.$$

2. *Find the corresponding adjoint state $\lambda \in {Z_{ref}}^*$ by solving the adjoint equation*

$$E_y(y(\tau),\tau)^*\lambda = -J_y(y(\tau),\tau).$$

3. *Calculate the reduced derivative $j'(\tau)$ via*

$$j'(\tau) = E_\tau(y(\tau),\tau)^*\lambda + J_\tau(y(\tau),\tau).$$

If the state equation is given in variational form, we can obtain the shape derivatives by the following algorithm:

Algorithm 3.2. ***(Calculation of Shape Derivatives for the variational formulation)*** *Let $\tau \in T_{ad}$ be given.*

1. *Find $y(\tau) \in Y_{ref}$ by solving the state equation*

$$\langle E(y(\tau),\tau),\phi\rangle_{Z_{ref},{Z_{ref}}^*} = 0 \quad \forall \phi \in {Z_{ref}}^*.$$

2. *Find the corresponding adjoint state $\lambda \in {Z_{ref}}^*$ by solving the adjoint equation*

$$\langle \lambda, E_y(y(\tau),\tau)\psi\rangle_{{Z_{ref}}^*,Z_{ref}} = -\langle J_y(y(\tau),\tau),\psi\rangle_{{Y_{ref}}^*,Y_{ref}} \quad \forall \psi \in {Y_{ref}}^*.$$

3. *Calculate the reduced derivative $j'(\tau)$ via*

$$\langle j'(\tau),\cdot\rangle_{S^*,S} = \langle \lambda, E_\tau(y(\tau),\tau)\cdot\rangle_{{Z_{ref}}^*,Z_{ref}} + \langle J_\tau(y(\tau),\tau),\cdot\rangle_{S^*,S}.$$

3.1.10 Shape Derivative Computation on the Physical Domain

Usually the structure of the transformed state equation $E(y,\tau) = 0$ is completely different from the original state equation $\bar{E}(y,\Omega) = 0$. The benefit of introducing a transformed state equation that is defined on a fixed reference domain with fixed function spaces usually comes with a more difficult state equation $E(y,\tau) = 0$.
For numerical applications it can be beneficial to solve instead of the transformed equations on the reference domain equivalent equations on the physical

domain $\Omega = \tau(\Omega_{\mathrm{ref}})$. In fact, solving the state equation $E(y, \tau) = 0$ on the reference domain is equivalent to solving the state equation $\bar{E}(\tilde{y}, \tau(\Omega_{\mathrm{ref}})) = 0$ on the domain $\tau(\Omega_{\mathrm{ref}})$. Furthermore for the original state equation $\bar{E}(y, \Omega) = 0$ there may already exist efficient PDE-solvers that we can reuse in this case. Similarly, equivalent equations for the calculation of the adjoint state and the shape derivative on the domain $\tau(\Omega_{\mathrm{ref}})$ can be derived. We will not go into details in this setting but demonstrate this for the Navier-Stokes equations.

3.1.11 Second Order Shape Derivatives

If J and E are twice continuously Fréchet differentiable we can also calculate second order shape derivatives. Again we can use techniques of optimal control to derive concrete formulas. We now apply a Lagrange function based approach to calculate second derivatives of the reduced objective function $j(\tau)$. In detail, we use a general approach for optimal control problems (see e.g. [31, Section 1.6.5]) for our shape optimization problem.
Second order derivatives are often needed to apply optimization algorithms that also use derivative information of second order, e.g. Newton's method. Usually, for applying these algorithms the whole operator $j''(\tau)$ is not needed. Instead, iterative solvers are used to solve linear systems like the Newton equation

$$j''(\tau^k)s^k = -j'(\tau^k)$$

or a perturbed version of it. However, these solvers only need to evaluate operator-vector-products $j''(\tau)s$ for $s \in S$. The following considerations show how $j''(\tau)s$ can be calculated efficiently. Note that for calculating second derivatives, we additionally assume that E and J are twice continuously differentiable and that $E_y(y(\tau), \tau)$ is invertible for all $\tau \in T_{\mathrm{ad}}$.
Using that $E(y(\tau), \tau) = 0$ for all $\tau \in T_{\mathrm{ad}}$ we have

$$j(\tau) = J(y(\tau), \tau) = J(y(\tau), \tau) + \langle \lambda, E(y(\tau), \tau) \rangle_{Z_{\mathrm{ref}}^*, Z_{\mathrm{ref}}} = \mathcal{L}(y(\tau), \tau, \lambda)$$

for arbitrary $\lambda \in Z_{\mathrm{ref}}^*$. Differentiating j we obtain for all $\psi \in S$

$$\langle j'(\tau), \psi \rangle_{S^*, S} = \langle \mathcal{L}_y(y(\tau), \tau, \lambda), y'(\tau)\psi \rangle_{Y_{\mathrm{ref}}^*, Y_{\mathrm{ref}}} + \langle \mathcal{L}_\tau(y(\tau), \tau, \lambda), \psi \rangle_{S^*, S}$$

For the second derivative we get for all $\phi, \psi \in S$

$$\begin{aligned}
\langle j''(\tau)\phi, \psi \rangle_{S^*, S} =& \langle \mathcal{L}_y(y(\tau), \tau, \lambda), y''(\tau)(\psi, \phi) \rangle_{Y_{\mathrm{ref}}^*, Y_{\mathrm{ref}}} \\
&+ \langle y'(\tau)^* \mathcal{L}_{yy}(y(\tau), \tau, \lambda) y'(\tau)\phi, \psi \rangle_{S^*, S} \\
&+ \langle y'(\tau)^* \mathcal{L}_{y\tau}(y(\tau), \tau, \lambda)\phi, \psi \rangle_{S^*, S} \\
&+ \langle \mathcal{L}_{\tau y}(y(\tau), \tau, \lambda) y'(\tau)\phi, \psi \rangle_{S^*, S} \\
&+ \langle \mathcal{L}_{\tau\tau}(y(\tau), \tau, \lambda)\phi, \psi \rangle_{S^*, S}.
\end{aligned}$$

If λ satisfies the adjoint equation, i.e. $E_y(y(\tau), \tau)^*\lambda = -J_y(y(\tau), \tau)$, we have $\mathcal{L}_y(y(\tau), \tau, \lambda) = 0$ and hence the term containing $y''(\tau)$ drops out and we obtain

$$\begin{aligned}
j''(\tau) &= y'(\tau)^* \mathcal{L}_{yy}(y(\tau), \tau, \lambda) y'(\tau) + y'(\tau)^* \mathcal{L}_{y\tau}(y(\tau), \tau, \lambda) \\
&\quad + \mathcal{L}_{\tau y}(y(\tau), \tau, \lambda) y'(\tau) + \mathcal{L}_{\tau\tau}(y(\tau), \tau, \lambda) \qquad (3.19) \\
&= Q(\tau)^* \mathcal{L}_{(y,\tau),(y,\tau)}(y(\tau), \tau, \lambda) Q(\tau)
\end{aligned}$$

with

$$Q(\tau) := \begin{pmatrix} y'(\tau) \\ I_S \end{pmatrix} \in L(S, Y_{\text{ref}} \times S), \quad \mathcal{L}_{(y,\tau),(y,\tau)} = \begin{pmatrix} \mathcal{L}_{yy} & \mathcal{L}_{y\tau} \\ \mathcal{L}_{\tau y} & \mathcal{L}_{\tau\tau} \end{pmatrix}.$$

Here $I_S \in L(S, S)$ is the identity.
To calculate $j''(\tau)s$ for $s \in S$ we thus have to evaluate

$$Q(\tau)^* \mathcal{L}_{(y,\tau),(y,\tau)}(y(\tau), \tau, \lambda) Q(\tau)s.$$

From (3.17) we know that $y'(\tau)$ solves

$$E_y(y(\tau), \tau) y'(\tau) = -E_\tau(y(\tau), \tau).$$

Therefore we can compute $j''(\tau)s$ with the following algorithm:

Algorithm 3.3. ***(Calculation of** $j''(\tau)s$**)*** *Let $\tau \in T_{ad}$ be given and the state $y(\tau)$ and the adjoint state $\lambda \in {Z_{ref}}^*$ be computed. Let furthermore $s \in S$.*

1. *Find the sensitivity $\delta_s y \in Y_{ref}$ by solving the equation*

$$E_y(y(\tau), \tau)\delta_s y = -E_\tau(y(\tau), \tau)s.$$

2. *Compute $h_1 \in {Y_{ref}}^*$ and $h_2 \in S^*$ via*

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{yy}(y(\tau), \tau, \lambda)\delta_s y - \mathcal{L}_{y\tau}(y(\tau), \tau, \lambda)s \\ \mathcal{L}_{\tau y}(y(\tau), \tau, \lambda)\delta_s y + \mathcal{L}_{\tau\tau}(y(\tau), \tau, \lambda)s \end{pmatrix}.$$

3. *Compute $h_3 \in S^*$ by solving the equation*

$$h_3 = y'(\tau)^* h_1 = -E_\tau(y(\tau), \tau)^* E_y(y(\tau), \tau)^{-*} h_1.$$

4. *Set $j''(\tau)s = h_2 + h_3$.*

The most effort is required to the linearized state equation in step 1 and the adjoint equation in step 3. Furthermore the state $y(\tau)$ and the adjoint state λ has to be computed. However, if the adjoint approach of Section 3.1.9 have been used to calculate the first order shape derivatives, $y(\tau)$ and λ are already available.

3.1.12 Derivatives with Respect to Shape Parameters

In applications the shapes of the objects to be optimized are often given by parametrizations using design parameters $u \in U$ with a finite or infinite dimensional design space U. For example, if the boundary curve Γ_B is parametrized via B-spline curves, U could be the space of B-spline parameters. See Section 5.1 for more details on various design parametrizations.
Hence, in many applications there exists a parametrization of the boundary curve and thus there exists a map $d : U \to S_{\text{bdry}}(\Omega_{\text{ref}}), u \mapsto d(u)$ where $S_{\text{bdry}}(\Omega_{\text{ref}})$ is the space of displacements of the reference domain boundary Γ_B^{ref} of Ω_{ref}. For instance, the displacement can be calculated by subtracting the

boundary curve of the reference object from the boundary curve of the actual object. Usually this map and its derivative are easy to evaluate. In fact, often the map $d : U \to S_{\text{bdry}}(\Omega_{\text{ref}}), u \mapsto d(u)$ is even linear or affine, see again Section 5.1.

However, to evaluate shape derivatives with respect to domain displacements, we have to transport the boundary displacements $d(u)$ to domain transformations $\tau(d) : \Omega_{\text{ref}} \to \mathbb{R}^d$. We consider now a setting where the displacement is transported by a linear elliptic partial differential equation, e.g. a linear elasticity equation or Poisson equation, to a domain displacement $V \in S$. To keep the boundary displacement we impose a Dirichlet boundary condition on $\partial\Omega_{\text{ref}}$, in particular we set $V = d(u)$ on Γ_B^{ref} and $V = 0$ on $\partial\Omega_{\text{ref}} \backslash \Gamma_B^{\text{ref}}$. Finally, the domain transformation $\tau \in T_{\text{ref}}$ is given by $\tau = \text{id} + V$. This can be abbreviated as

$$A(\tau, d(u)) = 0, \tag{3.20}$$

where $A : T_{\text{ref}} \times S_{\text{bdry}}(\Omega_{\text{ref}}) \to W$ describes the linear PDE with Dirichlet boundary conditions and the identity shift and we finally obtain the chain

$$u \mapsto d(u) \mapsto \tau(d(u)),$$

where $\tau = \tau(d(u))$ is the unique solution of (3.20). If we can describe T_{ad} via a subset $U_{\text{ad}} \subset U$ such that

$$U_{\text{ad}} = \{u \in U \mid \tau(d(u)) \in T_{\text{ad}}\},$$

then the reduced problem 3.15 can be written as

$$\min j(\tau) \quad \text{s.t. } A(\tau, d(u)) = 0, \;\; u \in U_{\text{ad}}. \tag{3.21}$$

Because the objective function depends on u or $d(u)$ we can also introduce the reduced objectives

$$\bar{j}(u) := j(\tau(d(u))), \quad \hat{j}(d) := j(\tau(d)), \tag{3.22}$$

where $\tau(d)$ is the solution of $A(\tau, d) = 0$ for a displacement $d \in S_{\text{bdry}}(\Omega_{\text{ref}})$ defined on Γ_B^{ref}. Because sensitivities of the map $u \mapsto d(u)$ are usually easy to evaluate, we are interested in an efficient calculation of $\hat{j}'(d)$.

Introducing the Lagrange function

$$\mathcal{L}(\tau, d, q) := j(\tau) + \langle q, A(\tau, d)\rangle_{W^*,W}$$

where $q \in W^*$ is the adjoint transformation, we arrive at the first order optimality conditions for (3.21):

$$A(\tau, d) = 0, \tag{3.23}$$

$$A_\tau(\tau, d)^* q = -j'(\tau), \tag{3.24}$$

$$\langle A_d(\tau, d)^* q, \hat{d} - d\rangle_{S_{\text{bdry}}(\Omega_{\text{ref}})^*, S_{\text{bdry}}(\Omega_{\text{ref}})} \geq 0 \quad \forall \hat{d} \in S^{\text{ad}}_{\text{bdry}}(\Omega_{\text{ref}}). \tag{3.25}$$

where $S^{\text{ad}}_{\text{bdry}}(\Omega_{\text{ref}})$ is the set of admissible boundary displacements corresponding to T_{ad}. Note again, that A is defined on the affine space T_{ref} and the derivative

$A_\tau(\tau, d)$ is defined on the displacement space S. The reduced derivative $\hat{j}'(d)$ is given by

$$\hat{j}'(d) = A_d(\tau, d)^* q,$$

where τ solves (3.23) and q solves (3.24). Shape derivatives with respect to the design parameters $u \in U_{\text{ad}}$ are then easily given by the chain rule

$$\bar{j}'(u) = d'(u)^* A_d(\tau, d(u))^* q.$$

If the map $u \mapsto d(u)$ is linear we simply have

$$\bar{j}'(u) = d(u)^* A_d(\tau, d(u))^* q.$$

We arrive at the following algorithm for calculating shape derivatives with respect to shape parameters:

Algorithm 3.4. ***(Calculation of derivatives w.r.t. shape parameters)*** *Let $u \in U_{ad}$ be given.*

1. *Find the boundary displacement $d(u) \in S_{bdry}(\Omega_{ref})$ using the concrete parametrization.*
2. *Calculate the domain transformation $\tau(d(u)) \in T_{ref}$ by solving* (3.23).
3. *Compute the adjoint transformation $q \in W^*$ by solving* (3.24).
4. *Find the reduced derivative $\hat{j}'(d) = A_d(\tau(d(u)), d(u))^* q$.*
5. *Calculate the reduced derivative $\bar{j}'(u)$ using $\hat{j}'(d)$ and $d'(u)$ of the concrete parametrization.*

Note that the main work of evaluating the reduced derivative is usually required in step 3. In fact, the presence of the term $j'(\tau)$ includes the solve of the state and adjoint equations of the underlying PDE as discussed in Section 3.1.9. However, in this approach we avoid computing sensitivities $\langle j'(\tau), \psi \rangle_{S^*,S}$ in direction of a concrete transformation $\psi \in S$. Instead, we compute the adjoint transformation only once and then find sensitivities $\langle \bar{j}'(u), v \rangle_{U^*,U}$ in directions v of the design space U. Because $d'(u)$ is usually easy to compute, step 5 of algorithm 3.4 is easy to evaluate, even if the number of design parameters, i.e. the dimension of U is very big. In fact, for a high dimensional U this approach can save very much computational effort in contrast to calculating sensitivities of $j'(\tau)$.

3.2 Shape Optimization with the Navier-Stokes Equations

We apply the presented approach to shape optimization problems governed by the instationary Navier-Stokes equations for a viscous, incompressible fluid on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ with Lipschitz boundary.
In this section we discuss the Navier-Stokes equations and state some regularity results for their solutions. We show how the state equations can be transformed to the reference domain and introduce the concrete transformation space, and the trial and test spaces. In the next section 3.3 we will then calculate first and second order shape derivatives for the Navier Stokes equations.

3.2.1 The Instationary Navier-Stokes Equations

We consider the instationary Navier-Stokes equations with homogeneous Dirichlet boundary conditions.
Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain with $d = 2$ or $d = 3$. Furthermore let $I = (0,T)$ be a time interval with a fixed end time $T > 0$. Then the instationary Navier-Stokes equations for a viscous, incompressible fluid can be stated as

$$\begin{aligned} \tilde{\boldsymbol{v}}_t - \nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} \text{ on } \Omega \times I, \\ \operatorname{div} \tilde{\boldsymbol{v}} &= 0 \text{ on } \Omega \times I, \\ \tilde{\boldsymbol{v}} &= \mathbf{0} \text{ on } \partial\Omega \times I, \\ \tilde{\boldsymbol{v}}(\cdot,0) &= \tilde{\boldsymbol{v}}_0 \text{ on } \Omega, \end{aligned} \tag{3.26}$$

where $\tilde{\boldsymbol{v}} : \Omega \times I \to \mathbb{R}^d$ denotes the velocity and $\tilde{p} : \Omega \times I \to \mathbb{R}$ the pressure of the fluid. Here $\nu > 0$ is the kinematic viscosity. Furthermore $\tilde{\boldsymbol{v}}_0$ is the given initial velocity at time $t = 0$ and $\tilde{\boldsymbol{f}}$ denotes the volume force.
The first equation is also known as *conservation of momentum.* The second equation is known as *conservation of mass* or *incompressibility condition* and states the solenoidality of $\tilde{\boldsymbol{v}}$. Furthermore the third equation is the homogeneous Dirichlet condition and the last one fixes the initial time for $\tilde{\boldsymbol{v}}$. Note that the homogeneous boundary condition imposes a *no slip condition* for the outer boundary and for the object B, respectively.
To derive a variational formulation, we define the spaces

$$\mathcal{V}(\Omega) := \{\tilde{\boldsymbol{v}} \in C_0^\infty(\Omega)^d \mid \operatorname{div} \tilde{\boldsymbol{v}} = 0\}, \quad V(\Omega) := \operatorname{cl}_{||\cdot||_{\mathbf{H}_0^1(\Omega)}}(\mathcal{V}(\Omega)),$$
$$H(\Omega) := \operatorname{cl}_{||\cdot||_{\mathbf{L}^2(\Omega)}}(\mathcal{V}(\Omega)), \quad L_0^2(\Omega) := \{\tilde{p} \in L^2(\Omega) : \int_\Omega \tilde{p} = 0\}.$$

The Bochner spaces are denoted by $L^p(I;X)$ as introduced in Section 2.1.6. As Ω is bounded, the space $L_0^2(\Omega)$ can be identified with $L^2(\Omega)/\mathbb{R}$ [59, Remark I.1.4], where

$$||\tilde{p}||_{L^2(\Omega)/\mathbb{R}} := \inf_{c \in \mathbb{R}} ||\tilde{p} + c||_{L^2(\Omega)}.$$

In fact, we have for all $\tilde{p} \in L_0^2(\Omega)$

$$||\tilde{p}||_{L_0^2(\Omega)} = ||\tilde{p}||_{L^2(\Omega)/\mathbb{R}}.$$

$H(\Omega)$ and $V(\Omega)$ are Hilbert spaces with the scalar products

$$(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})_{H(\Omega)} := (\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})_{\mathbf{L}^2(\Omega)}, \quad (\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})_{V(\Omega)} := (\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})_{\mathbf{H}_0^1(\Omega)} = \int_\Omega \sum_{i=1}^{d} (\tilde{\boldsymbol{v}}_{x_i}^T \tilde{\boldsymbol{w}}_{x_i}) \, dx.$$

Furthermore we introduce the corresponding Gelfand triple $V(\Omega) \hookrightarrow H(\Omega) = H(\Omega)^* \hookrightarrow V(\Omega)^*$, and recall the definition of the spaces

$$\begin{aligned} W(I; V(\Omega)) &:= \{\tilde{\boldsymbol{v}} \in L^2(I; V(\Omega)) \mid \tilde{\boldsymbol{v}}_t \in L^2(I; V(\Omega)^*)\}, \\ W(I; \mathbf{H}_0^1(\Omega)) &:= \{\tilde{\boldsymbol{v}} \in L^2(I; \mathbf{H}_0^1(\Omega)) \mid \tilde{\boldsymbol{v}}_t \in L^2(I; \mathbf{H}^{-1}(\Omega))\}. \end{aligned}$$

The weak formulation of (3.26) is: Find $\tilde{\boldsymbol{v}} \in W(I; V(\Omega))$ such that

$$\begin{aligned} \langle \tilde{\boldsymbol{v}}_t(\cdot, t), \tilde{\boldsymbol{w}} \rangle_{V(\Omega)^*, V(\Omega)} + \int_\Omega \tilde{\boldsymbol{v}}(\tilde{x}, t)^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, t) \tilde{\boldsymbol{w}}(\tilde{x}) \, d\tilde{x} + \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x}, t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x}) \, d\tilde{x} \\ = \int_\Omega \tilde{\boldsymbol{f}}(\tilde{x}, t)^T \tilde{\boldsymbol{w}}(\tilde{x}) \, d\tilde{x} \quad \forall \tilde{\boldsymbol{w}} \in V(\Omega) \text{ for a.a. } t \in I, \\ \tilde{\boldsymbol{v}}(\cdot, 0) = \tilde{\boldsymbol{v}}_0. \end{aligned} \tag{3.27}$$

In this setting the pressure term $\nabla \tilde{p}$ has vanished because the equation is tested with solenoidal functions $\tilde{\boldsymbol{w}} \in V(\Omega)$. The pressure $\tilde{p}$ can be recovered using regularity results for $\tilde{\boldsymbol{v}}$ and the equation of conservation of momentum. In fact, we can use the following lemma that is a combination of Proposition I.1.2 and Remark I.1.4 in [59].

Lemma 3.6. *Let $\Omega \subset \mathbb{R}^d$ be a bounded, open set with Lipschitz boundary. Then:*

1. *If for a distribution $\tilde{p}$ it holds that $D_i \tilde{p} \in L^2(\Omega)$ for $i = 1, \ldots, d$, then*

   $$\tilde{p} \in L^2(\Omega), \quad ||\tilde{p}||_{L_0^2(\Omega)} \leq c(\Omega) ||\nabla p||_{\mathbf{L}^2(\Omega)}$$

   for a constant $c(\Omega)$.

2. *If for a distribution $\tilde{p}$ it holds that $D_i \tilde{p} \in H^{-1}(\Omega)$ for $i = 1, \ldots, d$, then*

   $$\tilde{p} \in L^2(\Omega), \quad ||\tilde{p}||_{L_0^2(\Omega)} \leq c(\Omega) ||\nabla p||_{\mathbf{H}^{-1}(\Omega)}$$

   for a constant $c(\Omega)$.

3. *If $\tilde{f} \in \mathbf{H}^{-1}(\Omega)$ and $\langle \tilde{f}, \tilde{w} \rangle_{\mathbf{H}^{-1}(\Omega), \mathbf{H}_0^1(\Omega)} = 0$ for all $\tilde{w} \in \mathcal{V}(\Omega)$, then there exists $\tilde{p} \in L^2(\Omega)$ with*

   $$\tilde{f} = \nabla \tilde{p}.$$

3.2.2 Regularity Results for the Navier-Stokes Equations

In this section, we collect some results on the regularity of the solution $(\tilde{\boldsymbol{v}}, \tilde{p})$ of the Navier-Stokes equations. Many of the following results and their proofs can be found in [59]. It is well known that so far the question of existence and uniqueness is answered satisfactorily only in the case $d \leq 2$. In fact, for $d = 2$ we have:

Lemma 3.7. *Let $d = 2$ and assume*

$$\tilde{\boldsymbol{f}} \in L^2(I; V(\Omega)^*), \tilde{\boldsymbol{v}}_0 \in H(\Omega). \tag{3.28}$$

Then there exists a unique solution $\tilde{\boldsymbol{v}}$ of the Navier-Stokes equations in weak formulation (3.27) *and $\tilde{\boldsymbol{v}}$ satisfies*

$$\tilde{\boldsymbol{v}} \in C(I; H(\Omega)), \;\; \tilde{\boldsymbol{v}} \in W(I; V(\Omega)). \tag{3.29}$$

Furthermore the pressure can be recovered as a distribution on $\Omega \times I$.

The proof can be found for example in [59, Theorem III.3.2].
Assuming that the data $\tilde{\boldsymbol{f}}$ and $\tilde{\boldsymbol{v}}_0$ are sufficiently regular, the solution has further regularity as stated by

Lemma 3.8. *Let $d = 2$ and assume*

$$\tilde{\boldsymbol{f}}, \tilde{\boldsymbol{f}}_t \in L^2(I; \mathbf{H}^{-1}(\Omega)), \tilde{\boldsymbol{f}}(\cdot, 0) \in H(\Omega), \tilde{\boldsymbol{v}}_0 \in V(\Omega) \cap \mathbf{H}^2(\Omega). \tag{3.30}$$

Then the solution $(\tilde{\boldsymbol{v}}, \tilde{p})$ of the Navier-Stokes equations satisfies

$$\tilde{\boldsymbol{v}} \in C(I; V(\Omega)), \;\; \tilde{\boldsymbol{v}}_t \in L^2(I, V(\Omega)) \cap L^\infty(I; H(\Omega)), \;\; \tilde{p} \in L^\infty(I; L^2_0(\Omega)). \tag{3.31}$$

Furthermore there exists a constant $c(\Omega) > 0$ with

$$\begin{aligned} ||\tilde{p}||_{L^\infty(I;L^2_0(\Omega))} \leq c(\Omega)(||\tilde{\boldsymbol{v}}_t||_{L^\infty(I;H(\Omega))} + \nu ||\tilde{\boldsymbol{v}}||_{L^\infty(I;V(\Omega))} + \\ ||\tilde{\boldsymbol{v}}||^2_{L^\infty(I;V(\Omega))} + ||\tilde{\boldsymbol{f}}||_{L^\infty(I;\mathbf{H}^{-1}(\Omega))}). \end{aligned} \tag{3.32}$$

Proof. The regularity results for the velocity can be found in [59, Theorem III.3.5]. For the pressure we use the embeddings $L^{4/3}(\Omega) \hookrightarrow H^{-1}(\Omega)$ and $H^1_0(\Omega) \hookrightarrow L^4(\Omega)$ and the estimate

$$\begin{aligned} ||\tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}}||_{L^{4/3}(\Omega)} = ||\tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}}||_{L^4(\Omega)^*} = \sup_{||\tilde{\boldsymbol{w}}||_{L^4(\Omega)}=1} \int_\Omega \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{w}} \\ \leq c \sup_{||\tilde{\boldsymbol{w}}||_{L^4(\Omega)}=1} ||\tilde{\boldsymbol{v}}||_{L^4(\Omega)} ||\nabla \tilde{\boldsymbol{v}}||_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{w}}||_{L^4(\Omega)} = c ||\tilde{\boldsymbol{v}}||_{L^4(\Omega)} ||\nabla \tilde{\boldsymbol{v}}||_{\mathbf{L}^2(\Omega)} \end{aligned}$$

with a constant c. Introducing $A(\tilde{\boldsymbol{v}}) \in L^\infty(I; \mathbf{H}^{-1}(\Omega))$ by defining $A(\tilde{\boldsymbol{v}})(t)$ for a.a. $t \in I$ via

$$\langle A(\tilde{\boldsymbol{v}})(t), \tilde{\boldsymbol{w}} \rangle_{\mathbf{H}^{-1}(\Omega), \mathbf{H}^1_0(\Omega)} := \nu \int_\Omega \nabla \tilde{\boldsymbol{v}}(t) : \nabla \tilde{\boldsymbol{w}} \, d\tilde{x},$$

we obtain

$$\begin{aligned}
||\tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}^{-1}(\Omega))} &\leq c_1 ||\tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}}||_{L^\infty(I;\mathbf{L}^{4/3}(\Omega))} \\
&\leq c_2 ||\tilde{\boldsymbol{v}}||_{L^\infty(I;\mathbf{L}^4(\Omega))} ||\nabla \tilde{\boldsymbol{v}}||_{L^\infty(I;\mathbf{L}^2(\Omega))} \\
&\leq c_3 ||\tilde{\boldsymbol{v}}||^2_{L^\infty(I,V(\Omega))}, \\
||A(\tilde{\boldsymbol{v}})||_{L^\infty(I;\mathbf{H}^{-1}(\Omega))} &\leq \nu \|\tilde{\boldsymbol{v}}\|_{L^\infty(I,\mathbf{H}^1_0(\Omega))} = \nu \|\tilde{\boldsymbol{v}}\|_{L^\infty(I,V(\Omega))},
\end{aligned}$$

where $c_1, c_2, c_3 > 0$ are constants.
We have $\tilde{\boldsymbol{v}}_t \in L^\infty(I;\mathbf{H}^{-1}(\Omega))$ because $H(\Omega) \hookrightarrow \mathbf{L}^2(\Omega) \hookrightarrow \mathbf{H}^{-1}(\Omega)$. Furthermore $\tilde{\boldsymbol{f}} \in L^\infty(I;\mathbf{H}^{-1}(\Omega))$ since $\tilde{\boldsymbol{f}}, \tilde{\boldsymbol{f}}_t \in L^2(I;\mathbf{H}^{-1}(\Omega))$ (see, e.g. [59, Lemma III.1.1]). Hence,

$$\boldsymbol{g} := -\tilde{\boldsymbol{v}}_t - \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} - A(\tilde{\boldsymbol{v}}) + \tilde{\boldsymbol{f}} \in L^\infty(I;\mathbf{H}^{-1}(\Omega)). \tag{3.33}$$

Using $\langle \boldsymbol{g}(t), \tilde{\boldsymbol{w}}(t)\rangle_{\mathbf{H}^{-1}(\Omega),\mathbf{H}^1_0(\Omega)} = 0$ for all $\tilde{\boldsymbol{w}} \in V(\Omega)$ and a.a. $t \in I$ there exists by Lemma 3.6 for a.a. t a unique $\tilde{p}(t) \in L^2_0(\Omega)$ with

$$\nabla \tilde{p}(t) = \boldsymbol{g}(t),$$

where $||\tilde{p}(t)||_{L^2_0(\Omega)} \leq c_4 ||\boldsymbol{g}(t)||_{\mathbf{H}^{-1}(\Omega)}$ by lemma 3.6 with a constant $c_4 > 0$. Hence there exists a unique pressure $\tilde{p} \in L^\infty(I;L^2_0(\Omega))$ that satisfies (3.32). □

Remark 3.3. *The same regularity results for $\tilde{\boldsymbol{v}}$ but only $\tilde{p} \in L^2(I;L^2_0(\Omega))$ would follow if we supposed instead of* (3.30) *that*

$$\tilde{\boldsymbol{f}} \in L^2(I;\mathbf{H}^{-1}(\Omega)), \tilde{\boldsymbol{f}}_t \in L^2(I;V(\Omega)^*), \tilde{\boldsymbol{f}}(\cdot,0) \in H(\Omega), \tilde{\boldsymbol{v}}_0 \in V(\Omega) \cap \mathbf{H}^2(\Omega).$$

In fact, instead of (3.33) *we obtain*

$$\boldsymbol{g} := -\tilde{\boldsymbol{v}}_t - \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} - \nu A(\tilde{\boldsymbol{v}}) + \tilde{\boldsymbol{f}} \in L^2(I;\mathbf{H}^{-1}(\Omega)),$$

because $\tilde{\boldsymbol{f}}$ is only in $L^2(I;\mathbf{H}^{-1}(\Omega))$. Using the same arguments as above and the embedding $L^\infty(I;\mathbf{H}^{-1}(\Omega)) \hookrightarrow L^2(I;\mathbf{H}^{-1}(\Omega))$ we find a unique pressure $\tilde{p} \in L^2(I;L^2_0(\Omega))$ with

$$\begin{aligned}
||\tilde{p}||_{L^2(I;L^2_0(\Omega))} \leq c(\Omega)(||\tilde{\boldsymbol{v}}_t||_{L^2(I;H(\Omega))} + \nu ||\tilde{\boldsymbol{v}}||_{L^2(I;V(\Omega))} + \\
||\tilde{\boldsymbol{v}}||^2_{L^2(I;V(\Omega))} + ||\tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{H}^{-1}(\Omega))}),
\end{aligned} \tag{3.34}$$

with a constant $c(\Omega)$.

For the three-dimensional case we have the following existence result that can be found in [59, Theorem III.3.3]:

Lemma 3.9. *Let $d = 3$ and assume*

$$\tilde{\boldsymbol{f}} \in L^2(I;V(\Omega)^*), \tilde{\boldsymbol{v}}_0 \in H(\Omega). \tag{3.35}$$

Then there exists a solution $\tilde{\boldsymbol{v}}$ of the Navier-Stokes equations in weak formulation (3.27) *and $\tilde{\boldsymbol{v}}$ satisfies*

$$\tilde{\boldsymbol{v}} \in L^2(I;V(\Omega)) \cap L^\infty(I;H(\Omega)) \cap L^{8/3}(I;\mathbf{L}^4(\Omega)), \quad \tilde{\boldsymbol{v}}_t \in L^{4/3}(I;V(\Omega)^*). \tag{3.36}$$

Furthermore $\tilde{\boldsymbol{v}}$ is weakly continuous from I to $H(\Omega)$.

In contrast to the two-dimenstional case, the lemma above does not guarantee uniqueness of $\tilde{\boldsymbol{v}}$. On the other hand the following lemma shows uniqueness of the solution $\tilde{\boldsymbol{v}}$, if it exists.

Lemma 3.10. *Let $d = 3$. Then there exists at most one solution $\tilde{\boldsymbol{v}}$ of (3.27) satisfying*

$$\tilde{\boldsymbol{v}} \in L^2(I; V(\Omega)) \cap L^\infty(I; H(\Omega)) \cap L^8(I; \mathbf{L}^4(\Omega)), \quad \tilde{\boldsymbol{v}}_t \in L^{4/3}(I; V(\Omega)^*). \tag{3.37}$$

If this solution exists, it is continuous from I to $H(\Omega)$.

Again the proof can be found in [59, Theorem III.3.4].
Under some further assumptions on the data we obtain an existence and uniqueness result also for the three-dimensional case. For this we introduce the trilinear continuous form

$$b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}}) := \sum_{i,j=1}^{d} \int_\Omega \tilde{\boldsymbol{u}}_i (D_i \tilde{\boldsymbol{v}}_j) \tilde{\boldsymbol{w}}_j \, d\tilde{x} = \int_\Omega \tilde{\boldsymbol{u}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{w}} \, d\tilde{x} \tag{3.38}$$

for $\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$. We have for $\tilde{\boldsymbol{v}} \in \mathbf{H}_0^1(\Omega) \cap \mathbf{H}^2(\Omega), \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$

$$|b(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| \leq c_1 ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}^2(\Omega)} ||\tilde{\boldsymbol{w}}||_{\mathbf{L}^2(\Omega)} \tag{3.39}$$

with a constant c_1 that depends on d and the Poincaré constant of Ω (see Lemma 4.1).
For an existence and uniqueness result for the three-dimensional case we need the assumption

(C) Let $d = 3$ and

$$d_1(\Omega) := ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)} + \nu c_0 ||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)} + c_1 ||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{H}^2(\Omega)},$$

where c_0 is a constant such that for all $\boldsymbol{v} \in \mathbf{H}^2(\Omega)$ we have $||\Delta \boldsymbol{v}||_{L^2(\Omega)} \leq c_0 ||\boldsymbol{v}||_{\mathbf{H}^2(\Omega)}$, and c_1 is the constant of (3.39) above. Furthermore let

$$d_2(\Omega) \quad := ||\tilde{\boldsymbol{f}}||^2_{L^\infty(I; V(\Omega)^*)}.$$

We assume that

$$\frac{d_2(\Omega)}{\nu} + (1 + d_1(\Omega)^2) \left(||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{L}^2(\Omega)} + \frac{T d_2(\Omega)}{\nu} \right)^{1/2} e^{\int_I ||\tilde{\boldsymbol{f}}_t(s)||_{\mathbf{L}^2(\Omega)} \, ds} < \frac{\nu^3}{c^2}.$$

Here c is a constant such that $|b(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w})| \leq c ||\boldsymbol{u}||_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{w}||_{\mathbf{H}_0^1(\Omega)}$ for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega)$, see also Lemma 4.1.

Note that (C) can be satisfied if ν is large enough or if $\tilde{\boldsymbol{f}}$ and $\tilde{\boldsymbol{v}}_0$ are chosen "small enough". Then we can show

Lemma 3.11. *Let $d = 3$ and assume*

$$\tilde{\boldsymbol{f}} \in L^\infty(I; H(\Omega)), \tilde{\boldsymbol{f}}_t \in L^1(I; H(\Omega)), \tilde{\boldsymbol{v}}_0 \in V(\Omega) \cap \mathbf{H}^2(\Omega) \text{ and } (C). \tag{3.40}$$

Then the solution $(\tilde{\boldsymbol{v}}, \tilde{p})$ of the Navier-Stokes equations is unique and satisfies

$$\tilde{\boldsymbol{v}} \in C(I; V(\Omega)),\ \tilde{\boldsymbol{v}}_t \in L^2(I, V(\Omega)) \cap L^\infty(I; H(\Omega)),\ \tilde{p} \in L^\infty(I; L^2_0(\Omega)). \tag{3.41}$$

Furthermore there exists a constant $c(\Omega) > 0$ with

$$\begin{aligned} ||\tilde{p}||_{L^\infty(I;L^2_0(\Omega))} \leq c(\Omega)(||\tilde{\boldsymbol{v}}_t||_{L^\infty(I;H(\Omega))} + \nu||\tilde{\boldsymbol{v}}||_{L^\infty(I;V(\Omega))} + \\ ||\tilde{\boldsymbol{v}}||^2_{L^\infty(I;V(\Omega))} + ||\tilde{\boldsymbol{f}}||_{L^\infty(I;\mathbf{H}^{-1}(\Omega))}). \end{aligned} \tag{3.42}$$

Proof. The part for the velocity can be found in [59, Theorem III.3.7]). The pressure regularity and uniqueness can be obtained in the very same way as in Lemma 3.8 since $\tilde{\boldsymbol{f}} \in L^\infty(I; H(\Omega)) \hookrightarrow L^\infty(I; \mathbf{H}^{-1}(\Omega))$. □

Assuming more regularity for the boundary of Ω implies even more regularity for the solution $\tilde{\boldsymbol{v}}$. For details we refer again to [59, Section III.3.5].

3.2.3 Basic Assumptions

In the following we will define the functions $\bar{E}, \bar{J}$ and E, J as introduced for the abstract shape optimization problem in Section 3.1 for the shape optimization problem with Navier-Stokes equations. For the transformations and the data of the Navier-Stokes problem we assume:

(N1) The reference domain $\Omega_{\text{ref}} \in \mathcal{O}_{\text{ad}}$ is a bounded Lipschitz domain such that there exists a bounded Lipschitz domain D with $\bar{\Omega} \subset D$ for all $\Omega \in \mathcal{O}_{\text{ad}}$.

(N2) There exists a closed and bounded set $T_{\text{ad}} \subset \mathcal{T}^{2,\infty} \cap T_{\text{ref}}$, where

$$T_{\text{ref}} := \{\tau : \mathbb{R}^d \to \mathbb{R}^d \mid (\tau - \text{id}) \in S\},$$

such that $\mathcal{O}_{\text{ad}} = \{\tau(\Omega_{\text{ref}}) \mid \tau \in T_{\text{ad}}\}$. Here

$$S := \{V \in \mathbf{W}^{2,\infty}(\mathbb{R}^d) \mid V \equiv 0 \text{ near the boundary } \Gamma_{\text{ext}}\} \tag{3.43}$$

where $\Gamma_{\text{ext}} := \partial\Omega_{\text{ref}} \backslash \Gamma_B$ is the fixed boundary part and Γ_B is the design boundary. Furthermore it holds that

$$||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} < c(\Omega_{\text{ref}})$$

with $c(\Omega_{\text{ref}})$ being the constant defined in Lemma 3.2.

(N3) For the data $\tilde{\boldsymbol{v}}_0$ and $\tilde{\boldsymbol{f}}$ it holds

$$\begin{aligned} &\tilde{\boldsymbol{f}} \in L^\infty(I; \mathbf{C}^1(\Omega)),\ \tilde{\boldsymbol{f}}_t \in L^2(I; \mathbf{H}^{-1}(\Omega)), \\ &\tilde{\boldsymbol{f}}(0) \in H(\Omega),\ \tilde{\boldsymbol{v}}_0 \in V(\Omega) \cap \mathbf{H}^2(\Omega) \cap \mathbf{C}^1(\Omega) \end{aligned}$$

for all $\Omega \in \mathcal{O}_{\text{ad}} = \{\tau(\Omega_{\text{ref}}) \mid \tau \in T_{ad}\}$. So the data $\tilde{\boldsymbol{v}}_0, \tilde{\boldsymbol{f}}_0$ are used on all $\Omega \in \mathcal{O}_{\text{ad}}$. For $d = 3$ we furthermore assume that condition (C) holds.

Assumption (N3) ensures that the assumptions of Lemma 3.8 and Lemma 3.11 are satisfied. (N2) guarantees for all $\tau \in T_{\text{ad}}$ that the domains $\tau(\Omega_{\text{ref}})$ still have Lipschitz boundary, c.f. Lemma 3.2, and that $\det \tau' > 0$. By (N2) for all $\tau \in T_{\text{ad}}$ we have that $\tau \equiv \text{id}$ near the exterior boundary $\Gamma_{\text{ext}} = \partial\Omega_{\text{ref}} \backslash \Gamma_B$. Furthermore the smoothness of the transformations allows us to transport the Navier-Stokes equations on a domain Ω back to the reference domain Ω_{ref} and to show differentiability of the design-to-state operator and the state equations using the higher regularity implied by (N3).
For the remainder of this chapter we assume that (N1)-(N3) are satisfied.

3.2.4 Transformation to the Reference Domain

Let $\Omega = \tau(\Omega_{\text{ref}})$ with $\tau \in T_{\text{ad}}$ be given. We want to transform the variational form of the Navier-Stokes equations (3.27) on the domain $\Omega = \tau(\Omega_{\text{ref}})$ back to the reference domain Ω_{ref} such that the whole problem can be defined on Ω_{ref}. However, the solenoidality is not preserved by the pullback operation, i.e. for $\tau \in T_{\text{ad}}, \Omega = \tau(\Omega_{\text{ref}})$ the spaces $V_\tau(\Omega) := \{\boldsymbol{v} = \tilde{\boldsymbol{v}} \circ \tau \mid \tilde{\boldsymbol{v}} \in V(\Omega)\}$ and $H_\tau(\Omega) := \{\boldsymbol{v} = \tilde{\boldsymbol{v}} \circ \tau \mid \tilde{\boldsymbol{v}} \in H(\Omega)\}$ depend on τ and contain functions that are not solenoidal on Ω_{ref}. Since this is not suitable, we reintroduce the pressure, and formulate the incompressibility condition explicitly. In fact, using the spaces $\mathbf{H}_0^1(\Omega)$ and $\mathbf{L}^2(\Omega)$ instead of $V(\Omega)$ and $H(\Omega)$, the solenoidality is not included in the test and trial spaces and we arrive at the following *weak velocity-pressure formulation* of problem (3.27):
Find $(\tilde{\boldsymbol{v}}, \tilde{p}) \in W(I; \mathbf{H}_0^1(\Omega)) \times L^2(I; L_0^2(\Omega))$ such that

$$\begin{aligned}
\langle \tilde{\boldsymbol{v}}_t(\cdot,t), \tilde{\boldsymbol{w}} \rangle_{\mathbf{H}^{-1}(\Omega),\mathbf{H}_0^1(\Omega)} + \int_\Omega \tilde{\boldsymbol{v}}(\tilde{x},t)^T \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x} + \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x} \\
- \int_\Omega \tilde{p}(\tilde{x},t)\ \operatorname{div}\, \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x} = \int_\Omega \tilde{\boldsymbol{f}}(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ \forall \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega) \ \text{ for a.a. } t \in I, \\
\int_\Omega \tilde{q}(\tilde{x})\ \operatorname{div}\, \tilde{\boldsymbol{v}}(\tilde{x},t)\, d\tilde{x} = 0 \qquad\qquad \forall \tilde{q} \in L_0^2(\Omega) \ \text{ for a.a. } t \in I, \\
\tilde{\boldsymbol{v}}(\cdot,0) = \tilde{\boldsymbol{v}}_0.
\end{aligned} \tag{3.44}$$

Note, that the requirement $\tilde{\boldsymbol{v}} \in W(I; \mathbf{H}_0^1(\Omega))$ is stronger than $\tilde{\boldsymbol{v}} \in W(I; V(\Omega))$ since $\tilde{\boldsymbol{v}}_t \in L^2(I; \mathbf{H}^{-1}(\Omega))$ is a stronger condition than $\tilde{\boldsymbol{v}}_t \in L^2(I; V(\Omega)^*)$. But under assumption (N3) $\tilde{\boldsymbol{v}}$ has even higher regularity than $W(I; \mathbf{H}_0^1(\Omega))$. In fact by Lemma 3.8 and 3.11, for $d = 2, 3$ we have $\tilde{\boldsymbol{v}}_t \in L^2(I; V(\Omega)) \cap L^\infty(I; H(\Omega))$ so that the first term can be represented by

$$\langle \tilde{\boldsymbol{v}}_t(\cdot,t), \tilde{\boldsymbol{w}} \rangle_{\mathbf{H}^{-1}(\Omega),\mathbf{H}_0^1(\Omega)} = \int_\Omega \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{w}}\ d\tilde{x}.$$

Furthermore (N3) guarantees that $\tilde{p} \in L^2(I; L_0^2(\Omega))$. By including also the initial condition on the velocity, we can express (3.44) in a weak space-time velocity-pressure formulation: Find $(\tilde{\boldsymbol{v}}, \tilde{p}) \in Y(\Omega)$ with

$$
\begin{aligned}
&\int_\Omega (\tilde{\boldsymbol{v}}(\tilde{x},0) - \tilde{\boldsymbol{v}}_0(\tilde{x}))^T \tilde{\boldsymbol{w}}_0(\tilde{x})\ d\tilde{x} + \int_I \int_\Omega \tilde{\boldsymbol{v}}_t(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \tilde{\boldsymbol{v}}(\tilde{x},t)^T \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt + \int_I \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt \\
&- \int_I \int_\Omega \tilde{p}(\tilde{x},t)\ \operatorname{div}\ \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt - \int_I \int_\Omega \tilde{\boldsymbol{f}}(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \tilde{q}(\tilde{x})\ \operatorname{div}\ \tilde{\boldsymbol{v}}(\tilde{x},t)\, d\tilde{x}\ dt = 0 \quad \forall\, (\tilde{\boldsymbol{w}}, \tilde{\boldsymbol{w}}_0, \tilde{q}) \in Z(\Omega)^*,
\end{aligned}
\tag{3.45}
$$

where

$$
\begin{aligned}
Y(\Omega) &:= W(I; \mathbf{H}_0^1(\Omega)) \times L^2(I; L_0^2(\Omega)), \\
Z(\Omega) &:= L^2(I; \mathbf{H}^{-1}(\Omega)) \times \mathbf{L}^2(\Omega) \times L^2(I; L_0^2(\Omega)), \\
Z(\Omega)^* &= L^2(I; \mathbf{H}_0^1(\Omega)) \times \mathbf{L}^2(\Omega) \times L^2(I; L_0^2(\Omega)).
\end{aligned}
$$

Now we transform the state equation (3.44), defined on the domain $\Omega = \tau(\Omega_{\text{ref}})$ for $\tau \in T_{\text{ad}}$, back to the domain Ω_{ref}. As already introduced we write $\sim$ to denote that a function is defined on $\tau(\Omega_{\text{ref}})$. For functions $\tilde{\boldsymbol{v}}, \tilde{p}$ defined on $\tau(\Omega_{\text{ref}})$ we define $\boldsymbol{v}, p$ with domain Ω_{ref} by

$$
\boldsymbol{v}(x,t) := \tilde{\boldsymbol{v}}(\tau(x),t), \quad p(x,t) := \tilde{p}(\tau(x),t).
$$

For the gradient of a function $\tilde{g}$ defined on $\tau(\Omega_{\text{ref}})$ we have for $x \in \Omega_{\text{ref}}$

$$
\nabla_{\tilde{x}} \tilde{g}(\tau(x)) = \tau'(x)^{-T} \nabla_x g(x).
$$

Using these formulas we can apply the transformation rule for integrals for the terms in (3.44). The transformation acts only on the space. We will omit in the following the dependence of the functions on x and t.

$$
\begin{aligned}
\langle \tilde{\boldsymbol{v}}_t, \tilde{\boldsymbol{w}} \rangle_{\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})), \mathbf{H}_0^1(\tau(\Omega_{\text{ref}}))} &= \langle \boldsymbol{v}_t, \boldsymbol{w} \det \tau' \rangle_{\mathbf{H}^{-1}(\Omega_{\text{ref}}), \mathbf{H}_0^1(\Omega_{\text{ref}})}, \\
\int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{w}} \; d\tilde{x} &= \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{w} \det \tau' \; dx, \\
\int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{v}}^T \nabla_{\tilde{x}} \tilde{\boldsymbol{v}} \tilde{\boldsymbol{w}} \; d\tilde{x} &= \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \boldsymbol{w} \det \tau' \; dx, \\
\int_{\tau(\Omega_{\text{ref}})} \nu \nabla_{\tilde{x}} \tilde{\boldsymbol{v}} : \nabla_{\tilde{x}} \tilde{\boldsymbol{w}} \; d\tilde{x} &= \int_{\tau(\Omega_{\text{ref}})} \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{v}}_i^T \nabla \tilde{\boldsymbol{w}}_i \; d\tilde{x}, \\
&= \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau' \; dx, \\
\int_{\tau(\Omega_{\text{ref}})} \tilde{p} \; \text{div} \; \tilde{\boldsymbol{w}} \; d\tilde{x} &= \int_{\tau(\Omega_{\text{ref}})} \tilde{p} \; \text{tr} \; (\nabla \tilde{\boldsymbol{w}}) \; d\tilde{x}, \\
&= \int_{\Omega_{\text{ref}}} p \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \; dx, \\
\int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{w}} \; d\tilde{x} &= \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau)^T \boldsymbol{w} \det \tau' \; dx, \\
\int_{\tau(\Omega_{\text{ref}})} \tilde{q} \; \text{div} \; \tilde{\boldsymbol{v}} \; d\tilde{x} &= \int_{\tau(\Omega_{\text{ref}})} \tilde{q} \; \text{tr} \; (\nabla \tilde{\boldsymbol{v}}) \; d\tilde{x}, \\
&= \int_{\Omega_{\text{ref}}} q \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \; dx,
\end{aligned}
$$

where we used that $\tau \in \mathbf{W}^{2,\infty}(\Omega_{\text{ref}})$ implies $(\boldsymbol{w} \det \tau') \in \mathbf{H}_0^1(\Omega_{\text{ref}})$. The transformed weak Navier-Stokes equations problem can then be written as:
Find $(\boldsymbol{v}, p) \in W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) \times L^2(I; L_0^2(\Omega_{\text{ref}}))$ such that

$$
\begin{aligned}
\langle \boldsymbol{v}_t(\cdot, t), \boldsymbol{w} \det \tau' \rangle_{\mathbf{H}^{-1}(\Omega_{\text{ref}}), \mathbf{H}_0^1(\Omega_{\text{ref}})} &+ \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau' \, dx \\
+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \; \boldsymbol{w} \det \tau' \; dx &- \int_{\Omega_{\text{ref}}} p \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \, dx \\
- \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{w} \det \tau' \, dx &= 0 \quad \forall \, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\text{ref}}) \;\; \text{for a.a. } t \in I, \\
\int_{\Omega_{\text{ref}}} q \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \, dx &= 0 \quad \forall \, q \in L_0^2(\Omega_{\text{ref}}) \;\; \text{for a.a. } t \in I, \\
\boldsymbol{v}(\cdot, 0) &= \tilde{\boldsymbol{v}}_0(\tau(\cdot)).
\end{aligned}
\tag{3.46}
$$

For $\tau = \text{id}$ we recover directly the weak formulation (3.44) on the domain $\Omega = \Omega_{\text{ref}}$. For general $\tau \in T_{\text{ad}}$ we obtain an equivalent form of (3.44) on the domain $\Omega = \tau(\Omega_{\text{ref}})$. In fact, in the next subsection we will show that there are homeomorphisms between $W(I; \mathbf{H}_0^1(\tau(\Omega_{\text{ref}})))$ and $W(I; \mathbf{H}_0^1(\Omega_{\text{ref}}))$, and between $L_0^2(\tau(\Omega_{\text{ref}}))$ and $L_0^2(\Omega_{\text{ref}})$, such that (3.44) and (3.46) are equivalent.

For the space-time variational formulation we seak $(\boldsymbol{v}, p)$ such that

$$\begin{aligned}
&\int_{\Omega_{\mathrm{ref}}} (\boldsymbol{v}(\cdot,0) - \tilde{\boldsymbol{v}}_0(\tau))^T \boldsymbol{w}_0 \det \tau' \; dx + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}_t^T \boldsymbol{w} \det \tau' \, dx \; dt \\
+ &\int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau' \, dx \; dt + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \; \boldsymbol{w} \det \tau' \; dx \; dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} p \; \mathrm{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \, dx \; dt - \int_I \int_{\Omega_{\mathrm{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{w} \det \tau' \, dx \; dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} q \; \mathrm{tr} \; (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \, dx \; dt = 0 \quad \forall \, (\boldsymbol{w}, \boldsymbol{w}_0, q) \in Z(\Omega_{\mathrm{ref}})^*.
\end{aligned} \tag{3.47}$$

3.2.5 A Homeomorphism between the State Spaces

Assumptions (N1) - (N3) ensure in particular (3.30) for $d = 2$ and (3.40) for $d = 3$. Furthermore assumption (A0) holds in the following obvious version for time dependent problems, where the transformation acts only in space.

Lemma 3.12. *Let* $d \in \{2, 3\}$. *Then the space* $W(I; \mathbf{H}_0^1(\Omega))$ *for the velocity satisfies assumption* (A0), *more precisely, we have for all* $\tau \in T_{ad}$

$$\begin{gathered}
W(I; \mathbf{H}_0^1(\Omega_{\mathrm{ref}})) = \{\tilde{\boldsymbol{v}}(\tau(\cdot)) : \tilde{\boldsymbol{v}} \in W(I; \mathbf{H}_0^1(\tau(\Omega_{\mathrm{ref}})))\}, \\
\tilde{\boldsymbol{v}} \in W(I; \mathbf{H}_0^1(\tau(\Omega_{\mathrm{ref}}))) \mapsto \boldsymbol{v} := \tilde{\boldsymbol{v}}(\tau(\cdot)) \in W(I; \mathbf{H}_0^1(\Omega_{\mathrm{ref}})) \textit{ is a homeomorphism.}
\end{gathered} \tag{3.48}$$

Proof. We will show that (3.48) holds for real valued functions, i.e. for all $\tau \in T_{\mathrm{ad}}$ we have

$$\begin{gathered}
W(I; H_0^1(\Omega_{\mathrm{ref}})) = \{\tilde{v}(\tau(\cdot)) : \tilde{v} \in W(I; H_0^1(\tau(\Omega_{\mathrm{ref}})))\}, \\
\tilde{v} \in W(I; H_0^1(\tau(\Omega_{\mathrm{ref}}))) \mapsto v := \tilde{v}(\tau(\cdot)) \in W(I; H_0^1(\Omega_{\mathrm{ref}})) \text{ is a homeomorphism}
\end{gathered} \tag{3.49}$$

Then the assertion for the product space follows directly.
Let $\tau \in T_{\mathrm{ad}}$ and $\tilde{v} \in W(I; H_0^1(\tau(\Omega_{\mathrm{ref}})))$. We identify $\tilde{x} = \tau(x)$ and define $v(x,t) := \tilde{v}(\tau(x), t)$. Then by the transformation formula we have $\nabla_{\tilde{x}} \tilde{v}(\tau(x), t) = \tau'^{-T} \nabla_x v(x, t)$ and obtain

$$\begin{aligned}
&\|\tilde{v}\|^2_{L^2(I; H_0^1(\tau(\Omega_{\mathrm{ref}})))} \\
&= \int_I \int_{\tau(\Omega_{\mathrm{ref}})} (\nabla_{\tilde{x}} \tilde{v}(\tilde{x}, t)^T \nabla_{\tilde{x}} \tilde{v}(\tilde{x}, t)) \, d\tilde{x} \, dt \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} (\nabla_{\tilde{x}} \tilde{v}(\tau(x), t)^T \nabla_{\tilde{x}} \tilde{v}(\tau(x), t)) \det(\tau'(x)) \, dx \, dt \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} (\nabla_x v(x,t)^T \tau'(x)^{-1} \tau'(x)^{-T} \nabla_x v(x,t)) \det(\tau'(x)) \, dx \, dt \\
&\leq \|\det(\tau')\|_{L^\infty(\Omega_{\mathrm{ref}})} \|(\tau')^{-1} (\tau')^{-T}\|_{L^\infty(\Omega_{\mathrm{ref}})^{d \times d}} \|v\|^2_{L^2(I; H_0^1(\Omega_{\mathrm{ref}}))}.
\end{aligned}$$

This shows that the linear mapping

$$\tilde{v} \in L^2(I; H_0^1(\tau(\Omega_{\text{ref}}))) \mapsto v = \tilde{v}(\tau(\cdot), \cdot) \in L^2(I; H_0^1(\Omega_{\text{ref}}))$$

is bounded and the same argument with τ^{-1} instead of τ shows that the inverse is also bounded. For $\tau \in T_{\text{ad}}$ we have $\det(\tau') \in W^{1,\infty}(\Omega_{\text{ref}})$ and $\det(\tau') \geq \delta$ for some $\delta > 0$. Therefore, the linear mapping

$$v \in L^2(I; H_0^1(\Omega_{\text{ref}})) \mapsto v \det(\tau') \in L^2(I; H_0^1(\Omega_{\text{ref}}))$$

is also bounded with bounded inverse. Here we used that $\tau \in \mathbf{W}^{2,\infty}(\Omega_{\text{ref}})$ implies $v(t)\ \det(\tau') \in H_0^1(\Omega_{\text{ref}})$ for all $t \in I$. We conclude that the linear operator

$$A(\tau) : \tilde{v} \in L^2(I; H_0^1(\tau(\Omega_{\text{ref}}))) \mapsto v \det(\tau') = \tilde{v}(\tau(\cdot), \cdot)\det(\tau') \in L^2(I; H_0^1(\Omega_{\text{ref}}))$$

is bounded with bounded inverse. Let $\tilde{v} \in W(I; H_0^1(\tau(\Omega_{\text{ref}})))$ be arbitrary. Then $\tilde{v}_t \in L^2(I; H^{-1}(\tau(\Omega_{\text{ref}})))$ and for all $\tilde{w} \in L^2(I; H_0^1(\tau(\Omega_{\text{ref}})))$

$$\begin{aligned}
&\langle \tilde{v}_t, \tilde{w} \rangle_{L^2(I;H^{-1}(\tau(\Omega_{\text{ref}}))),L^2(I;H_0^1(\tau(\Omega_{\text{ref}})))} \\
&= \langle \tilde{v}_t, A(\tau)^{-1}(\tilde{w}(\tau(\cdot), \cdot)\det(\tau')) \rangle_{L^2(I;H^{-1}(\tau(\Omega_{\text{ref}}))),L^2(I;H_0^1(\tau(\Omega_{\text{ref}})))} \\
&= \langle A(\tau)^{-*}\tilde{v}_t, \tilde{w}(\tau(\cdot), \cdot)\det(\tau') \rangle_{L^2(I;H^{-1}(\Omega_{\text{ref}})),L^2(I;H_0^1(\Omega_{\text{ref}}))}.
\end{aligned}$$

Hence, we have for all $\tilde{w} \in H_0^1(\tau(\Omega_{\text{ref}}))$ and all $\phi \in C_0^\infty(I; \mathbb{R})$:

$$\begin{aligned}
&\langle A(\tau)^{-*}\tilde{v}_t, \phi(\cdot)\tilde{w}(\tau(\cdot))\det(\tau') \rangle_{L^2(I;H^{-1}(\Omega_{\text{ref}})),L^2(I;H_0^1(\Omega_{\text{ref}}))} = \\
&= \int_I \langle \tilde{v}_t(\cdot, t), \tilde{w} \rangle_{H^{-1}(\tau(\Omega_{\text{ref}})),H_0^1(\tau(\Omega_{\text{ref}}))} \phi(t)\, dt = -\int_I \int_{\tau(\Omega_{\text{ref}})} \tilde{v}(\tilde{x}, t)\tilde{w}(\tilde{x})\phi'(t)\, d\tilde{x}\, dt \\
&= -\int_I \int_{\Omega_{\text{ref}}} \tilde{v}(\tau(x), t)\tilde{w}(\tau(x))\det(\tau'(x))\phi'(t)\, dx\, dt \\
&= -\int_I \langle \tilde{v}(\tau(\cdot), t), \tilde{w}(\tau(\cdot)) \det \tau' \rangle_{H^{-1}(\Omega_{\text{ref}}),H_0^1(\Omega_{\text{ref}})} \phi'(t)\ dt \\
&= \langle \tilde{v}(\tau(\cdot), \cdot), \phi'(\cdot)\tilde{w}(\tau(\cdot))\det(\tau') \rangle_{L^2(I;H^{-1}(\Omega_{\text{ref}})),L^2(I;H_0^1(\Omega_{\text{ref}}))}.
\end{aligned}$$

Therefore, $v = \tilde{v}(\tau(\cdot), \cdot)$ has the weak time derivative

$$v_t = A(\tau)^{-*}\tilde{v}_t \in L^2(I; H^{-1}(\Omega_{\text{ref}})),$$

since the operator $A(\tau)^{-*}$ is bounded.
This concludes the proof that the linear mapping

$$\tilde{v} \in W(I; H_0^1(\tau(\Omega_{\text{ref}}))) \mapsto v = \tilde{v}(\tau(\cdot), \cdot) \in W(I; H_0^1(\Omega_{\text{ref}}))$$

is bounded. The same arguments with τ^{-1} instead of τ yield (3.49) and therefore (3.48). □

A similar result can be shown for the pressure space if we define a topology on $\{p \mid p(\cdot,t) \in L^2_0(\Omega)\ \forall t \in I\}$ like $L^p(I; L^2_0(\Omega))$ as guaranteed by Lemma 3.8 and 3.11. In fact, we have a homeomorphism $\tilde{q} \in L^2_0(\tau(\Omega_{\text{ref}})) \mapsto q \in L^2_0(\Omega_{\text{ref}})$ by

$$q(x) := \tilde{q}(\tau(x)) - \frac{1}{\mu(\Omega_{\text{ref}})} \int_{\Omega_{\text{ref}}} \tilde{q}(\tau(y))\ dy.$$

Note that the last term implies that $q \in L^2_0(\Omega_{\text{ref}})$ but not necessarily $\tilde{q}(\tau(\cdot))$. However as $||\tilde{q}(\tau)||_{L^2(\Omega_{\text{ref}})/\mathbb{R}} = ||q||_{L^2_0(\Omega_{\text{ref}})}$ we just choose the corresponding representative in $L^2_0(\Omega_{\text{ref}})$.

3.2.6 The Shape Optimization Problem

Let $\bar{J}$ be an objective function of type

$$\bar{J}(\tilde{\boldsymbol{v}}, \Omega) := \underbrace{\int_I \int_\Omega f_1(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x},t), \nabla\tilde{\boldsymbol{v}}(\tilde{x},t))\ d\tilde{x}\ dt}_{=:\bar{J}^D(\tilde{\boldsymbol{v}},\Omega)} + \underbrace{\int_\Omega f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x},T))\ d\tilde{x}}_{=:\bar{J}^T(\tilde{\boldsymbol{v}},\Omega)}. \quad (3.50)$$

Here, $f_1 : D \times \mathbb{R}^d \times \mathbb{R}^{d\times d} \to \mathbb{R}$ and $f_2 : D \times \mathbb{R}^d \to \mathbb{R}$ are at least twice continuously differentiable functions. f_2 describes the part of the objective function that depends on the velocity at end time T. Note that we only allow an impact of $\tilde{\boldsymbol{v}}$ (and not of $\tilde{p}$) on the objective and this ensures that the adjoint velocity is solenoidal in the adjoint Navier-Stokes equations. In many applications the objective functions indeed depend only on $\boldsymbol{v}$, e.g. the drag of one or more objects.

We can transform the objective function to an objective that is defined on the reference domain Ω_{ref} by the transformation rule for integrals and arrive at

$$\begin{aligned} J(\boldsymbol{v}, \tau) := & \underbrace{\int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \boldsymbol{v}(x,t), \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t)) \det\tau'\ dx\ dt}_{=:J^D(\boldsymbol{v},\tau)} \\ & + \underbrace{\int_{\Omega_{\text{ref}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \det\tau'\ dx,}_{=:J^T(\boldsymbol{v},\tau)} \end{aligned} \quad (3.51)$$

where $\boldsymbol{v}$ is a function defined on Ω_{ref}. We have $\bar{J}(\tilde{\boldsymbol{v}}, \tau(\Omega_{\text{ref}})) = J(\boldsymbol{v}, \tau)$ where $\tilde{\boldsymbol{v}} \circ \tau = \boldsymbol{v}$.

We arrive at the optimization problem:

Problem 3.4. *We call*

$$\min_{(\boldsymbol{v},p,\tau)} \int_I \int_{\Omega_{ref}} f_1(\cdot, \boldsymbol{v}, \tau'^{-T}\nabla \boldsymbol{v})\ dx\ dt + \int_{\Omega_{ref}} f_2(\cdot, \boldsymbol{v}(\cdot, T))\ dx\ s.t.$$

$$\langle \boldsymbol{v}_t(\cdot,t), \boldsymbol{w} \det \tau' \rangle_{\mathbf{H}^{-1}(\Omega_{ref}),\mathbf{H}_0^1(\Omega_{ref})} + \sum_{i=1}^{d} \int_{\Omega_{ref}} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau'\, dx$$

$$+ \int_{\Omega_{ref}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v}\ \boldsymbol{w} \det \tau'\ dx - \int_{\Omega_{ref}} p\ tr\ (\tau'^{-T}\nabla \boldsymbol{w}) \det \tau'\, dx$$

$$- \int_{\Omega_{ref}} \tilde{\boldsymbol{f}}(\tau(x),t)^T \boldsymbol{w} \det \tau'\, dx = 0 \quad \forall\, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{ref}) \ \ \textit{for a.a. } t \in I,$$

$$\int_{\Omega_{ref}} q\ tr\ (\tau'^{-T}\nabla \boldsymbol{v}) \det \tau'\, dx = 0 \quad \forall\, q \in L_0^2(\Omega_{ref}) \ \ \textit{for a.a. } t \in I,$$

$$\boldsymbol{v}(\cdot,0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot))$$

the ***shape optimization problem for the instationary Navier-Stokes equations****.*

In Section 3.3 we will derive the shape derivatives of the reduced objective function $j(\tau) := J(\boldsymbol{v}(\tau), \tau)$ using the setting introduced in Section 3.1.9.

3.2.7 The Instationary Navier-Stokes Equations with Inhomogeneous Boundary Conditions

In many applications, e.g. when considering the flow around a cylinder, there are different boundary conditions for the state equation. To cover these scenarios, we consider the Navier-Stokes equations with inhomogeneous Dirichlet boundary conditions and a free outflow on the outer boundary Γ_{ext}. The state equation on a domain Ω is then given by

$$\begin{aligned}
\tilde{\boldsymbol{v}}_t - \nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} && \text{on } \Omega \times I,\\
\operatorname{div} \tilde{\boldsymbol{v}} &= 0 && \text{on } \Omega \times I,\\
\tilde{\boldsymbol{v}} &= \tilde{\boldsymbol{v}}_{D_{\text{ext}}} && \text{on } \Gamma_{D_{\text{ext}}} \times I,\\
\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_B \times I,\\
\tilde{p}\,\tilde{\boldsymbol{n}} - \nu\frac{\partial}{\partial\tilde{n}}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_N \times I,\\
\tilde{\boldsymbol{v}}(\cdot,0) &= \tilde{\boldsymbol{v}}_0 && \text{on } \Omega.
\end{aligned}$$

Here Γ_B is the boundary of the design object where we impose homogeneous Dirichlet boundary conditions. For the remaining outer boundary, we have a Dirichlet part $\Gamma_{D_{\text{ext}}} \neq \emptyset$ and a Neumann part $\Gamma_N \neq \emptyset$. On Γ_N we have a free outflow condition. We denote the Dirichlet boundary by $\Gamma_D := \Gamma_{D_{\text{ext}}} \cup \Gamma_B$.
For the variational form we introduce the space $\mathbf{H}_0^1(\Omega, \Gamma_D)$ of $\mathbf{H}^1$ functions $\tilde{\boldsymbol{w}}$ with $\tilde{\boldsymbol{w}} = 0$ on Γ_D. Testing the momentum equation with $\tilde{\boldsymbol{w}} \in H_0^1(\Omega, \Gamma_D)$ we

have for a.a. $t \in I$:

$$
\begin{aligned}
\int_\Omega \sum_{i=1}^{d} -\nu \ \mathrm{div}\ (\nabla \tilde{\boldsymbol{v}}_i(\tilde{x},t))\tilde{\boldsymbol{w}}_i(\tilde{x})\ d\tilde{x} &+ \int_\Omega \sum_{i=1}^{d} \frac{\partial}{\partial \tilde{x}_i}\tilde{p}(\tilde{x},t)\tilde{\boldsymbol{w}}_i(\tilde{x})\ d\tilde{x} \\
&= \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x} - \int_\Omega \tilde{p}(\tilde{x},t)\ \mathrm{div}\ \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x} \\
&\quad - \int_{\partial\Omega} \nu \frac{\partial}{\partial \tilde{n}} \tilde{\boldsymbol{v}}(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{S} + \int_{\partial\Omega} \tilde{p}(\tilde{x},t)\tilde{n}^T \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{S} \\
&= \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x} - \int_\Omega \tilde{p}(\tilde{x},t)\ \mathrm{div}\ \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x} \\
&\qquad - \int_{\Gamma_N} \nu \frac{\partial}{\partial \tilde{n}} \tilde{\boldsymbol{v}}(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x}) + \tilde{p}(\tilde{x},t)\tilde{n}^T \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{S} \\
&= \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x} - \int_\Omega \tilde{p}(\tilde{x},t)\ \mathrm{div}\ \tilde{\boldsymbol{w}}(\tilde{x})\ d\tilde{x},
\end{aligned}
$$

where we used that $\tilde{\boldsymbol{w}} = 0$ on Γ_D and $\tilde{p}\tilde{\boldsymbol{n}} - \nu \frac{\partial}{\partial \tilde{n}} \tilde{\boldsymbol{v}} = 0$ on Γ_N for a.a. $t \in I$.
Let $\bar{\boldsymbol{v}}$ be an extension of the Dirichlet boundary values, i.e. $\bar{\boldsymbol{v}} = \tilde{\boldsymbol{v}}_{D_{\text{ext}}}$ on $\Gamma_{D_{\text{ext}}}$ and $\bar{\boldsymbol{v}} = 0$ on Γ_B. Furthermore we assume enough regularity for $\tilde{\boldsymbol{v}}$ and $\tilde{p}$. Then the velocity-pressure variational formulation of the inhomogenous problem is: Find $(\tilde{\boldsymbol{v}}, \tilde{p}) \in \{\bar{\boldsymbol{v}} + \hat{\boldsymbol{v}} \mid \hat{\boldsymbol{v}} \in W(I; \mathbf{H}_0^1(\Omega, \Gamma_D))\} \times L^2(I; L^2(\Omega))$ with

$$
\begin{aligned}
&\int_\Omega (\tilde{\boldsymbol{v}}(\tilde{x},0) - \tilde{\boldsymbol{v}}_0)^T \tilde{\boldsymbol{w}}_0\ d\tilde{x} + \int_I \int_\Omega \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{w}}\ d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \tilde{\boldsymbol{v}}(\tilde{x},t)^T \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt + \int_I \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}(\tilde{x},t) : \nabla \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt \\
&- \int_I \int_\Omega \tilde{p}(\tilde{x},t)\ \ \mathrm{div}\ \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt - \int_I \int_\Omega \tilde{\boldsymbol{f}}(\tilde{x},t)^T \tilde{\boldsymbol{w}}(\tilde{x})\, d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \tilde{q}(\tilde{x})\ \ \mathrm{div}\ \tilde{\boldsymbol{v}}(\tilde{x},t)\, d\tilde{x}\ dt = 0 \quad \forall\, (\tilde{\boldsymbol{w}}, \tilde{\boldsymbol{w}}_0, \tilde{q}) \in \bar{Z}(\Omega)^*,
\end{aligned}
\tag{3.52}
$$

where $\bar{Z}(\Omega)^* := L^2(I; \mathbf{H}_0^1(\Omega, \Gamma_D)) \times \mathbf{L}^2(\Omega) \times L^2(I; L^2(\Omega))$. Note that $\tilde{p}$ is uniquely defined if $\Gamma_N \neq \emptyset$. Therefore we replaced $L^2(I; L_0^2(\Omega))$ by $L^2(I; L^2(\Omega))$ in contrast to the homogeneous problem without outflow.
There are also weak formulations of the problem where the solenoidality is included in the trial and test spaces. Then $\bar{\boldsymbol{v}}$ has to be a *solenoidal* extension of the Dirichlet boundary values, i.e. div $\bar{\boldsymbol{v}} = 0$ and $\bar{\boldsymbol{v}} = \tilde{\boldsymbol{v}}_{D_{\text{ext}}}$ on $\Gamma_{D_{\text{ext}}}$, $\bar{\boldsymbol{v}} = 0$ on Γ_B. For the concrete formulation and the existence of such a solenoidal extension $\bar{\boldsymbol{v}}$, see the comments in [28] and [20].
The system (3.52) is the inhomogeneous version of (3.45), assuming enough regularity for the state. We will not specify a corresponding version of (3.44) for weaker states and the impact on a well-posed shape optimization problem. In fact, the existence and uniqueness theory for inhomogeneous Navier-Stokes equations with inflow is very involved and in part still an open topic. This also concerns the regularity of the solutions. For existence and uniqueness results in a concrete setting with inflow see, e.g., [28].

3.3 Shape Derivatives for the Shape Optimization Problem with Navier-Stokes Equations

We want to calculate the shape derivatives of the reduced objective function

$$j(\tau) := J(\boldsymbol{v}(\tau), \tau),$$

where $(\boldsymbol{v}(\tau), p(\tau))$ is the solution of the instationary Navier-Stokes equations. In this section, we assume that the data and the space of transformations T_{ref} are regular enough such that the state equation can be expressed as

$$\begin{aligned}
&\langle(\boldsymbol{w}, \boldsymbol{w}_0, q), E((\boldsymbol{v}, p), \tau)\rangle_{Z(\Omega_{\text{ref}})^*, Z(\Omega_{\text{ref}})} := \\
&\int_{\Omega_{\text{ref}}} (\boldsymbol{v}(\cdot, 0) - \tilde{\boldsymbol{v}}_0(\tau))^T \boldsymbol{w}_0 \det \tau' \; dx + \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{w} \det \tau' \, dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau' \, dx \; dt + \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \boldsymbol{w} \det \tau' \; dx \; dt \\
&- \int_I \int_{\Omega_{\text{ref}}} p \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \; dx \; dt - \int_I \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{w} \det \tau' \, dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} q \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \; dx \; dt = 0 \quad \forall \, (\boldsymbol{w}, \boldsymbol{w}_0, q) \in Z(\Omega_{\text{ref}})^*
\end{aligned} \tag{3.53}$$

and that assumptions (A1) - (A4) (c.f. Section 3.1.8) are satisfied. For evaluating second derivatives of the reduced objective function we need even more assumptions regarding second derivatives of E and J. In the following we calculate the shape derivatives on a formal level without substantiating the technical details. A rigorous setting in a suitable function space framework will be introduced in Chapter 4 and is one of the main parts of this work.
To calculate the shape derivatives of the reduced objective function we use the adjoint approach as already introduced in the setting in Section 3.1.9. For the first shape derivatives we apply Algorithm 3.2 to the instationary Navier-Stokes equations. Here, we need the evaluation of $E_{(\boldsymbol{v},p)}$, E_τ and $J_{(\boldsymbol{v},p)}$. For the evaluation of second shape derivatives as decribed in Algorithm 3.3 in the general setting we need the evaluation of the second derivatives of the Lagrange function $\mathcal{L}$ using the second derivatives of E and J.

3.3.1 First Derivatives of the State Equation and the Objective Function

For evaluating the first order shape derivatives we calculate the derivatives of E and J. For E we use the variational formulation (3.53) and test $E((\boldsymbol{v}, p), \tau)$ with $(\boldsymbol{\lambda}, \lambda_0, \mu) \in Z(\Omega_{\text{ref}})^*$. Then we differentiate with respect to $(\boldsymbol{v}, p)$ and τ to obtain directional derivatives. The directional derivatives with respect to τ are computed in directions $V \in S \subset \mathbf{W}^{2,\infty}(\mathbb{R}^d)$.

We assume that the objective function has the form (3.51)

$$J(\boldsymbol{v},\tau) = \int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \boldsymbol{v}(x,t), \tau'(x)^{-T}\nabla \boldsymbol{v}(x,t)) \det \tau' \, dx \, dt \\ + \int_{\Omega_{\text{ref}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \det \tau' \, dx$$

and derive the derivatives for J in this setting. Note that J only depends on $\boldsymbol{v}$ and τ but not on p. Therefore we define the restriction $\hat{Y}_{\text{ref}}$ as the velocity part of Y_{ref}. Furthermore we interpret $J : Y_{\text{ref}} \times T_{\text{ad}} \to \mathbb{R}$ as a function $J : \hat{Y}_{\text{ref}} \times T_{\text{ad}} \to \mathbb{R}$.

3.3.1.1 First derivative E_τ. Let $((\boldsymbol{v},p),\tau) \in Y_{\text{ref}} \times T_{\text{ad}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\text{ref}}}^*$ and $V \in S$. Then we have

$$\begin{aligned}
&\langle(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_\tau((\boldsymbol{v},p),\tau)V\rangle_{{Z_{\text{ref}}}^*, Z_{\text{ref}}} = \\
&= \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda} \text{ tr } (\tau'^{-1}V') \det \tau' \, dx \, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} (\text{tr}(\tau'^{-1}V')I - V'\tau'^{-1} - \tau'^{-T}V'^T)\tau'^{-T}\nabla \boldsymbol{\lambda}_i \det \tau' \, dx \, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T (\text{ tr } (\tau'^{-1}V')I - \tau'^{-T}V'^T)\tau'^{-T}\nabla \boldsymbol{v} \boldsymbol{\lambda} \det \tau' \, dx \, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} p \left(\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla \boldsymbol{\lambda}) - \text{ tr } (\tau'^{-T}\nabla \boldsymbol{\lambda}) \text{ tr } (\tau'^{-1}V')\right) \det \tau' \, dx \, dt \\
&- \int_I \int_{\Omega_{\text{ref}}} \left(\tilde{\boldsymbol{f}}(\tau(x),t)^T \text{ tr } (\tau'^{-1}V') + V^T \nabla \tilde{\boldsymbol{f}}(\tau(x),t)\right) \boldsymbol{\lambda} \det \tau' \, dx \, dt \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}(x,0)^T \boldsymbol{\lambda}_0 \text{ tr } (\tau'^{-1}V') \det \tau' \, dx \\
&- \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{v}}_0(\tau(x))^T \boldsymbol{\lambda}_0 \text{ tr } (\tau'^{-1}V') \det \tau' \, dx - \int_{\Omega_{\text{ref}}} V^T \nabla \tilde{\boldsymbol{v}}_0(\tau(x)) \boldsymbol{\lambda}_0 \det \tau' \, dx \\
&- \int_I \int_{\Omega_{\text{ref}}} \mu \left(\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla \boldsymbol{v}) - \text{ tr } (\tau'^{-T}\nabla \boldsymbol{v}) \text{ tr } (\tau'^{-1}V')\right) \det \tau' \, dx \, dt.
\end{aligned} \tag{3.54}$$

In 2D the third term can be written as

$$\int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T V'^{-T} \nabla \boldsymbol{v} \lambda \det V' \, dx \, dt,$$

the fourth term equals

$$\int_I \int_{\Omega_{\text{ref}}} -p \text{ tr } (V'^{-T}\nabla \boldsymbol{\lambda}) \det V' \, dx \, dt,$$

and the last term is

$$\int_I \int_{\Omega_{\text{ref}}} \mu \text{ tr } (V'^{-T}\nabla \boldsymbol{v}) \det V' \, dx \, dt.$$

So in 2D we have

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu),E_\tau((\boldsymbol{v},p),\tau)V\rangle_{Z_{\mathrm{ref}}{}^*,Z_{\mathrm{ref}}}=\\
&\qquad\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}_t^T\boldsymbol{\lambda}\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx\ dt\\
&\quad+\int_I\int_{\Omega_{\mathrm{ref}}}\sum_{i=1}^d\nu\nabla\boldsymbol{v}_i^T\tau'^{-1}(\mathrm{tr}(\tau'^{-1}V')I-V'\tau'^{-1}-\tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{\lambda}_i\det\tau'\ dx\ dt\\
&\quad+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^TV'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\det V'\ dx\ dt-\int_I\int_{\Omega_{\mathrm{ref}}}p\ \mathrm{tr}\ (V'^{-T}\nabla\boldsymbol{\lambda})\det V'\ dx\ dt\\
&\quad-\int_I\int_{\Omega_{\mathrm{ref}}}\Big(\tilde{\boldsymbol{f}}(\tau(x),t)^T\ \mathrm{tr}\ (\tau'^{-1}V')+V^T\nabla\tilde{\boldsymbol{f}}(\tau(x),t)\Big)\boldsymbol{\lambda}\det\tau'\ dx\ dt\\
&\quad+\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}(x,0)^T\boldsymbol{\lambda}_0\mathrm{tr}(\tau'^{-1}V')\det\tau'\ dx-\int_{\Omega_{\mathrm{ref}}}\tilde{\boldsymbol{v}}_0(\tau(x))^T\boldsymbol{\lambda}_0\mathrm{tr}(\tau'^{-1}V')\det\tau'\ dx\\
&\quad-\int_{\Omega_{\mathrm{ref}}}V^T\nabla\tilde{\boldsymbol{v}}_0(\tau(x))\boldsymbol{\lambda}_0\det\tau'\ dx-\int_I\int_{\Omega_{\mathrm{ref}}}\mu\ \mathrm{tr}\ (V'^{-T}\nabla\boldsymbol{v})\det V'\ dx\ dt.
\end{aligned}
$$

3.3.1.2 First derivative E_τ at $\tau=\mathrm{id}$. Let $(\boldsymbol{v},p)\in Y_{\mathrm{ref}}$, $(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu)\in Z_{\mathrm{ref}}{}^*$ and $V\in S$. Then in 2D and 3D we have

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu),E_\tau((\boldsymbol{v},p),\mathrm{id})V\rangle_{Z_{\mathrm{ref}}{}^*,Z_{\mathrm{ref}}}=\\
&\quad-\int_{\Omega_{\mathrm{ref}}}V^T\nabla\tilde{\boldsymbol{v}}_0\boldsymbol{\lambda}_0\ dx\\
&\quad+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}_t^T\boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt+\int_I\int_{\Omega_{\mathrm{ref}}}\nu\nabla\boldsymbol{v}:\nabla\boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt\\
&\quad-\int_I\int_{\Omega_{\mathrm{ref}}}\sum_{i=1}^d\nu\nabla\boldsymbol{v}_i^T(V'+V'^T)\nabla\boldsymbol{\lambda}_i\ dx\ dt\\
&\quad-\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^TV'^T\nabla\boldsymbol{v}\boldsymbol{\lambda}\ dx\ dt+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^T\nabla\boldsymbol{v}\boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt\\
&\quad+\int_I\int_{\Omega_{\mathrm{ref}}}p\ \mathrm{tr}\ (V'^T\nabla\boldsymbol{\lambda})\ dx\ dt-\int_I\int_{\Omega_{\mathrm{ref}}}p\ \mathrm{div}\ \boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt\\
&\quad-\int_I\int_{\Omega_{\mathrm{ref}}}\tilde{\boldsymbol{f}}^T\boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt-\int_I\int_{\Omega_{\mathrm{ref}}}V^T\nabla\tilde{\boldsymbol{f}}\boldsymbol{\lambda}\ dx\ dt\\
&\quad-\int_I\int_{\Omega_{\mathrm{ref}}}\mu\ \mathrm{tr}\ (V'^T\nabla\boldsymbol{v})\ dx\ dt+\int_I\int_{\Omega_{\mathrm{ref}}}\mu\ \mathrm{div}\ \boldsymbol{v}\ \mathrm{div}\ V\ dx\ dt\\
&\quad+\int_{\Omega_{\mathrm{ref}}}(\boldsymbol{v}(x,0)-\tilde{\boldsymbol{v}}_0(x))^T\boldsymbol{\lambda}_0\ \mathrm{div}\ V\ dx.
\end{aligned}
\tag{3.55}
$$

For 2D this formula can be simplified using the same equalities as above.

3.3.1.3 First derivative J_τ.

Let $(\boldsymbol{v}, \tau) \in \hat{Y}_{\text{ref}} \times T_{\text{ad}}$ and $V \in S$. Then we have

$$
\begin{aligned}
&\langle J_\tau(\boldsymbol{v}, \tau), V\rangle_{S^*,S} = \\
&\quad \int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \text{ tr } (\tau'^{-1} V') \det \tau' \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \, \tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v} \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) V \ \det \tau' \ dx \ dt \\
&\quad + \int_{\Omega_{\text{ref}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \text{ tr } (\tau'^{-1} V') \det \tau' \ dx \\
&\quad + \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_2(\tau(x), \boldsymbol{v}(x,T)) V \det \tau' \ dx.
\end{aligned}
\tag{3.56}
$$

3.3.1.4 First derivative J_τ at $\tau = \text{id}$.

Let $\boldsymbol{v} \in \hat{Y}_{\text{ref}}$ and $V \in S$. Then

$$
\begin{aligned}
&\langle J_\tau(\boldsymbol{v}, \text{id}), V\rangle_{S^*,S} = \\
&\quad + \int_I \int_{\Omega_{\text{ref}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \text{ div } V \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \, V'^T \nabla \boldsymbol{v} \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \, V \ dx \ dt \\
&\quad + \int_{\Omega_{\text{ref}}} f_2(x, \boldsymbol{v}(x,T)) \text{ div } V \ dx \\
&\quad + \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_2(x, \boldsymbol{v}(x,T)) V \ dx.
\end{aligned}
\tag{3.57}
$$

3.3.1.5 First derivative $E_{(v,p)}$.

Let $((\boldsymbol{v}, p), \tau) \in Y_{\text{ref}} \times T_{\text{ad}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\text{ref}}}^*$ and $(\boldsymbol{w}, q) \in Y_{\text{ref}}$. Then

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{(\boldsymbol{v},p)}((\boldsymbol{v}, p), \tau)(\boldsymbol{w}, q)\rangle_{{Z_{\text{ref}}}^*, Z_{\text{ref}}} = \\
&\quad \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \det \tau' \ dt \ dx + \int_{\Omega_{\text{ref}}} \boldsymbol{w}(x,0)^T \boldsymbol{\lambda}_0 \det \tau' \ dx \\
&\quad + \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{w}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{\lambda}_i \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\text{ref}}} \left(\boldsymbol{w}^T \tau'^{-T} \nabla \boldsymbol{v} + \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{w}\right) \boldsymbol{\lambda} \det \tau' \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\text{ref}}} q \text{ tr } (\tau'^{-T} \nabla \boldsymbol{\lambda}) \det \tau' \ dx \ dt + \int_I \int_{\Omega_{\text{ref}}} \mu \text{ tr } (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \ dx \ dt.
\end{aligned}
\tag{3.58}
$$

3.3.1.6 First derivative J_v. Let $(\boldsymbol{v},\tau) \in \hat{Y}_{\text{ref}} \times T_{\text{ad}}$ and $w \in \hat{Y}_{\text{ref}}$. Then

$$\begin{aligned}
&\langle J_{\boldsymbol{v}}(\boldsymbol{v},\tau),\boldsymbol{w}\rangle_{\hat{Y}^*_{\text{ref}},\hat{Y}_{\text{ref}}} = \\
&= \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla \boldsymbol{v}(x,t))\boldsymbol{w} \det \tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla \boldsymbol{v}(x,t))\tau'^{-T}\nabla \boldsymbol{w} \det \tau' \; dx \; dt \\
&+ \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tau(x),\boldsymbol{v}(x,T))\boldsymbol{w}(x,T) \det \tau' \; dx.
\end{aligned} \tag{3.59}$$

3.3.2 The Adjoint Equation and First Order Shape Derivatives

For calculating the first order shape derivative $j'(\tau)$ for a transformation $\tau \in T_{\text{ad}}$ we follow Algorithm 3.2. For the instationary Navier-Stokes equations we obtain:

Algorithm 3.5. ***(Calculation of Shape Derivatives for the Navier-Stokes equations)*** *Let $\tau \in T_{ad}$ be given.*

1. *Find $(\boldsymbol{v},p) \in Y_{ref}$ by solving the state equation*

$$\langle E((\boldsymbol{v},p),\tau),(\boldsymbol{w},\boldsymbol{w}_0,q)\rangle_{Z_{ref},{Z_{ref}}^*} = 0 \quad \forall (\boldsymbol{w},\boldsymbol{w}_0,q) \in {Z_{ref}}^*.$$

2. *Find the corresponding adjoint state $(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu) \in {Z_{ref}}^*$ via the adjoint equation such that $\forall (\boldsymbol{w},q) \in Y_{ref}$:*

$$\langle (\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu), E_{(\boldsymbol{v},p)}((\boldsymbol{v},p),\tau)(\boldsymbol{w},q)\rangle_{{Z_{ref}}^*,Z_{ref}} = -\langle J_{\boldsymbol{v}}(\boldsymbol{v},\tau),\boldsymbol{w}\rangle_{\hat{Y}^*_{ref},\hat{Y}_{ref}}.$$

3. *Calculate the reduced derivative $j'(\tau)$ via*

$$\langle j'(\tau),\cdot\rangle_{S^*,S} = \langle (\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu), E_\tau((\boldsymbol{v},p),\tau)\cdot\rangle_{{Z_{ref}}^*,Z_{ref}} + \langle J_\tau((\boldsymbol{v},p),\tau),\cdot\rangle_{S^*,S}.$$

We will now give concrete formulas for the three step above. The first one is simply solving the transformed Navier-Stokes system (3.53).
For step 2 we use (3.58). In fact, for the first term in (3.58) we have

$$\begin{aligned}
\int_I \int_{\Omega_{\text{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \det \tau' \; dt \; dx = &- \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{w}^T \boldsymbol{\lambda}_t \det \tau' \; dx \; dt \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{w}(\cdot,T)^T \boldsymbol{\lambda}(\cdot,T) \det \tau' \; dx \\
&- \int_{\Omega_{\text{ref}}} \boldsymbol{w}(\cdot,0)^T \boldsymbol{\lambda}(\cdot,0) \det \tau' \; dx,
\end{aligned}$$

where we applied integration by parts for the time variable. Using this identity the adjoint equation reads

$$
\begin{aligned}
&- \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}^T \boldsymbol{\lambda}_t \det \tau' \; dx \; dt + \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}(\cdot, T)^T \boldsymbol{\lambda}(\cdot, T) \det \tau' \; dx \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{w}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{\lambda}_i \det \tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \left(\boldsymbol{w}^T \tau'^{-T} \nabla \boldsymbol{v} + \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{w} \right) \boldsymbol{\lambda} \det \tau' \; dx \; dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} q \; \mathrm{tr} \; (\tau'^{-T} \nabla \boldsymbol{\lambda}) \det \tau' \; dx \; dt + \int_I \int_{\Omega_{\mathrm{ref}}} \mu \; \mathrm{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \; dx \; dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}(\cdot, 0)^T (\boldsymbol{\lambda}_0 - \boldsymbol{\lambda}(\cdot, 0)) \det \tau' \; dx = -\langle J_{\boldsymbol{v}}(\boldsymbol{v}, \tau), \boldsymbol{w} \rangle_{\hat{Y}_{\mathrm{ref}}^*, \hat{Y}_{\mathrm{ref}}} \forall (\boldsymbol{w}, q) \in Y_{\mathrm{ref}},
\end{aligned}
\tag{3.60}
$$

Having calculated $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu)$ we obtain $j'(\tau)$ directly by using (3.54) and (3.56).

Let $V \in S$. Then:

$$
\begin{aligned}
&\langle j'(\tau), V\rangle_{S^*,S} \\
&= \langle(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_\tau((\boldsymbol{v},p),\tau)V\rangle_{Z_{\text{ref}}^*,Z_{\text{ref}}} + \langle J_\tau((\boldsymbol{v},p),\tau), V\rangle_{S^*,S} \\
&= \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda} \text{ tr } (\tau'^{-1}V') \det\tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} (\text{tr } (\tau'^{-1}V')I - V'\tau'^{-1} - \tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{\lambda}_i \det\tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(\text{ tr } (\tau'^{-1}V')I - \tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda} \det\tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} p \left(\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{\lambda}) - \text{ tr } (\tau'^{-T}\nabla\boldsymbol{\lambda}) \text{ tr } (\tau'^{-1}V')\right) \det\tau' \; dx \; dt \\
&- \int_I \int_{\Omega_{\text{ref}}} \left(\tilde{\boldsymbol{f}}(\tau(x),t)^T \text{ tr } (\tau'^{-1}V') + V^T\nabla\tilde{\boldsymbol{f}}(\tau(x),t)\right) \boldsymbol{\lambda} \det\tau' \; dx \; dt \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}(x,0)^T\boldsymbol{\lambda}_0 \text{ tr } (\tau'^{-1}V') \det\tau' \; dx \\
&- \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{v}}_0(\tau(x))^T\boldsymbol{\lambda}_0 \text{ tr } (\tau'^{-1}V') \det\tau' \; dx - \int_{\Omega_{\text{ref}}} V^T\nabla\tilde{\boldsymbol{v}}_0(\tau(x))\boldsymbol{\lambda}_0 \det\tau' \; dx \\
&- \int_I \int_{\Omega_{\text{ref}}} \mu \left(\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v}) - \text{ tr } (\tau'^{-T}\nabla\boldsymbol{v}) \text{ tr } (\tau'^{-1}V')\right) \det\tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t)) \text{ tr } (\tau'^{-1}V') \det\tau' \; dx \; dt \\
&- \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial(\nabla\tilde{\boldsymbol{v}})} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t)) \, \tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v} \det\tau' \; dx \; dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{x}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))V \; \det\tau' \; dx \; dt \\
&+ \int_{\Omega_{\text{ref}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \text{ tr } (\tau'^{-1}V') \det\tau' \; dx \\
&+ \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{x}} f_2(\tau(x), \boldsymbol{v}(x,T))V \det\tau' \; dx.
\end{aligned} \tag{3.61}
$$

3.3.3 Evaluation of the Shape Derivative on the Physical Domain

As already described in Section 3.1.10 we can compute the shape derivative for a given iterate $\tau \in T_{\text{ad}}$ by solving equivalent systems on the actual physical domain $\Omega = \tau(\Omega_{\text{ref}})$. In fact, we can transform the integrals back to Ω. By construction, in step 1 of Algorithm 3.5, we can equivalently calculate the solution $(\tilde{\boldsymbol{v}}, \tilde{p})$ of the Navier-Stokes equations on the domain $\tau(\Omega_{\text{ref}})$. This is very useful as we can use existent high-performance solvers for solving the Navier-Stokes equations.
Transforming the adjoint equation of step 2 yields the equivalent task:

Find $(\tilde{\boldsymbol{\lambda}}, \tilde{\boldsymbol{\lambda}}_0, \tilde{\mu})$ such that $\forall(\tilde{\boldsymbol{w}}, \tilde{q}) \in Y(\tau(\Omega_{\text{ref}}))$

$$
\begin{aligned}
&- \int_I \int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{\lambda}}_t \; dx \; dt + \int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{w}}(\cdot, T)^T \tilde{\boldsymbol{\lambda}}(\cdot, T) \; dx \\
&+ \int_I \int_{\tau(\Omega_{\text{ref}})} \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{w}}_i^T \nabla \tilde{\boldsymbol{\lambda}}_i \; dx \; dt + \int_I \int_{\tau(\Omega_{\text{ref}})} \left(\tilde{\boldsymbol{w}}^T \nabla \tilde{\boldsymbol{v}} + \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{w}} \right) \tilde{\boldsymbol{\lambda}} \; dx \; dt \\
&- \int_I \int_{\tau(\Omega_{\text{ref}})} \tilde{q} \; \text{tr} \; (\nabla \tilde{\boldsymbol{\lambda}}) \; dx \; dt + \int_I \int_{\tau(\Omega_{\text{ref}})} \tilde{\mu} \; \text{tr} \; (\nabla \tilde{\boldsymbol{w}}) \; dx \; dt \\
&+ \int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{w}}(\cdot, 0)^T (\tilde{\boldsymbol{\lambda}}_0 - \tilde{\boldsymbol{\lambda}}(\cdot, 0)) \; dx = -\langle \bar{J}_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}}, \tau(\Omega_{\text{ref}})), \tilde{\boldsymbol{w}} \rangle_{\hat{Y}(\tau(\Omega_{\text{ref}}))^*, \hat{Y}(\tau(\Omega_{\text{ref}}))}.
\end{aligned}
$$

This is the variational form of the standard adjoint Navier-Stokes equations. In strong form we have

$$
\begin{aligned}
-\tilde{\boldsymbol{\lambda}}_t - \nu \Delta \tilde{\boldsymbol{\lambda}} + (\nabla \tilde{\boldsymbol{v}}) \tilde{\boldsymbol{\lambda}} - (\nabla \tilde{\boldsymbol{\lambda}})^T \tilde{\boldsymbol{v}} - \nabla \tilde{\mu} &= -\bar{J}^D_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}}, \tau(\Omega_{\text{ref}})) && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\
- \text{ div } \tilde{\boldsymbol{\lambda}} &= 0 && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\
\tilde{\boldsymbol{\lambda}} &= 0 && \text{on } \partial(\tau(\Omega_{\text{ref}})) \times I, \\
\tilde{\boldsymbol{\lambda}}(\cdot, 0) &= \tilde{\boldsymbol{\lambda}}_0 && \text{on } \tau(\Omega_{\text{ref}}), \\
\tilde{\boldsymbol{\lambda}}(\cdot, T) &= -\bar{J}^T_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}}, \tau(\Omega_{\text{ref}})) && \text{on } \tau(\Omega_{\text{ref}}).
\end{aligned}
$$

Again we can use existent solvers to solve the adjoint Navier-Stokes equations. Furthermore we can use existence and uniqueness theory for the adjoint Navier-Stokes equations system and thus also derive existence and uniqueness results for (3.60), c.f. [30], [63] and [8].

Note that if $\bar{J}^D$ also depended on the pressure p, the second equation would read

$$
- \text{ div } \tilde{\boldsymbol{\lambda}} = -\bar{J}^D_{\tilde{p}}(\tilde{\boldsymbol{v}}, \tilde{p}, \tau(\Omega_{\text{ref}})) \qquad \text{on } \tau(\Omega_{\text{ref}}) \times I.
$$

Finally, we can evaluate the reduced gradient on the domain $\tau(\Omega_{\text{ref}})$. In fact, for fixed $\tau \in T_{\text{ad}}$ we introduce the objective function $\tilde{j}(\tilde{\tau}) := j(\tilde{\tau} \circ \tau) = j(\hat{\tau})$ where $\tilde{\tau} \circ \tau = \hat{\tau}$ is a transformation defined on T_{ref} while $\tilde{\tau}$ is the corresponding transformation defined on $\tau(\Omega_{\text{ref}})$. Note that this is well defined if either τ or $\tilde{\tau}$ is near id such that $\hat{\tau} \in T_{\text{ad}}$. In particular, $\tilde{j}$ is the corresponding reduced objective function associated with $\bar{J}(\tilde{\boldsymbol{v}}, \tau(\Omega))$, defined on a function space over $\tau(\Omega_{\text{ref}})$. Hence we have $\tilde{j}(\text{id}) = j(\tau)$ and for $V \in S$

$$
\langle j'(\tau), V \rangle_{S^*,S} = \langle \tilde{j}'(\text{id}), \tilde{V} \rangle_{S^*,S},
$$

where $\tilde{V} := V \circ \tau^{-1}$. So, for evaluating $j'(\tau)$ we can use formula (3.56), using $\tilde{V}$ instead of V, integrating over $\tau(\Omega_{\text{ref}})$ instead of Ω_{ref} and evaluating at $\tau = \text{id}$.

For details, see also [9]. Using this formalism we have

$$
\begin{aligned}
&\langle j'(\tau), V\rangle_{S^*,S} \\
&\quad = \langle \tilde{j}'(\mathrm{id}), \tilde{V}\rangle_{S^*,S} \\
&\quad = \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \ \mathrm{tr}\ (\tilde{V}')\ d\tilde{x}\ dt \\
&\qquad + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{v}}_i^T (\ \mathrm{tr}\ (\tilde{V}')I - \tilde{V}' - \tilde{V}'^T) \nabla \tilde{\boldsymbol{\lambda}}_i \ d\tilde{x}\ dt \\
&\qquad + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{v}}^T (\ \mathrm{tr}\ (\tilde{V}')I - \tilde{V}'^T) \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \ d\tilde{x}\ dt \\
&\qquad + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{p} \Big(\ \mathrm{tr}\ (\tilde{V}'^T \nabla \tilde{\boldsymbol{\lambda}}) -\ \mathrm{tr}\ (\nabla \tilde{\boldsymbol{\lambda}})\ \mathrm{tr}\ (\tilde{V}')\Big)\ d\tilde{x}\ dt \\
&\qquad - \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \Big(\tilde{\boldsymbol{f}}^T\ \mathrm{tr}\ (\tilde{V}') + \tilde{V}^T \nabla \tilde{\boldsymbol{f}}\Big) \tilde{\boldsymbol{\lambda}} \ d\tilde{x}\ dt \\
&\qquad - \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0 \tilde{\boldsymbol{\lambda}}_0 \ d\tilde{x} \\
&\qquad - \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\mu} \Big(\ \mathrm{tr}\ (\tilde{V}'^T \nabla \tilde{\boldsymbol{v}}) -\ \mathrm{tr}\ (\nabla \tilde{\boldsymbol{v}})\ \mathrm{tr}\ (\tilde{V}')\Big)\ d\tilde{x}\ dt \\
&\qquad + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\ \mathrm{tr}\ (\tilde{V}')\ d\tilde{x}\ dt \\
&\qquad - \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial(\nabla \tilde{\boldsymbol{v}})} \tilde{f}_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \ d\tilde{x}\ dt \\
&\qquad + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial \tilde{x}} \tilde{f}_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \tilde{V}\ \ d\tilde{x}\ dt \\
&\qquad + \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{f}_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T))\ \mathrm{tr}\ (\tilde{V}')\ d\tilde{x} \\
&\qquad + \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial \tilde{x}} \tilde{f}_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}\ d\tilde{x},
\end{aligned}
\tag{3.62}
$$

where $\tilde{V} = V \circ \tau^{-1}$.

Note that $\operatorname{tr}(\tilde{V}') = \operatorname{div} \tilde{V}$ so that we can group some terms and arrive at

$$
\begin{aligned}
&\langle j'(\tau), V\rangle_{S^*,S} \\
&= \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \; d\tilde{x}\; dt + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \; d\tilde{x}\; dt \\
&- \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{v}}_i^T (\tilde{V}' + \tilde{V}'^T) \nabla \tilde{\boldsymbol{\lambda}}_i \; d\tilde{x}\; dt \\
&- \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{v}}^T \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x}\; dt + \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \; d\tilde{x}\; dt \\
&+ \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{p} \Big(\operatorname{tr}(\tilde{V}'^T \nabla \tilde{\boldsymbol{\lambda}}) - \operatorname{div} \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \Big) \; d\tilde{x}\; dt \\
&- \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \; d\tilde{x}\; dt - \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x}\; dt \\
&- \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0 \tilde{\boldsymbol{\lambda}}_0 \; d\tilde{x} \\
&- \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{\mu} \Big(\operatorname{tr}(\tilde{V}'^T \nabla \tilde{\boldsymbol{v}}) - \operatorname{div} \tilde{\boldsymbol{v}} \operatorname{div} \tilde{V} \Big) \; d\tilde{x}\; dt \\
&+ \int_I \int_{\tau(\Omega_{\mathrm{ref}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \operatorname{div} \tilde{V} \; d\tilde{x}\; dt \\
&- \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} \tilde{f}_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \; d\tilde{x}\; dt \\
&+ \int_I \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial \tilde{x}} \tilde{f}_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \tilde{V} \; d\tilde{x}\; dt \\
&+ \int_{\tau(\Omega_{\mathrm{ref}})} \tilde{f}_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \operatorname{div} \tilde{V} \; d\tilde{x} + \int_{\tau(\Omega_{\mathrm{ref}})} \frac{\partial}{\partial \tilde{x}} \tilde{f}_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V} \; d\tilde{x}.
\end{aligned}
\tag{3.63}
$$

Note that in 2D this derivative can be further simplified using the comments after (3.54).
In the literature shape derivatives are often formulated as boundary integrals. If the states and adjoint states are smooth enough, we can achieve such a formulation using integration by parts for the integrals in formula (3.63). All domain integrals and some boundary integrals cancel out because of the boundary conditions and after some computations we arrive at a representation that contains only boundary integrals. In Appendix A the derivation is shown in

detail. Finally we arrive at:

$$
\begin{aligned}
&\langle j'(\tau), V\rangle_{S^*,S} = \\
&\int_I \int_{\Gamma_B} (\nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} - \tilde{p} \text{ div } \tilde{\boldsymbol{\lambda}} + \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}}) \tilde{V}^T \tilde{n} \; dS \; dt \\
&+ \int_I \int_{\Gamma_B} (\partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}})^T (\nu \partial_{\tilde{n}} \tilde{\boldsymbol{v}} - \tilde{p} \tilde{n}) \tilde{V}^T \tilde{n} \; dS \; dt \\
&- \int_I \int_{\Gamma_B} ((\partial_{\tilde{n}} \tilde{\boldsymbol{v}})^T (\nu \partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{v}}^T \tilde{n} + \tilde{\mu} \tilde{n}) \tilde{V}^T \tilde{n} \; dS \; dt \\
&+ \int_I \int_{\Gamma_B} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \tilde{V}^T \tilde{n} \; dS \; dt + \int_{\Gamma_B} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(x, T)) \tilde{V}^T \tilde{n} \; dS \; dt
\end{aligned}
\tag{3.64}
$$

where $\tilde{V} = V \circ \tau^{-1}$. Note that $\tilde{V}^T \tilde{n}$ is the normal component of the displacement $\tilde{V}$. Hence, under regularity assumptions on state and adjoint state the shape derivative depends only on the normal part of the displacement. This fits into the Hadamard representation of shape derivatives which states that the shape derivative is a boundary integral and depends only on the normal part of $\tilde{V}$, see Section 3.1.2.

However, for our numerical implementation we will use (3.63) for the calculation of the shape derivatives because a formulation as a boundary integral requires more regularity for the states and adjoint states. In fact, in our numericals tests we use Finite-Element-Galerkin discretizations like Taylor-Hood elements that are usually not continuously differentiable across element boundaries. Therefore the integration by parts that we used to derive the boundary representation is not well-founded is this context.

3.3.4 Second Order Shape Derivatives

For the calculation of second shape derivatives, see Algorithm 3.3, we need the evaluation of the second derivatives of the Lagrange function $\mathcal{L}$, i.e. the second derivatives of E and J. However, the calculation is tedious so that we moved it to the Appendix B. We give here only the results for the second derivatives of E at $\tau = \text{id}$. As already described for the first order shape derivatives, also for the second derivatives an equivalent set of equations can be solved on the actual physical domain $\tau(\Omega_{\text{ref}})$. For this only the second derivatives of E and J at $\tau = \text{id}$ are required.

Now we state the second derivatives of E for $d \in \{2, 3\}$. Note that for $d = 2$ some terms cancel out and we obtain shorter formulas. We refer to Appendix B where all formulas are given in detail. Let $(\boldsymbol{v}, p) \in Y_{\text{ref}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\text{ref}}}^*$,

$V, W \in S$ and $(\boldsymbol{w}, q), (\boldsymbol{u}, s) \in Y_{\text{ref}}$. Then

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau\tau}((\boldsymbol{v}, p), \text{id})(V)(W)\rangle_{Z_{\text{ref}}^*, Z_{\text{ref}}} \\
&= \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda}(\text{ div } V \text{ div } W - \text{ tr } (W'V'))\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{v}_i^T \kappa_2 \nabla \boldsymbol{\lambda}_i \, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T (- \text{ tr } (W'V')\; I + W'^T V'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda}\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T (- \text{ div } V W'^T + V'^T W'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda}\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T (\text{ div } V \text{ div } W\; I - \text{ div } W V'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda}\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} p(\text{ tr } (V'^T \nabla \boldsymbol{\lambda}) \text{ div } W + \text{ tr } (W'^T \nabla \boldsymbol{\lambda}) \text{ div } V)\, dx\, dt \\
&- \int_I \int_{\Omega_{\text{ref}}} p(\text{ tr } (W'^T V'^T \nabla \boldsymbol{\lambda}) + \text{ tr } (V'^T W'^T \nabla \boldsymbol{\lambda}))\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} p \text{ div } \boldsymbol{\lambda}(\text{ tr } (W'V') - \text{ div } (V) \text{ div } (W))\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} W^T \nabla \tilde{\boldsymbol{f}}(x,t) \boldsymbol{\lambda} \text{ div } V\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(x,t)^T \boldsymbol{\lambda}(\text{ div } V \text{ div } W - \text{ tr } (W'V'))\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} V^T (\sum_{i=1}^d \nabla^2 \tilde{\boldsymbol{f}}_i(x,t) W \lambda_i + \nabla \tilde{\boldsymbol{f}}(x,t)) \boldsymbol{\lambda} \text{ div } W\, dx\, dt \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}(\cdot, 0)^T \boldsymbol{\lambda}_0(\text{ div } V \text{ div } W - \text{ tr } (W'V'))\, dx \\
&+ \int_{\Omega_{\text{ref}}} W^T \nabla \tilde{\boldsymbol{v}}_0 \boldsymbol{\lambda}_0 \text{ div } V\, dx \\
&+ \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{v}}_0^T \boldsymbol{\lambda}_0(\text{ div } V \text{ div } W - \text{ tr } (W'V'))\, dx \\
&+ \int_{\Omega_{\text{ref}}} V^T (\sum_{i=1}^d \nabla^2 (\boldsymbol{v}_0)_i W \lambda_0 + \nabla \tilde{\boldsymbol{v}}_0 \boldsymbol{\lambda}_0 \text{ div } W\, dx \\
&- \int_I \int_{\Omega_{\text{ref}}} \mu(\text{ tr } (V'^T \nabla \boldsymbol{v}) \text{ div } W + \text{ tr } (W'^T \nabla \boldsymbol{v}) \text{ div } V)\, dx\, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \mu(\text{ tr } (W'^T V'^T \nabla \boldsymbol{v}) + \text{ tr } (V'^T W'^T \nabla \boldsymbol{v}))\, dx\, dt \\
&- \int_I \int_{\Omega_{\text{ref}}} \mu \text{ div } \boldsymbol{v}(\text{ tr } (W'V') - \text{ div } (V) \text{ div } (W))\, dx\, dt.
\end{aligned}
$$

with

$$\begin{aligned}\kappa_2 := & \text{ div } (V)(-W' - W'^T) + \text{ div } (W)(-V' - V'^T) \\ & + (\text{ div } (V) \text{ div } (W) - \text{ tr } (W'V'))I \\ & + V'(W' + W'^T) + W'(V' + V'^T) + V'^T W'^T + W'^T V'^T.\end{aligned}$$

Furthermore we have

$$\begin{aligned}& \langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau,(\boldsymbol{v},p)}((\boldsymbol{v}, p), \mathrm{id})(V)(\boldsymbol{w}, q)) \rangle_{Z_{\mathrm{ref}}^*, Z_{\mathrm{ref}}} \\ & = \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \text{ div } V \, dx \, dt + \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}(\cdot, 0)^T \boldsymbol{\lambda}_0 \text{ div } V \, dx \\ & + \sum_{i=1}^d \int_I \int_{\Omega_{\mathrm{ref}}} \nu \nabla \boldsymbol{w}_i^T (\text{ div } (V)I - V' - V'^T) \nabla \boldsymbol{\lambda}_i \, dx \, dt \\ & + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}^T (\text{ div } V)I - V'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda} \, dx \, dt \\ & + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T (\text{ div } V)I - V'^T) \nabla \boldsymbol{w} \boldsymbol{\lambda} \, dx \, dt \\ & + \int_I \int_{\Omega_{\mathrm{ref}}} q \left(\text{ tr } (V'^T \nabla \boldsymbol{\lambda}) - \text{ div } \boldsymbol{\lambda} \text{ div } V) \right) \, dx \, dt \\ & - \int_I \int_{\Omega_{\mathrm{ref}}} \mu (\text{ tr } (V'^T \nabla \boldsymbol{w}) - \text{ div } \boldsymbol{w} \text{ div } V) \, dx \, dt.\end{aligned}$$

A short calculation shows

$$\begin{aligned}& \langle (\boldsymbol{\lambda}, \mu), E_{(\boldsymbol{v},p),\tau}((\boldsymbol{v}, p), \mathrm{id})(\boldsymbol{w}, q)(V)) \rangle_{Z_{\mathrm{ref}}^*, Z_{\mathrm{ref}}} \\ & = \langle (\boldsymbol{\lambda}, \mu), E_{\tau,(\boldsymbol{v},p)}((\boldsymbol{v}, p), \mathrm{id})(V)(\boldsymbol{w}, q)) \rangle_{Z_{\mathrm{ref}}^*, Z_{\mathrm{ref}}}.\end{aligned}$$

Finally,

$$\begin{aligned}& \langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{(\boldsymbol{v},p),(\boldsymbol{v},p)}((\boldsymbol{v}, p), \mathrm{id})(\boldsymbol{w}, q)(\boldsymbol{u}, s) \rangle_{Z_{\mathrm{ref}}^*, Z_{\mathrm{ref}}} \\ & = \int_I \int_{\Omega_{\mathrm{ref}}} \left(\boldsymbol{w}^T \nabla \boldsymbol{u} + \boldsymbol{u}^T \nabla \boldsymbol{w} \right) \boldsymbol{\lambda} \, dx \, dt.\end{aligned} \tag{3.65}$$

For the derivatives of J we again refer to Appendix B, because the derivatives are derived for the general objective functional (3.50) and hence are also abstract.

With the second derivatives of E and J we can determine the derivatives $\mathcal{L}_{(\tilde{\boldsymbol{v}},\tilde{p}),(\tilde{\boldsymbol{v}},\tilde{p})}, \mathcal{L}_{\tau,(\tilde{\boldsymbol{v}},\tilde{p})}, \mathcal{L}_{(\tilde{\boldsymbol{v}},\tilde{p}),\tau}$ and $\mathcal{L}_{\tau,\tau}$ of the Lagrange function. Hence, we can calculate for $s \in S$ the second derivative $j''(\mathrm{id})s$ with the following algorithm based on Algorithm 3.3.

Algorithm 3.6. ***(Calculation of second order shape derivatives for the Navier-Stokes equations)*** *Let $\tau \in T_{ad}$. Let the state $(\tilde{\boldsymbol{v}}, \tilde{p}) \in Y_{ref}$ and the adjoint state $(\tilde{\boldsymbol{\lambda}}, \tilde{\boldsymbol{\lambda}}_0, \tilde{\mu}) \in Z_{ref}^*$ be computed. Let furthermore $s \in S$.*

1. *Find the sensitivity $(\delta_s \tilde{\boldsymbol{v}}, \delta_s \tilde{p}) \in Y_{ref}$ by solving the equation*

$$E_{(\tilde{\boldsymbol{v}},\tilde{p})}((\tilde{\boldsymbol{v}}, \tilde{p}), \tau)(\delta_s \tilde{\boldsymbol{v}}, \delta_s \tilde{p}) = -E_\tau((\tilde{\boldsymbol{v}}, \tilde{p}), \tau)s.$$

2. *Compute* $h_1 \in {Y_{ref}}^*$ *and* $h_2 \in S^*$ *via*

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{(\tilde{\boldsymbol{v}},\tilde{p}),(\tilde{\boldsymbol{v}},\tilde{p})}(z)(\delta_s\tilde{\boldsymbol{v}},\delta_s\tilde{p}) - \mathcal{L}_{(\tilde{\boldsymbol{v}},\tilde{p}),\tau}(z)s \\ \mathcal{L}_{\tau,(\tilde{\boldsymbol{v}},\tilde{p})}(z)(\delta_s\tilde{\boldsymbol{v}},\delta_s\tilde{p}) + \mathcal{L}_{\tau\tau}(z)s \end{pmatrix}$$

where $z = ((\tilde{\boldsymbol{v}},\tilde{p}),\tau,\tilde{\boldsymbol{\lambda}},\tilde{\boldsymbol{\lambda}}_0,\tilde{\mu})$.

3. *Compute* $h_3 \in S^*$ *by solving the equation*

$$h_3 = (\tilde{\boldsymbol{v}},\tilde{p})^* h_1 = -E_\tau((\tilde{\boldsymbol{v}},\tilde{p}),\tau)^* E_{(\tilde{\boldsymbol{v}},\tilde{p})}((\tilde{\boldsymbol{v}},\tilde{p}),\tau)^{-*} h_1.$$

4. *Set* $j''(\tau)s = h_2 + h_3$.

Again we can do this computations in the physical domain $\tau(\Omega_{\text{ref}})$. Then we need the evaluation of the second derivatives of E and J only at $\tau = \text{id}$.

3.3.5 First Order Shape Derivatives for the Inhomogeneous Navier-Stokes Equations

As already described in Section 3.2.7, in many applications we also have inhomogeneous Dirichlet boundary conditions and/or a free outflow region. In this section we sketch how the shape derivative calculation changes, if we have a Dirichlet part and/or a Neumann part on the exterior boundary Γ_{ext}. Consider the case

$$\begin{aligned} \tilde{\boldsymbol{v}}_t - \nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\ \operatorname{div}\tilde{\boldsymbol{v}} &= 0 && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\ \tilde{\boldsymbol{v}} &= \tilde{\boldsymbol{v}}_{D_{\text{ext}}} && \text{on } \Gamma_{D_{\text{ext}}} \times I, \\ \tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_B \times I, \\ \tilde{p}\,\tilde{\boldsymbol{n}} - \nu\frac{\partial}{\partial\tilde{n}}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_N \times I, \\ \tilde{\boldsymbol{v}}(\cdot,0) &= \tilde{\boldsymbol{v}}_0 && \text{on } \tau(\Omega_{\text{ref}}). \end{aligned}$$

as already done in Section 3.2.7. Here let $\Gamma_{D_{\text{ext}}} \neq \emptyset$, but Γ_N may be empty. The concept of deriving shape derivatives can be applied also for this case. We will demonstrate this for the calculation on the actual physical domain.
After calculating the solution of the inhomogeneous Navier-Stokes system above on the actual physical domain $\Omega = \tau(\Omega_{\text{ref}})$, we have to solve the corresponding adjoint system. Because of the different boundary conditions, the adjoint inhomogeneous Navier-Stokes equations read

$$\begin{aligned} -\tilde{\boldsymbol{\lambda}}_t - \nu\Delta\tilde{\boldsymbol{\lambda}} + (\nabla\tilde{\boldsymbol{v}})\tilde{\boldsymbol{\lambda}} - (\nabla\tilde{\boldsymbol{\lambda}})^T\tilde{\boldsymbol{v}} - \nabla\tilde{\mu} &= -\bar{J}^D_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}},\tau(\Omega_{\text{ref}})) && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\ -\operatorname{div}\tilde{\boldsymbol{\lambda}} &= 0 && \text{on } \tau(\Omega_{\text{ref}}) \times I, \\ \tilde{\boldsymbol{\lambda}} &= 0 && \text{on } (\Gamma_B \cup \Gamma_{D_{\text{ext}}}) \times I, \\ \nu\partial_{\tilde{n}}\tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{v}}^T\tilde{n}\tilde{\boldsymbol{\lambda}} - \tilde{\mu}\tilde{n} &= 0 && \text{on } \Gamma_N \times I, \\ \tilde{\boldsymbol{\lambda}}(\cdot,0) &= \tilde{\boldsymbol{\lambda}}_0 && \text{on } \tau(\Omega_{\text{ref}}), \\ \tilde{\boldsymbol{\lambda}}(\cdot,T) &= -\bar{J}^T_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}},\tau(\Omega_{\text{ref}})) && \text{on } \tau(\Omega_{\text{ref}}). \end{aligned}$$

Given the state $(\tilde{\boldsymbol{v}}, \tilde{p})$ and the adjoint state $(\tilde{\boldsymbol{\lambda}}, \tilde{\boldsymbol{\lambda}}_0, \tilde{\mu})$ we can use formula (3.63) to evaluate the shape derivative. In fact, by (N2) we assumed that for every transformation $\tau \in T_{\text{ad}}$ we have $\tau \equiv \text{id}$ in a neighbourhood of the boundary $\Gamma_{D_{\text{ext}}} \cup \Gamma_N$. Thus, we have no contribution of these boundaries to the shape derivative.

3.3.6 First Order Shape Derivatives for the Stationary Navier-Stokes Equations

Until now we just considered the instationary Navier-Stokes equations. For the stationary Navier-Stokes equations the shape derivatives can be calculated in a very similar way. However, the functions do not depend on t and the term with the time derivative for the velocity is missing in the state equation. We consider the Navier-Stokes equations with inhomogeneous Dirichlet conditions on the exterior boundary and a free outflow boundary. Then the state equation on the physical domain $\Omega = \tau(\Omega_{\text{ref}})$ is given by:

$$\begin{aligned}
-\nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} && \text{on } \Omega,\\
\operatorname{div} \tilde{\boldsymbol{v}} &= 0 && \text{on } \Omega,\\
\tilde{\boldsymbol{v}} &= \tilde{\boldsymbol{v}}_{D_{\text{ext}}} && \text{on } \Gamma_{D_{\text{ext}}},\\
\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_B,\\
\tilde{p}\,\tilde{\boldsymbol{n}} - \nu\frac{\partial}{\partial\tilde{n}}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_N.
\end{aligned}$$

Here $\tilde{\boldsymbol{v}} : \Omega \to \mathbb{R}^d$ is the velocity and $\tilde{p} : \Omega \to \mathbb{R}$ is the pressure variable. $\nu > 0$ is the kinematic viscosity and the data $\tilde{\boldsymbol{f}} : \Omega \to \mathbb{R}^d$, $\tilde{\boldsymbol{v}}_{D_{\text{ext}}} : \Gamma_{D_{\text{ext}}} \to \mathbb{R}^d$ are given. Furthermore we consider an objective function $\bar{J}^{\text{st}}$ of type

$$\bar{J}^{\text{st}}(\tilde{\boldsymbol{v}}, \Omega) := \int_\Omega f^{\text{st}}(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}), \nabla\tilde{\boldsymbol{v}}(\tilde{x}))\, d\tilde{x}. \tag{3.66}$$

A short computation (see e.g. [56, Section 3.1]) shows that the adjoint equations in strong form are given by

$$\begin{aligned}
-\nu\Delta\tilde{\boldsymbol{\lambda}} + (\nabla\tilde{\boldsymbol{v}})\tilde{\boldsymbol{\lambda}} - (\nabla\tilde{\boldsymbol{\lambda}})^T\tilde{\boldsymbol{v}} - \nabla\tilde{\mu} &= -\bar{J}^{\text{st}}_{\tilde{\boldsymbol{v}}}(\tilde{\boldsymbol{v}}, \Omega) && \text{on } \Omega,\\
-\operatorname{div} \tilde{\boldsymbol{\lambda}} &= 0 && \text{on } \Omega,\\
\tilde{\boldsymbol{\lambda}} &= 0 && \text{on } \Gamma_{D_{\text{ext}}} \cup \Gamma_B,\\
\nu\partial_{\tilde{n}}\tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{v}}^T\tilde{n}\tilde{\boldsymbol{\lambda}} + \tilde{\mu}\tilde{n} &= 0 && \text{on } \Gamma_N.
\end{aligned}$$

Using the same techniques as for the instationary case we obtain the first shape derivative on the physical domain $\Omega = \tau(\Omega_{\text{ref}})$ as a variant of (3.63).

$$
\begin{aligned}
\langle j'(\tau), V\rangle_{S^*,S} = \quad & \int_\Omega \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} \;\mathrm{div}\; \tilde{V} \; d\tilde{x} \\
& - \int_\Omega \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{v}}_i^T (\tilde{V}' + \tilde{V}'^T) \nabla \tilde{\boldsymbol{\lambda}}_i \; d\tilde{x} \\
& - \int_\Omega \tilde{\boldsymbol{v}}^T \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x} + \int_\Omega \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \;\mathrm{div}\; \tilde{V} \; d\tilde{x} \\
& + \int_\Omega \tilde{p} \Big(\;\mathrm{tr}\; (\tilde{V}'^T \nabla \tilde{\boldsymbol{\lambda}}) - \;\mathrm{div}\; \tilde{\boldsymbol{\lambda}} \;\mathrm{div}\; \tilde{V} \Big) \; d\tilde{x} \\
& - \int_\Omega \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \;\mathrm{div}\; \tilde{V} \; d\tilde{x} - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x} \qquad (3.67) \\
& - \int_\Omega \tilde{\mu} \Big(\;\mathrm{tr}\; (\tilde{V}'^T \nabla \tilde{\boldsymbol{v}}) - \;\mathrm{div}\; \tilde{\boldsymbol{v}} \;\mathrm{div}\; \tilde{V} \Big) \; d\tilde{x} \\
& + \int_\Omega f^{\text{st}}(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \;\mathrm{div}\; \tilde{V} \; d\tilde{x} \\
& - \int_\Omega \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f^{\text{st}}(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \; d\tilde{x} \\
& + \int_\Omega \frac{\partial}{\partial \tilde{x}} f^{\text{st}}(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \tilde{V} \; d\tilde{x}.
\end{aligned}
$$

4 A Differentiability Result for the Design-to-State Map

In this section we want to go into details for the concrete functional analytic setting for shape optimization with the instationary Navier-Stokes equations. As discussed in the introduction of Section 4.2 in detail, Bello et al. ([6],[7],[5]) analyzed the differentiability of the state with respect to domain variations for the stationary Navier-Stokes equations. In the instationary case additional complications occur that we will deal with in this chapter. We will show Fréchet differentiability of the design-to-state operator $\tau \mapsto \boldsymbol{v}(\tau)$, where $\boldsymbol{v}(\tau)$ is the velocity part of the solution of the instationary Navier-Stokes equations on $\tau(\Omega_{\text{ref}})$. In this context we will also show the unique solvability of the linearized Navier-Stokes equations.

4.1 Differentiability of the State Equation

We recall the weak space-time formulation of the transformed Navier-Stokes equations, as already stated in (3.47):
Find $(\boldsymbol{v}, p) \in Y_{\text{ref}}$ such that

$$\begin{aligned}
&\int_{\Omega_{\text{ref}}} (\boldsymbol{v}(\cdot,0) - \tilde{\boldsymbol{v}}_0(\tau))^T \boldsymbol{w}_0 \det \tau' \, dx + \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{w} \det \tau' \, dx \, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} \tau'^{-T} \nabla \boldsymbol{w}_i \det \tau' \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \; \boldsymbol{w} \det \tau' \, dx \, dt \\
&- \int_I \int_{\Omega_{\text{ref}}} p \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \, dx \, dt - \int_I \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{w} \det \tau' \, dx \, dt \\
&+ \int_I \int_{\Omega_{\text{ref}}} q \; \text{tr} \; (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \, dx \, dt = 0 \quad \forall \, (\boldsymbol{w}, \boldsymbol{w}_0, q) \in {Z_{\text{ref}}}^*
\end{aligned} \tag{4.1}$$

where

$$\begin{aligned}
Y_{\text{ref}} &:= W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) \times L^2(I; L_0^2(\Omega_{\text{ref}})) \\
Z_{\text{ref}} &:= L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}})) \times \mathbf{L}^2(\Omega_{\text{ref}}) \times L^2(I; L_0^2(\Omega_{\text{ref}})) \\
{Z_{\text{ref}}}^* &= L^2(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) \times \mathbf{L}^2(\Omega_{\text{ref}}) \times L^2(I; L_0^2(\Omega_{\text{ref}}))
\end{aligned}$$

In this section we will show Fréchet differentiability of the state equation E, i.e. the transformed instationary Navier-Stokes equations (4.1). The crucial term of E is the transformed nonlinear convection term. We recall the definition of $b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})$ in (3.38):

$$b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}}) := \sum_{i,j=1}^{d} \int_{\Omega} \tilde{\boldsymbol{u}}_i (D_i \tilde{\boldsymbol{v}}_j) \tilde{\boldsymbol{w}}_j \, d\tilde{x} = \int_{\Omega} \tilde{\boldsymbol{u}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{w}} \, d\tilde{x} \tag{4.2}$$

for $\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$. We have the following lemma:

Lemma 4.1. *For $d = 2$ we have for all $\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$*

$$|b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| \leq 2^{1/2} ||\tilde{\boldsymbol{u}}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{u}}||^{1/2}_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/2}_{\mathbf{H}_0^1(\Omega)}.$$

For $d = 3$ we obtain

$$|b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| \leq 2 ||\tilde{\boldsymbol{u}}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{u}}||^{3/4}_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{w}}||^{3/4}_{\mathbf{H}_0^1(\Omega)}.$$

Furthermore for $d = 2, 3$ we have for $\tilde{\boldsymbol{v}} \in \mathbf{H}_0^1(\Omega) \cap \mathbf{H}^2(\Omega), \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$

$$|b(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}}) \leq c_1 ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}^2(\Omega)} ||\tilde{\boldsymbol{w}}||_{\mathbf{L}^2(\Omega)}$$

with a constant c_1 that depends on d and the Poincaré constant of Ω.

Proof. Using Lemma III.3.3 for $d = 2$ and Lemma III.3.5 for $d = 3$ in [59] we obtain for all $\tilde{q} \in H_0^1(\Omega)$

$$||\tilde{q}||_{L^4(\Omega)} \leq 2^{1/4} ||\tilde{q}||^{1/2}_{L^2(\Omega)} ||\tilde{q}||^{1/2}_{H_0^1(\Omega)} \quad \text{for } d = 2, \tag{4.3}$$

$$||\tilde{q}||_{L^4(\Omega)} \leq 2^{1/2} ||\tilde{q}||^{1/4}_{L^2(\Omega)} ||\tilde{q}||^{3/4}_{H_0^1(\Omega)} \quad \text{for } d = 3. \tag{4.4}$$

For $\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$ and $d = 2, 3$ we have

$$\begin{aligned}
|b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| &\leq \sum_{i,j=1}^{d} \int_\Omega |\tilde{\boldsymbol{u}}_i (D_i \tilde{\boldsymbol{v}}_j) \tilde{\boldsymbol{w}}_j| d\tilde{x} \\
&\leq \sum_{i,j=1}^{d} ||\tilde{\boldsymbol{u}}_i||_{L^4(\Omega)} ||D_i \tilde{\boldsymbol{v}}_j||_{L^2(\Omega)} ||\tilde{\boldsymbol{w}}_j||_{L^4(\Omega)} \\
&\leq \left(\sum_{i,j=1}^{d} ||D_i \tilde{\boldsymbol{v}}_j||^2_{L^2(\Omega)} \right)^{1/2} \cdot \left(\sum_{i=1}^{d} ||\tilde{\boldsymbol{u}}_i||^2_{L^4(\Omega)} \right)^{1/2} \cdot \left(\sum_{j=1}^{d} ||\tilde{\boldsymbol{w}}_j||^2_{L^4(\Omega)} \right)^{1/2}.
\end{aligned}$$

Using (4.3) and (4.4) we obtain

$$\begin{aligned}
|b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| &\leq 2^{1/2} ||\tilde{\boldsymbol{u}}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{u}}||^{1/2}_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/2}_{\mathbf{H}_0^1(\Omega)} \quad \text{for } d = 2, \\
|b(\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| &\leq 2 ||\tilde{\boldsymbol{u}}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{u}}||^{3/4}_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{w}}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\tilde{\boldsymbol{w}}||^{3/4}_{\mathbf{H}_0^1(\Omega)} \quad \text{for } d = 3.
\end{aligned}$$

Finally for $d = 2, 3$ and $\tilde{\boldsymbol{v}} \in \mathbf{H}_0^1(\Omega) \cap \mathbf{H}^2(\Omega), \tilde{\boldsymbol{w}} \in \mathbf{H}_0^1(\Omega)$ we have

$$\begin{aligned}
|b(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}}, \tilde{\boldsymbol{w}})| &= \sum_{i,j=1}^{d} \int_\Omega |\tilde{\boldsymbol{v}}_i (D_i \tilde{\boldsymbol{v}}_j) \tilde{\boldsymbol{w}}_j| \, dx \\
&\leq \sum_{i,j=1}^{d} ||\tilde{\boldsymbol{v}}_i||_{L^4(\Omega)} ||D_i \tilde{\boldsymbol{v}}_j||_{L^4(\Omega)} ||\tilde{\boldsymbol{w}}_j||_{L^2(\Omega)} \\
&\leq \tilde{c}_1 ||\tilde{\boldsymbol{v}}||_{\mathbf{L}^4(\Omega)} ||\nabla \tilde{\boldsymbol{v}}||_{L^4(\Omega)^{d \times d}} ||\tilde{\boldsymbol{w}}||_{\mathbf{L}^2(\Omega)} \\
&\leq c_1 ||\tilde{\boldsymbol{v}}||_{\mathbf{H}_0^1(\Omega)} ||\tilde{\boldsymbol{v}}||_{\mathbf{H}^2(\Omega)} ||\tilde{\boldsymbol{w}}||_{\mathbf{L}^2(\Omega)}
\end{aligned}$$

where we used Poincaré's inequality. □

Now, we introduce the corresponding multilinear form $\tilde{b}$ for the transformed Navier-Stokes equations. For $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega)$ and $T \in L^\infty(\Omega)^{d\times d}$ we define:

$$\tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, T) := \int_\Omega \boldsymbol{u}^T T \nabla \boldsymbol{v} \boldsymbol{w} \; dx = \sum_{i,j,k=1}^{d} \int_\Omega u_i T_{ij} (v_k)_{x_j} w_k \; dx. \tag{4.5}$$

We can show the continuity of $\tilde{b}$:

Lemma 4.2. *Let $d = 2$ and $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega), T \in L^\infty(\Omega)^{d\times d}$. Then with a constant $C > 0$:*

$$\begin{aligned}
&|\tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, T)| \\
&\leq 2||\boldsymbol{u}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{1/2}_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{w}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{w}||^{1/2}_{\mathbf{H}_0^1(\Omega)} ||T||_{L^\infty(\Omega)^{2\times 2}} \\
&\leq C ||\nabla \boldsymbol{u}||_{L^2(\Omega)^{2\times 2}} ||\nabla \boldsymbol{v}||_{L^2(\Omega)^{2\times 2}} ||\nabla \boldsymbol{w}||_{L^2(\Omega)^{2\times 2}} ||T||_{L^\infty(\Omega)^{2\times 2}}.
\end{aligned}$$

For $d = 3$ we have with a constant $C > 0$:

$$\begin{aligned}
&|\tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, T)| \\
&\leq 2\sqrt{3}||\boldsymbol{u}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{3/4}_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)} ||\boldsymbol{w}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{w}||^{3/4}_{\mathbf{H}_0^1(\Omega)} ||T||_{L^\infty(\Omega)^{3\times 3}} \\
&\leq C ||\nabla \boldsymbol{u}||_{L^2(\Omega)^{3\times 3}} ||\nabla \boldsymbol{v}||_{L^2(\Omega)^{3\times 3}} ||\nabla \boldsymbol{w}||_{L^2(\Omega)^{3\times 3}} ||T||_{L^\infty(\Omega)^{3\times 3}}.
\end{aligned}$$

Proof. We first show that for $\boldsymbol{u}, \boldsymbol{w} \in \mathbf{L}^4(\Omega), \boldsymbol{v} \in \mathbf{H}_0^1(\Omega), T \in L^\infty(\Omega)^{d\times d}$ it holds:

$$\begin{aligned}
&|\tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, T)| \\
&\leq \sqrt{d} \left(\sum_{i=1}^{d} ||u_i||^2_{L^4(\Omega)} \right)^{1/2} \left(\sum_{k=1}^{d} ||w_k||^2_{L^4(\Omega)} \right)^{1/2} ||T||_{L^\infty(\Omega)^{d\times d}} ||\nabla \boldsymbol{v}||_{L^2(\Omega)^{d\times d}}.
\end{aligned}$$

In fact, we use Schwarz and Hölder inequalities and obtain:

$$|\tilde{b}(\boldsymbol{u},\boldsymbol{v},\boldsymbol{w},T)| = |\sum_{i,j,k=1}^{d}\int_{\Omega} u_i T_{ij}(v_k)_{x_j} w_k \ dx|$$

$$\leq \sum_{i,j,k=1}^{d} ||u_i||_{L^4(\Omega)}||T_{ij}||_{L^\infty(\Omega)}||(v_k)_{x_j}||_{L^2(\Omega)}||w_k||_{L^4(\Omega)}$$

$$\leq \left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2}\left(\sum_{i=1}^{d}\left(\sum_{j,k=1}^{d}||T_{ij}||_{L^\infty(\Omega)}||(v_k)_{x_j}||_{L^2(\Omega)}||w_k||_{L^4(\Omega)}\right)^2\right)^{1/2}$$

$$\leq \left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2} \cdot$$

$$\left(\sum_{i=1}^{d}\left(\left(\sum_{k=1}^{d}\left(\sum_{j=1}^{d}||T_{ij}||_{L^\infty(\Omega)}||(v_k)_{x_j}||_{L^2(\Omega)}\right)^2\right)^{1/2}\left(\sum_{k=1}^{d}||w_k||^2_{L^4(\Omega)}\right)^{1/2}\right)^2\right)^{1/2}$$

$$= \left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2} \cdot$$

$$\left(\sum_{i=1}^{d}\left(\left(\sum_{k=1}^{d}\left(\sum_{j=1}^{d}||T_{ij}||_{L^\infty(\Omega)}||(v_k)_{x_j}||_{L^2(\Omega)}\right)^2\right)\left(\sum_{k=1}^{d}||w_k||^2_{L^4(\Omega)}\right)\right)\right)^{1/2}$$

$$= \left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2}\left(\sum_{k=1}^{d}||w_k||^2_{L^4(\Omega)}\right)^{1/2} \cdot$$

$$\left(\sum_{i,k=1}^{d}\left(\sum_{j=1}^{d}||T_{ij}||_{L^\infty(\Omega)}||(v_k)_{x_j}||_{L^2(\Omega)}\right)^2\right)^{1/2}$$

$$\leq \left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2}\left(\sum_{k=1}^{d}||w_k||^2_{L^4(\Omega)}\right)^{1/2} \cdot$$

$$||T||_{L^\infty(\Omega)^{d\times d}}\left(\sum_{i,j,k=1}^{d}||(v_k)_{x_j}||^2_{L^2(\Omega)}\right)^{1/2}$$

$$=\sqrt{d}\left(\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)}\right)^{1/2}\left(\sum_{k=1}^{d}||w_k||^2_{L^4(\Omega)}\right)^{1/2}||T||_{L^\infty(\Omega)^{d\times d}}||\nabla\boldsymbol{v}||_{L^2(\Omega)^{d\times d}}.$$

Using (4.3) and

$$\begin{aligned}\sum_{i=1}^{d}||u_i||^2_{L^4(\Omega)} &\leq 2^{1/2}\sum_{i=1}^{d}||u_i||_{L^2(\Omega)}||\nabla u_i||_{\mathbf{L}^2(\Omega)}\\ &\leq 2^{1/2}||\boldsymbol{u}||_{\mathbf{L}^2(\Omega)}||\boldsymbol{u}||_{\mathbf{H}^1_0(\Omega)}\end{aligned}$$

for $d = 2$ and (4.4) and

$$\begin{aligned}\sum_{i=1}^{d} ||u_i||^2_{L^4(\Omega)} &\le 2\sum_{i=1}^{d} ||u_i||^{1/2}_{L^2(\Omega)} ||\nabla u_i||^{3/2}_{\mathbf{L}^2(\Omega)} \\ &\le 2^{1/2} ||\boldsymbol{u}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{3/2}_{\mathbf{H}^1_0(\Omega)}\end{aligned}$$

for $d = 3$ the assertions follow directly. □

We will now show the differentiability by analyzing (4.1) term by term. We show that each multilinear form is bounded, using the higher regularity given by (N3). However, we do not assume additional regularity for the test function $\boldsymbol{w} \in L^2(I; \mathbf{H}^1_0(\Omega_{\text{ref}})$.
We start with the term $\tilde{b}$.

Lemma 4.3. *For $d = 2$ the multilinear form*

$$\begin{aligned}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S) \in\ & (L^\infty(I; \mathbf{L}^2(\Omega)) \cap L^3(I; \mathbf{H}^1_0(\Omega))) \times L^3(I; \mathbf{H}^1_0(\Omega)) \\ & \times L^2(I; \mathbf{H}^1_0(\Omega)) \times L^\infty(\Omega)^{d\times d} \\ & \mapsto \int_I \tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S)\ dt \in \mathbb{R}\end{aligned}$$

is bounded.

Proof. Using Lemma 4.2 and the Hölder inequality, we have for $d = 2$:

$$\begin{aligned}&\int_I \tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S)\ dt \\ &\le C \int_I ||\boldsymbol{u}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{1/2}_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{w}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{w}||^{1/2}_{\mathbf{H}^1_0(\Omega)} ||S||_{L^\infty(\Omega)^{2\times 2}}\ dt \\ &\le C \int_I ||\boldsymbol{u}||^{1/2}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{1/2}_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{w}||_{\mathbf{H}^1_0(\Omega)} ||S||_{L^\infty(\Omega)^{2\times 2}}\ dt \\ &\le C ||\boldsymbol{u}||^{1/2}_{L^\infty(I;\mathbf{L}^2(\Omega))} ||\boldsymbol{u}||^{1/2}_{L^3(I;\mathbf{H}^1_0(\Omega))} ||\boldsymbol{v}||_{L^3(I;\mathbf{H}^1_0(\Omega))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}^1_0(\Omega))} ||S||_{L^\infty(\Omega)^{2\times 2}}\end{aligned}$$

with a constant $C > 0$. □

For the three-dimensional case, we have to assume additional regularity for $\boldsymbol{u}$ and $\boldsymbol{v}$:

Lemma 4.4. *For $d = 3$ the multilinear form*

$$\begin{aligned}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S) \in\ & (L^\infty(I; \mathbf{L}^2(\Omega)) \cap L^{7/2}(I; \mathbf{H}^1_0(\Omega))) \times L^{7/2}(I; \mathbf{H}^1_0(\Omega)) \\ & \times L^2(I; \mathbf{H}^1_0(\Omega)) \times L^\infty(\Omega)^{d\times d} \\ & \mapsto \int_I \tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S)\ dt \in \mathbb{R}\end{aligned}$$

is bounded.

Proof. Using Lemma 4.2 we have for $d = 3$ and a constant $C > 0$:

$$\begin{aligned}
&\int_I \tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S)\ dt \\
&\leq C \int_I ||\boldsymbol{u}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{3/4}_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{w}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{w}||^{3/4}_{\mathbf{H}^1_0(\Omega)} ||S||_{L^\infty(\Omega)^{3\times 3}}\ dt \\
&\leq C \int_I ||\boldsymbol{u}||^{1/4}_{\mathbf{L}^2(\Omega)} ||\boldsymbol{u}||^{3/4}_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{w}||_{\mathbf{H}^1_0(\Omega)} ||S||_{L^\infty(\Omega)^{3\times 3}}\ dt.
\end{aligned}$$

Now we use again the Hölder inequality. For $||\boldsymbol{w}||_{\mathbf{H}^1_0(\Omega)}$ we use the Hölder index $\frac{1}{2}$. Choosing the Hölder index $\frac{2}{7}$ for $||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)}$ and $\frac{3}{14}$ for $||\boldsymbol{u}||^{3/4}_{\mathbf{H}^1_0(\Omega)}$ we have

$$\frac{3}{14} + \frac{2}{7} + \frac{1}{2} = 1$$

and arrive at

$$\begin{aligned}
&\int_I \tilde{b}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, S)\ dt \leq \\
&C ||\boldsymbol{u}||^{1/2}_{L^\infty(I;\mathbf{L}^2(\Omega))} ||\boldsymbol{u}||^{1/2}_{L^{7/2}(I;\mathbf{H}^1_0(\Omega))} ||\boldsymbol{v}||_{L^{7/2}(I;\mathbf{H}^1_0(\Omega))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}^1_0(\Omega))} ||S||_{L^\infty(\Omega)^{3\times 3}}.
\end{aligned}$$

□

The boundedness of the other terms is obtained in a similar but easier way, which we state in the following lemmas.

Lemma 4.5. *For $d \in \{2, 3\}$ the multilinear form*

$$\begin{aligned}
&(\boldsymbol{v}, \boldsymbol{w}, S) \in L^2(I; \mathbf{H}^1_0(\Omega)) \times L^2(I; \mathbf{H}^1_0(\Omega)) \times L^\infty(\Omega)^{d\times d} \\
&\mapsto \int_I \int_\Omega \sum_{i=1}^d \nabla \boldsymbol{v}_i^T S \nabla \boldsymbol{w}_i \, dx\ dt \in \mathbb{R}
\end{aligned}$$

is bounded.

Proof.

$$\begin{aligned}
&\int_I \int_\Omega \sum_{i=1}^d \nabla \boldsymbol{v}_i^T S \nabla \boldsymbol{w}_i \, dx\ dt \\
&\leq C ||S||_{L^\infty(\Omega)^{d\times d}} \int_I ||\boldsymbol{v}||_{\mathbf{H}^1_0(\Omega)} ||\boldsymbol{w}||_{\mathbf{H}^1_0(\Omega)}\ dt \\
&\leq C ||S||_{L^\infty(\Omega)^{d\times d}} ||\boldsymbol{v}||_{L^2(I;\mathbf{H}^1_0(\Omega))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}^1_0(\Omega))}.
\end{aligned}$$

□

Lemma 4.6. *For $d \in \{2, 3\}$ the multilinear form*

$$\begin{aligned}
&(\boldsymbol{v}, p, S) \in L^2(I; \mathbf{H}^1_0(\Omega)) \times L^2(I; L^2(\Omega)) \times L^\infty(\Omega)^{d\times d} \\
&\mapsto \int_I \int_\Omega p\ tr\ (S \nabla \boldsymbol{v})\, dx\ dt \in \mathbb{R}
\end{aligned}$$

is bounded.

Proof.

$$\begin{aligned}
&\int_I \int_\Omega p \ \mathrm{tr}\ (S\nabla \boldsymbol{v})\, dx\ dt \\
&\leq C||S||_{L^\infty(\Omega)^{d\times d}} \int_I ||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)} ||p||_{L^2(\Omega)}\ dt \\
&\leq C||S||_{L^\infty(\Omega)^{d\times d}} ||\boldsymbol{v}||_{L^2(I;\mathbf{H}_0^1(\Omega))} ||p||_{L^2(I;L^2(\Omega))}.
\end{aligned}$$

□

Lemma 4.7. *For $d \in \{2,3\}$ the multilinear form*

$$\begin{aligned}
&(\boldsymbol{v}, \boldsymbol{w}, s) \in L^2(I;\mathbf{L}^2(\Omega)) \times L^2(I;\mathbf{L}^2(\Omega)) \times L^\infty(\Omega) \\
&\mapsto \int_I \int_\Omega \boldsymbol{v}^T \boldsymbol{w} s\, dx\ dt \in \mathbb{R}
\end{aligned}$$

is bounded.

Proof.

$$\begin{aligned}
&\int_I \int_\Omega \boldsymbol{v}^T \boldsymbol{w} s\, dx\ dt \\
&\leq ||s||_{L^\infty(\Omega)} \int_I ||\boldsymbol{v}||_{\mathbf{L}^2(\Omega)} ||\boldsymbol{w}||_{\mathbf{L}^2(\Omega)}\ dt \\
&\leq ||s||_{L^\infty(\Omega)} ||\boldsymbol{v}||_{L^2(I;\mathbf{L}^2(\Omega))} ||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega))}.
\end{aligned}$$

□

We finally arrive at a differentiability result for E:

Theorem 4.1. *For $d = 2$ the map*

$$\begin{aligned}
(\boldsymbol{v}, p, \tau, \boldsymbol{w}, \boldsymbol{w}_0, q) \in \quad & \{\boldsymbol{v} \in L^3(I;\mathbf{H}_0^1(\Omega_{ref})) \mid \boldsymbol{v}_t \in L^2(I;\mathbf{L}^2(\Omega_{ref}))\} \\
& \times L^2(I;L^2(\Omega_{ref})) \times \mathbf{W}^{1,\infty}(\Omega_{ref}) \\
& \times L^2(I;\mathbf{H}_0^1(\Omega_{ref})) \cap L^\infty(I;\mathbf{L}^2(\Omega_{ref})) \\
& \times \mathbf{L}^2(\Omega_{ref}) \times L^2(I;L^2(\Omega_{ref})) \to \mathbb{R}
\end{aligned}$$

defined by

$$(\boldsymbol{v}, p, \tau, \boldsymbol{w}, \boldsymbol{w}_0, q) \mapsto \langle (\boldsymbol{w}, \boldsymbol{w}_0, q), E((\boldsymbol{v}, p), \tau) \rangle_{{Z_{ref}}^*, Z_{ref}}$$

is Fréchet differentiable with E defined via (4.1).

Proof. We have

$$\{\boldsymbol{v} \in L^3(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}) \mid \boldsymbol{v}_t \in L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))\} \hookrightarrow L^\infty(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))$$

and furthermore by Lemma 3.4 we know the differentiability of the terms $\det \tau'$, τ'^{-1} and τ'^{-T} with respect to τ. Furthermore the multilinear forms of Lemmas 4.3 to 4.7 are bounded and thus Fréchet differentiable. Since E is a composition of these terms, we can use the lemmas above to establish the result. □

Using the same proof we obtain for $d = 3$:

Theorem 4.2. *For $d = 3$ the map*

$$\begin{aligned}(\boldsymbol{v}, p, \tau, \boldsymbol{w}, \boldsymbol{w}_0, q) \in \quad & \{\boldsymbol{v} \in L^{7/2}(I; \mathbf{H}_0^1(\Omega_{ref}) \mid \boldsymbol{v}_t \in L^2(I; \mathbf{L}^2(\Omega_{ref}))\} \\ & \times L^2(I; L^2(\Omega_{ref})) \times \mathbf{W}^{1,\infty}(\Omega_{ref}) \\ & \times L^2(I; \mathbf{H}_0^1(\Omega_{ref})) \cap L^\infty(I; \mathbf{L}^2(\Omega_{ref})) \\ & \times \mathbf{L}^2(\Omega_{ref}) \times L^2(I; L^2(\Omega_{ref})) \to \mathbb{R}\end{aligned}$$

defined by

$$(\boldsymbol{v}, p, \tau, \boldsymbol{w}, \boldsymbol{w}_0, q) \mapsto \langle (\boldsymbol{w}, \boldsymbol{w}_0, q), E((\boldsymbol{v}, p), \tau) \rangle_{Z_{ref}^*, Z_{ref}}$$

is Fréchet differentiable with E defined via (4.1)*.*

Note that (N3) guarantees the additional regularity of $\boldsymbol{v}$ and p needed for the differentiability result for $d = 2$ and $d = 3$.

4.2 Fréchet Differentiability of the State with respect to Domain Variations

In this section we will show the Fréchet differentiability of the design-to-state operator for the instationary Navier-Stokes equations. In the whole section we assume that (N1)-(N3) are fulfilled.
We will use the weak formulation of the transformed NSE, as already stated in (3.46): Find $(\boldsymbol{v}, p) \in W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) \times L^2(I; L_0^2(\Omega_{\text{ref}}))$ such that

$$\begin{aligned} &\int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{w} \det \tau' \, dx + \sum_{i=1}^d \int_{\Omega_{\text{ref}}} \nu \nabla v_i^T \tau'^{-1} \tau'^{-T} \nabla w_i \det \tau' \, dx \\ &+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{v} \; \boldsymbol{w} \det \tau' \; dx - \int_{\Omega_{\text{ref}}} p \text{ tr } (\tau'^{-T} \nabla \boldsymbol{w}) \det \tau' \, dx \\ &- \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{w} \det \tau' \, dx = 0 \quad \forall \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\text{ref}}) \text{ for a.a. } t \in I \\ &\int_{\Omega_{\text{ref}}} q \text{ tr } (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau' \, dx = 0 \quad \forall q \in L_0^2(\Omega_{\text{ref}}) \text{ for a.a. } t \in I \\ &\boldsymbol{v}(\cdot, 0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)). \end{aligned} \tag{4.6}$$

We will now prove the Fréchet differentiablility of the velocity $\boldsymbol{v}(\tau)$ in an appropriate setting, where $\boldsymbol{v}(\tau)$ solves (4.6).
Usually the analysis of the Navier-Stokes equations uses the space $V(\Omega)$ which includes the incompressibility condition. However, since the solenoidality of the functions is not preserved when we transform the equations to the reference domain, additional difficulties occur. There are different possibilities to surmount this. In [55] J. Simon uses a variant of the implicit funtion theorem to show differentiability with respect to transformations for stationary Stokes flow when Ω is a $W^{2,\infty}$ domain. J.A. Bello, E. Fernández-Cara and J. Simon [7], [6] showed differentiability of the drag in the case of stationary Navier-Stokes equations

when Ω is a $W^{2,\infty}$ domain and J.A. Bello, E. Fernández-Cara, J. Lemoine and J. Simon [5] extended this result even for Lipschitz domains under $W^{1,\infty}$ transformations. To treat the incompressibility condition Bello et al. introduced in [7], [6] a family of isomorphisms to rewrite the equation $\operatorname{div} \boldsymbol{v}(\tau) = 0$ appropriately. In [5] the authors state the incompressibility equations explicitly as we have already done by introducing the velocity-pressure formulation (4.6).
In the time-dependent case significant additional complications appear (see also [10]) as we exemplary discuss in the case $d = 2$: They are caused by the fact that in the standard $W(I; V(\Omega))$-setting (3.27) with standard data regularity (3.28) the time regularity of the pressure is very low. In fact, the $\nabla\tilde{p}$ term takes care of those parts of the residual that are not seen when tested with solenoidal functions. We can only show that $\tilde{\boldsymbol{v}}_t \in L^2(I; V(\Omega)^*)$ in the standard setting. Now $L^2(I; V(\Omega)^*)$ is a weaker space than $L^2(I; \mathbf{H}^{-1}(\Omega))$, since $V(\Omega) \subsetneq \mathbf{H}_0^1(\Omega)$ is a closed subspace strictly smaller than $\mathbf{H}_0^1(\Omega)$. Therefore, the fact that $\tilde{\boldsymbol{v}}_t \in L^2(I; V(\Omega)^*)$ cannot be used to derive time regularity results for the pressure. This causes difficulties since after transformation to the reference domain the velocity field is no longer solenoidal. Thus, the pressure cannot be eliminated and the skew symmetry of the trilinear convection form cannot be used since it only holds if the first argument is solenoidal. For achieving that the required regularity properties of solutions are maintained under transformation, we need the requirement $\tau \in T_{\text{ad}} \subset \mathbf{W}^{2,\infty}(\Omega')$. This especially concerns the regularity of the time derivative.
As already shown in [5] and [9] it is sufficient to consider the differentiability of $\boldsymbol{v}(\tau)$ at $\tau = \text{id}$, since $\tau(\Omega_{\text{ref}})$ can be taken as the current reference domain and the derivative with respect to variations of this domain can be transformed to derivatives with respect to domain variations of Ω_{ref}.

4.2.1 Boundedness of the State

In a first step we show that the norm of the states $\boldsymbol{v}$ and p is bounded for small variations of the domain, i.e. that there exists $\epsilon > 0$ and $C > 0$ such that for all $\tau \in T_{\text{ad}}$:

$$\begin{gathered}||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\text{ref}})} < \epsilon \quad \Longrightarrow \\ ||\boldsymbol{v} - \bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} \leq C,\ ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} \leq C, \\ ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^\infty(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \leq C,\ ||p - \bar{p}||_{L^2(I;L_0^2(\Omega_{\text{ref}}))} \leq C\end{gathered}$$

where $(\boldsymbol{v}, p) = (\boldsymbol{v}(\tau), p(\tau))$ is the solution for the Navier-Stokes equations on $\tau(\Omega_{\text{ref}})$ and $(\bar{\boldsymbol{v}}, \bar{p})$ is the solution on Ω_{ref}.
This will be done in several steps. First we show, for given $\tau \in T_{\text{ad}}$ and a function $\tilde{h}$ defined on $\tau(\Omega_{\text{ref}})$, that the map $\tilde{h} \mapsto h := \tilde{h} \circ \tau$ is linear and continuous for some appropriate choices of the image and range function spaces. Using this we will demonstrate that the norms of the velocity part of the instationary Navier-Stokes equations solution is bounded for small domain variations. Finally we conclude that also the norm of the pressure ist bounded.
We begin with the following lemma which shows that for $a \in W^{1,\infty}(\Omega_{\text{ref}})$ and $b \in H^1(\Omega_{\text{ref}})^*$ also $ab \in H^1(\Omega_{\text{ref}})^*$:

Lemma 4.8. *Let $d \in \{2,3\}$. Let $a \in W^{1,\infty}(\Omega_{ref})$ and $b \in H^1(\Omega_{ref})^*$. Then there exists a constant $c(\Omega_{ref}) > 0$ with*

$$||ab||_{H^1(\Omega_{ref})^*} \leq c(\Omega_{ref})||a||_{W^{1,\infty}(\Omega_{ref})}||b||_{H^1(\Omega_{ref})^*}. \tag{4.7}$$

The constant $c(\Omega_{ref})$ is bounded for small $\mathbf{W}^{2,\infty}$-transformations of Ω_{ref}.

Proof. We have

$$\begin{aligned}
||ab||^2_{H^1(\Omega_{\text{ref}})^*} &= |\sup_{||c||_{H^1(\Omega_{\text{ref}})}=1} \int_{\Omega_{\text{ref}}} abc\ dx|^2 \\
&\leq \sup_{||c||_{H^1(\Omega_{\text{ref}})}=1} ||ac||^2_{H^1(\Omega_{\text{ref}})}||b||^2_{H^1(\Omega_{\text{ref}})^*} \\
&\leq \sup_{||c||_{H^1(\Omega_{\text{ref}})}=1} (||a||^2_{L^\infty(\Omega_{\text{ref}})} + ||\nabla a||^2_{\mathbf{L}^\infty(\Omega_{\text{ref}})})||c||^2_{H^1(\Omega_{\text{ref}})}||b||^2_{H^1(\Omega_{\text{ref}})^*} \\
&\leq c(\Omega_{\text{ref}})||a||^2_{W^{1,\infty}(\Omega_{\text{ref}})}||b||^2_{H^1(\Omega_{\text{ref}})^*}.
\end{aligned}$$

In fact we use here that $a \in W^{1,\infty}(\Omega_{\text{ref}})$ such that $ac \in H^1(\Omega_{\text{ref}})$. The constant is obviously bounded for small $\mathbf{W}^{2,\infty}$-transformations of Ω_{ref}. □

In Lemma 3.3 we showed that L^p- and Sobolev spaces are conserved for transformed domains. The following lemma shows the continuity of the transformation in the Sobolev spaces.

Lemma 4.9. *For given $\tau \in T_{ad}$ the operator $\tilde{h} \mapsto h := \tilde{h}(\tau(\cdot))$ is linear and continuous from $L^p(\tau(\Omega_{ref}))$ to $L^p(\Omega_{ref})$, from $H^1_0(\tau(\Omega_{ref}))$ to $H^1_0(\Omega_{ref})$, and from $H^2(\tau(\Omega_{ref}))$ to $H^2(\Omega_{ref})$.*
Furthermore the operator $\tilde{\boldsymbol{h}} \mapsto \boldsymbol{h}$ with $\boldsymbol{h}(x,t) := \tilde{\boldsymbol{h}}(\tau(x),t)$ is linear and continuous from $L^2(I;\mathbf{H}^{-1}(\tau(\Omega_{ref})))$ to $L^2(I;\mathbf{H}^{-1}(\Omega_{ref}))$ and from $L^\infty(I;\mathbf{H}^{-1}(\tau(\Omega_{ref})))$ to $L^\infty(I;\mathbf{H}^{-1}(\Omega_{ref}))$.

Proof. We have for $J(x) := \det \tau'(x)$

$$\begin{aligned}
||h||^p_{L^p(\Omega_{\text{ref}})} &= \int_{\Omega_{\text{ref}}} |h(x)|^p\ dx = \int_{\tau(\Omega_{\text{ref}})} |\tilde{h}(\tilde{x})|^p J^{-1}(\tau^{-1}(\tilde{x}))\ d\tilde{x} \\
&\leq ||J^{-1}||_{L^\infty(\Omega_{\text{ref}})}||\tilde{h}||^p_{L^p(\tau(\Omega_{\text{ref}}))}, \\
||\nabla h||^p_{\mathbf{L}^p(\Omega_{\text{ref}})} &= \int_{\Omega_{\text{ref}}} ||\nabla h(x)||^p_2\ dx = \int_{\Omega_{\text{ref}}} ||\tau(x)'^T \nabla_{\tilde{x}}\tilde{h}(\tau(x))||^p_2\ dx \\
&= \int_{\tau(\Omega_{\text{ref}})} ||\tau'(\tau^{-1}(\tilde{x}))^T \nabla_{\tilde{x}}\tilde{h}(\tilde{x})||^p_2 J^{-1}(\tau^{-1}(\tilde{x}))\ d\tilde{x} \\
&\leq ||J^{-1}||_{L^\infty(\Omega_{\text{ref}})}||\tau'||^p_{L^\infty(\Omega_{\text{ref}})}||\nabla_{\tilde{x}}\tilde{h}||^p_{L^p(\tau(\Omega_{\text{ref}}))}.
\end{aligned}$$

Here we used that $J^{-1}(\tau^{-1}(\tilde{x})) = \det(\tau^{-1})'(\tilde{x})$ for all $\tilde{x} \in \tau(\Omega_{\text{ref}})$.

$$
\begin{aligned}
&||\nabla^2 h||^p_{L^p(\Omega_{\text{ref}})^{d\times d}} = \int_{\Omega_{\text{ref}}} ||\nabla^2 h(x)||_2^p \; dx \\
&= \int_{\Omega_{\text{ref}}} ||\tau'^T \nabla^2_{\tilde{x}} \tilde{h}(\tau(x)) + \sum_{i=1}^d \frac{d}{d\tilde{x}_i} \tilde{h}(\tau(x)) \nabla^2 \tau_i(x)||_2^p \; dx \\
&= \int_{\tau(\Omega_{\text{ref}})} ||\tau'(\tau^{-1}(\cdot))^T \nabla^2_{\tilde{x}} \tilde{h}(\cdot) + \sum_{i=1}^d \frac{d}{d\tilde{x}_i} \tilde{h}(\cdot) \nabla^2 \tau_i(\tau^{-1}(x))||_2^p J^{-1}(\tau^{-1}(x)) \; d\tilde{x} \\
&\leq ||J^{-1}||_{L^\infty(\Omega_{\text{ref}})} \cdot \\
&\quad \left(||\tau'||^p_{L^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla^2_{\tilde{x}} \tilde{h}||^p_{L^p(\tau(\Omega_{\text{ref}}))^{d\times d}} + d ||\nabla_{\tilde{x}} \tilde{h}||^p_{\mathbf{L}^p(\tau(\Omega_{\text{ref}}))} ||\tau''||^p_{L^\infty(\Omega_{\text{ref}})^{d\times d\times d}} \right).
\end{aligned}
$$

For $\tilde{\boldsymbol{h}} \mapsto \boldsymbol{h} = \tilde{\boldsymbol{h}}(\tau(\cdot), t)$ as map between $L^2(I; \mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))$ and $L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}}))$ we have

$$
\begin{aligned}
&||\boldsymbol{h}||^2_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} = \int_I ||\boldsymbol{h}(t)||^2_{\mathbf{H}^{-1}(\Omega_{\text{ref}})} \; dt \\
&= \int_I |\sup_{||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}=1} \langle \boldsymbol{h}(t), \boldsymbol{v} \rangle_{\mathbf{H}^{-1}(\Omega_{\text{ref}}), \mathbf{H}_0^1(\Omega_{\text{ref}})}|^2 \; dt \\
&= \int_I |\sup_{||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}=1} \int_{\Omega_{\text{ref}}} \boldsymbol{h}(t)^T \boldsymbol{v} \; dx|^2 \; dt \\
&= \int_I |\sup_{||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}=1} \int_{\tau(\Omega_{\text{ref}})} \tilde{\boldsymbol{h}}(\tilde{x}, t)^T \boldsymbol{v}(\tau^{-1}(\tilde{x})) J^{-1}(\tau^{-1}(\tilde{x})) \; d\tilde{x}|^2 \; dt \\
&= \int_I |\sup_{||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}=1} \langle \tilde{\boldsymbol{h}}(t) J^{-1}(\tau^{-1}(\cdot)), \boldsymbol{v}(\tau^{-1}(\cdot)) \rangle_{\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})), \mathbf{H}_0^1(\tau(\Omega_{\text{ref}}))}|^2 \; dt \\
&\leq \int_I |\sup_{||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}=1} ||\tilde{\boldsymbol{h}}(t) J^{-1}(\tau^{-1}(\cdot))||_{\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}}))} ||\boldsymbol{v}(\tau^{-1}(\cdot))||_{\mathbf{H}_0^1(\tau(\Omega_{\text{ref}}))}|^2 \; dt \\
&\leq C^2 \int_I ||\tilde{\boldsymbol{h}}(t) J^{-1}(\tau^{-1}(\cdot))||^2_{\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}}))} \; dt \\
&\leq \tilde{C} ||\tilde{\boldsymbol{h}}||^2_{L^2(I;\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))} ||J^{-1}||^2_{W^{1,\infty}(\Omega_{\text{ref}})}.
\end{aligned}
$$

where we used that $\tilde{\boldsymbol{h}}(t)$ has a representation in $\mathbf{L}^2(\tau(\Omega_{\text{ref}}))$. In the last step we used Lemma 4.8 where the constant $\tilde{C}$ can be chosen not to depend on the domain $\tau(\Omega_{\text{ref}})$ for transformations τ near id. Furthermore we introduced the constant $C := ||(\tau')^{-1}(\tau')^{-T}||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||J||_{L^\infty(\Omega_{\text{ref}})}$ since

$$
\begin{aligned}
&||\boldsymbol{v}(\tau^{-1}(\cdot))||_{\mathbf{H}_0^1(\tau(\Omega_{\text{ref}}))}\\
&= \sum_{i=1}^{d} \int_{\tau(\Omega_{\text{ref}})} \nabla_{\tilde{x}} v_i(\tau^{-1}(\tilde{x}))^T \nabla_{\tilde{x}} v_i(\tau^{-1}(\tilde{x}))\ d\tilde{x}\\
&= \sum_{i=1}^{d} \int_{\tau(\Omega_{\text{ref}})} \nabla_{x} v_i(\tau^{-1}(\tilde{x}))^T (\tau^{-1})'(\tilde{x})((\tau^{-1})'(\tilde{x}))^T \nabla_{x} v_i(\tau^{-1}(\tilde{x}))\ d\tilde{x}\\
&= \sum_{i=1}^{d} \int_{\tau(\Omega_{\text{ref}})} \nabla_{x} v_i(\tau^{-1}(\tilde{x}))^T \tau'(\tau^{-1}(\tilde{x}))^{-1} \tau'(\tau^{-1}(\tilde{x}))^{-T} \nabla_{x} v_i(\tau^{-1}(\tilde{x}))\ d\tilde{x}\\
&= \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nabla_{x} v_i(x)^T \tau'(x)^{-1} \tau'(x)^{-T} \nabla_{x} v_i(x) \det \tau'\ dx\\
&\leq ||(\tau')^{-1}(\tau')^{-T}||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||J||_{L^\infty(\Omega_{\text{ref}})} \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nabla_x v_i(x)^T \nabla_x v_i(x)\ dx\\
&= ||(\tau')^{-1}(\tau')^{-T}||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||J||_{L^\infty(\Omega_{\text{ref}})}||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}
\end{aligned}
$$

by $(\tau^{-1})'(\tilde{x}) = (\tau'(\tau^{-1}(\tilde{x})))^{-1}$ for all $\tilde{x} \in \tau(\Omega_{\text{ref}})$.
This shows that the operator $\tilde{\boldsymbol{h}} \mapsto \boldsymbol{h} := \tilde{\boldsymbol{h}}(\tau(\cdot), t)$ is linear and continuous from $L^2(I; \mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))$ to $L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}}))$. For the same map from $L^\infty(I; \mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))$ to $L^\infty(I; \mathbf{H}^{-1}(\Omega_{\text{ref}}))$ we use nearly the same proof:

$$
\begin{aligned}
&||\boldsymbol{h}||_{L^\infty(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} = \sup_{t\in I} ||\boldsymbol{h}(t)||_{\mathbf{H}^{-1}(\Omega_{\text{ref}})}\\
&\leq C \sup_{t\in I} ||\tilde{\boldsymbol{h}}(t) J^{-1}(\tau^{-1}(\cdot))||_{\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}}))}\\
&\leq \hat{C}||\tilde{\boldsymbol{h}}||_{L^\infty(I;\mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))}||J^{-1}||_{W^{1,\infty}(\Omega_{\text{ref}})},
\end{aligned}
$$

where $\hat{C}$ can be chosen not to depend on the domain $\tau(\Omega_{\text{ref}})$ for transformations τ near id by Lemma 4.8. ☐

4.2.1.1 Boundedness of the velocity Using Lemma 4.9 we can show the boundedness of the velocity and of the time derivative of the velocity. We start with the the 2D case:

Lemma 4.10. *Let $d = 2$ and $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of* (4.6) *for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ the solutions for arbitrary $\tau \in T_{ad}$. Then there exists $\epsilon, C > 0$ with*

$$
\begin{aligned}
&||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})} < \epsilon \quad \Longrightarrow\\
&||\boldsymbol{v} - \bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{ref}))} \leq C,\ ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))} \leq C, \qquad (4.8)\\
&||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^\infty(I;\mathbf{L}^2(\Omega_{ref}))} \leq C.
\end{aligned}
$$

Proof. We will analyze the proofs of the existence and regularity of the solutions in Theorem III.3.1 and Theorem III.3.5 in [59] to show the boundedness of the norms. In fact we will show, that in the regularity proofs the velocity norms

considered on a domain Ω depend only on the data $\tilde{\boldsymbol{f}}, \tilde{\boldsymbol{v}}_0, \nu$ and constants that are bounded for small transformations of Ω.
We apply the Galerkin procedure as done in the proof of Theorem III.3.1 in [59]: For $d = 2, 3$ there exists a sequence $\tilde{\boldsymbol{w}}_1, \ldots, \tilde{\boldsymbol{w}}_m, \ldots$ of elements in $\mathcal{V}(\Omega)$, which is free and total in $V(\Omega)$. For each m we define an approximate solution $\tilde{\boldsymbol{v}}_m$ of (3.27) as follows

$$\tilde{\boldsymbol{v}}_m = \sum_{i=1}^{m} g_{im}(t)\tilde{\boldsymbol{w}}_i, \tag{4.9}$$

and

$$\begin{aligned} ((\tilde{\boldsymbol{v}}_m(t))_t, \tilde{\boldsymbol{w}}_j)_{\mathbf{L}^2(\Omega)} + \nu(\tilde{\boldsymbol{v}}_m(t), \tilde{\boldsymbol{w}}_j)_{\mathbf{H}_0^1(\Omega)} + b(\tilde{\boldsymbol{v}}_m(t), \tilde{\boldsymbol{v}}_m(t), \tilde{\boldsymbol{w}}_j) \\ = (\tilde{\boldsymbol{f}}(t), \tilde{\boldsymbol{w}}_j)_{\mathbf{L}^2(\Omega)}, \qquad t \in [0,T], j = 1, \ldots, m \\ \tilde{\boldsymbol{v}}_m(0) = \tilde{\boldsymbol{v}}_{0m}, \end{aligned}$$

where $\tilde{\boldsymbol{v}}_{0m}$ is the orthogonal projection in $H(\Omega)$ of $\tilde{\boldsymbol{v}}_0$ onto the space spanned by $\tilde{\boldsymbol{w}}_1, \ldots, \tilde{\boldsymbol{w}}_m$.
In the proof of Theorem III.3.1 in [59] it is shown that

$$\begin{aligned} \sup_{s \in I} ||\tilde{\boldsymbol{v}}_m(s)||^2_{\mathbf{L}^2(\Omega)} \leq ||\tilde{\boldsymbol{v}}_0||_{\mathbf{L}^2(\Omega)} + \nu^{-1} \int_I ||\tilde{\boldsymbol{f}}(t)||^2_{V(\Omega)^*}\, dt, \\ ||\tilde{\boldsymbol{v}}_m(T)||^2_{\mathbf{L}^2(\Omega)} + \nu \int_I ||\tilde{\boldsymbol{v}}_m(t)||^2_{\mathbf{H}_0^1(\Omega)}\, dt \leq ||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{L}^2(\Omega)} + \nu^{-1} \int_I ||\tilde{\boldsymbol{f}}(t)||^2_{V(\Omega)^*}\, dt, \end{aligned} \tag{4.10}$$

and that a subsequence of $(\tilde{\boldsymbol{v}}_m)$ converges to a $\tilde{\boldsymbol{v}} \in \mathbf{L}^2(I; V(\Omega)) \cap \mathbf{L}^\infty(I; H(\Omega))$ that solves (3.27).
Now $||\tilde{\boldsymbol{f}}(t)||_{V(\Omega)^*} \leq c(\Omega)||\tilde{\boldsymbol{f}}(t)||_{\mathbf{H}^{-1}(\Omega)}$ with a constant $c(\Omega)$ that is bounded for small variations of Ω. Thus (4.10) shows that $\tilde{\boldsymbol{v}} \in \mathbf{L}^2(I; V(\Omega)) \cap \mathbf{L}^\infty(I; H(\Omega))$ and that the bound of the norm depends continuously on ν and the norms $||\tilde{\boldsymbol{v}}_0||_{\mathbf{L}^2(\Omega)}$ and $||\tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{H}^{-1}(\Omega))}$.
Furthermore (N3) permits further regularity as $\tilde{\boldsymbol{v}}_0 \in V(\Omega) \cap \mathbf{H}^2(\Omega)$. We use a similar approximation $\tilde{\boldsymbol{v}}_m$ as above but choose $\tilde{\boldsymbol{v}}_{0m}$ as the orthogonal projection in $V(\Omega) \cap \mathbf{H}^2(\Omega)$ of $\tilde{\boldsymbol{v}}_0$ onto the space spanned by $\tilde{\boldsymbol{w}}_1, \ldots, \tilde{\boldsymbol{w}}_m$. Then $\tilde{\boldsymbol{v}}_{0m} \to \tilde{\boldsymbol{v}}_0$ in $\mathbf{H}^2(\Omega)$ and $||\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{H}^2(\Omega)} \leq ||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)}$.
Then in Theorem III.3.5 in [59] it is shown that for $d = 2$ we have for all $t \in I$

$$\begin{aligned} ||(\tilde{\boldsymbol{v}}_m)_t(t)||^2_{\mathbf{L}^2(\Omega)} \leq \left(||(\tilde{\boldsymbol{v}}_m)_t(0)||^2_{\mathbf{L}^2(\Omega)} + \frac{2}{\nu} \int_I ||\tilde{\boldsymbol{f}}_t(s)||^2_{V(\Omega)^*}\, ds \right) e^{\int_I \frac{2}{\nu} ||\tilde{\boldsymbol{v}}_m(s)||^2_{\mathbf{H}_0^1(\Omega)}\, ds} \\ \frac{\nu}{2} ||(\tilde{\boldsymbol{v}}_m)_t(t)||^2_{\mathbf{H}_0^1(\Omega)} \leq \frac{2}{\nu} ||\tilde{\boldsymbol{f}}_t(t)||^2_{V(\Omega)^*} + \frac{2}{\nu} ||\tilde{\boldsymbol{v}}_m(t)||^2_{\mathbf{H}_0^1(\Omega)} ||(\tilde{\boldsymbol{v}}_m)_t(t)||^2_{\mathbf{L}^2(\Omega)} \end{aligned} \tag{4.11}$$

where

$$||(\tilde{\boldsymbol{v}}_m)_t(0)||_{\mathbf{L}^2(\Omega)} \leq ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)} + \nu||\Delta \tilde{\boldsymbol{v}}_{0m}||_{\mathbf{L}^2(\Omega)} + ||B\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{L}^2(\Omega)} \tag{4.12}$$

and $B\boldsymbol{v} \in V(\Omega)^*$ is defined by $< B\boldsymbol{v}, \boldsymbol{w} >_{V(\Omega)^*, V(\Omega)} := b(\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{w})$ for all $\boldsymbol{w} \in V(\Omega)$.

For the second term in (4.12) we obtain

$$||\Delta\tilde{\boldsymbol{v}}_{0m}||_{L^2(\Omega)} \le c_0||\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{H}^2(\Omega)} \le c_0||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)}$$

Here c_0 depends only on d because $\Delta\tilde{\boldsymbol{v}}_{0m} = \sum_{i=1}^{d} \frac{\partial^2 \tilde{\boldsymbol{v}}_{0m}}{\partial^2 x_i}$.
By Lemma 4.1 we have

$$|b(\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{w})| \le c_1||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)}||\boldsymbol{v}||_{\mathbf{H}^2(\Omega)}||\boldsymbol{w}||_{\mathbf{L}^2(\Omega)}$$

where c_1 is a constant that depends only on d and the Poincaré constant $c_P(\Omega)$ of Ω.
Therefore

$$||B\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{L}^2(\Omega)} \le c_1||\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{H}_0^1(\Omega)}||\tilde{\boldsymbol{v}}_{0m}||_{\mathbf{H}^2(\Omega)} \le c_1||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{H}^2(\Omega)}. \tag{4.13}$$

Because the Poincaré constant $c_P(\Omega)$ is bounded for $W^{1,\infty}$ -transformations near id of the domain Ω, we can choose c_1 also domain-independent for small $W^{1,\infty}$ variations of Ω_{ref}. In fact, for star-shaped domains $c_P(\Omega)$ is uniformly bounded, c.f. [35] or the comments in [66] and [1]. With Lemma 4.12 we can also use this result for Lipschitz domains. We finally get

$$||(\tilde{\boldsymbol{v}}_m)_t(0)||_{\mathbf{L}^2(\Omega)} \le ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)} + \nu c_0||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)} + c_1||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{H}^2(\Omega)}. \tag{4.14}$$

From this using (4.11) we see that the bounds of the $L^\infty(I; H(\Omega))$ and $L^2(I; V(\Omega))$-norm of $\tilde{\boldsymbol{v}}_t$ depend continuously on $||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)}, ||\tilde{\boldsymbol{f}}_t||_{L^2(I;\mathbf{H}^{-1}(\Omega))}, ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)}$ and $||\tilde{\boldsymbol{v}}||_{L^2(I;V(\Omega))}$.
So to obtain (4.17) it suffices to show, that for given $\tau \in T_{\text{ad}}$ the operator $\tilde{h} \mapsto h = \tilde{h}(\tau(\cdot))$ is linear and continuous from $L^p(\tau(\Omega_{\text{ref}}))$ to $L^p(\Omega_{\text{ref}})$, from $H_0^1(\tau(\Omega_{\text{ref}}))$ to $H_0^1(\Omega_{\text{ref}})$, and from $H^2(\tau(\Omega_{\text{ref}}))$ to $H^2(\Omega_{\text{ref}})$. Furthermore we need to show that $\tilde{h} \mapsto h = \tilde{h}(\tau(\cdot), t)$ is linear and continuous from $L^2(I; \mathbf{H}^{-1}(\tau(\Omega_{\text{ref}})))$ to $L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}}))$. This was already shown in Lemma 4.9. $\square$

We can show the same result also for the 3D case:

Lemma 4.11. *Let $d = 3$ and $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of (4.6) for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ the solutions for arbitrary $\tau \in T_{ad}$. Then there exists $\epsilon > 0$ and $C > 0$ with*

$$\begin{aligned} &||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})} < \epsilon \quad \Longrightarrow \\ &||\boldsymbol{v} - \bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{ref}))} \le C,\ ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))} \le C, \\ &||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^\infty(I;\mathbf{L}^2(\Omega_{ref}))} \le C. \end{aligned} \tag{4.15}$$

Proof. We use the same approximate solutions $(\tilde{\boldsymbol{v}}_m)$ as in the 2D case. The estimates in (4.10) also hold for $d = 3$. Furthermore, using Lemma 4.1, we arrive at the same estimate (4.14) as in the 2D case

$$||(\tilde{\boldsymbol{v}}_m)_t(0)||_{\mathbf{L}^2(\Omega)} \le ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)} + \nu c_0||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)} + c_1||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{H}^2(\Omega)} =: d_1(\Omega) \tag{4.16}$$

where for transformations near id we can choose the same constants c_0 and c_1 for $\Omega = \Omega_{\text{ref}}$ and $\Omega = \tau(\Omega_{\text{ref}})$.
Let $c > 0$ such that $2c_P(\Omega) \le c$ for $\Omega = \Omega_{\text{ref}}$ and $\Omega = \tau(\Omega_{\text{ref}})$. Then for $d = 3$ for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega)$ we have

$$|b(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w})| \le c||\boldsymbol{u}||_{\mathbf{H}_0^1(\Omega)}||\boldsymbol{v}||_{\mathbf{H}_0^1(\Omega)}||\boldsymbol{w}||_{\mathbf{H}_0^1(\Omega)}.$$

In the proof of Theorem III.3.7 in [59] it is shown that for all $0 \le t \le T$

$$\frac{d}{dt}||(\tilde{\boldsymbol{v}}_m)_t||^2_{\mathbf{L}^2(\Omega)} + 2\left(\nu - c\sqrt{\frac{d_3(\Omega)}{\nu}}\right)||(\tilde{\boldsymbol{v}}_m)_t||^2_{\mathbf{H}_0^1(\Omega)} \le 2||\tilde{\boldsymbol{f}}_t||_{\mathbf{L}^2(\Omega)}||(\tilde{\boldsymbol{v}}_m)_t||_{\mathbf{L}^2(\Omega)},$$

$$1 + ||(\tilde{\boldsymbol{v}}_m)_t||^2_{\mathbf{L}^2(\Omega)} \le (1 + d_1(\Omega)^2)e^{\int_I ||\tilde{\boldsymbol{f}}_t(s)||_{\mathbf{L}^2(\Omega)}\ ds}.$$

Now for transformations τ near id we can show that there exists a $c^* > 0$ such that $d_3(\tau(\Omega_{\text{ref}})) < c^* < \frac{\nu^3}{c^2}$ where c^* is domain-independent. In fact, by assumption (N3) we have a $c^*(\Omega)$ such that

$$\begin{aligned} d_3(\Omega) &:= \frac{d_2(\Omega)}{\nu} + (1 + d_1(\Omega)^2)\left(||\tilde{\boldsymbol{v}}_0||^2_{\mathbf{L}^2(\Omega)} + \frac{Td_2(\Omega)}{\nu}\right)^{1/2} e^{\int_I ||\tilde{\boldsymbol{f}}_t(s)||_{\mathbf{L}^2(\Omega)}\ ds} \\ &\le c^*(\Omega) < \frac{\nu^3}{c^2}. \end{aligned}$$

Now by lemma 4.9 $d_1(\Omega)$, $d_2(\Omega)$ and $||\tilde{\boldsymbol{f}}_t||_{L^1(I;H(\Omega))}$ have a bound that depends continuously on τ. This implies that we can find such a c^* independent of Ω for τ near id.
From the second inequality we see that $(\tilde{\boldsymbol{v}}_m)_t \in L^\infty(I; \mathbf{L}^2(\Omega))$ and that the bound of the norm depends continuously on $d_1(\Omega)$ and $||\tilde{\boldsymbol{f}}_t||_{L^1(I;\mathbf{L}^2(\Omega))}$. Using this and the first inequality we also obtain $(\tilde{\boldsymbol{v}}_m)_t \in L^2(I; \mathbf{H}_0^1(\Omega))$. In fact we use that $(\nu - c\sqrt{\frac{d_3(\Omega)}{\nu}})$ is uniformly bounded away from 0 for $\Omega = \tau(\Omega_{\text{ref}})$ and $||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\text{ref}})} < \epsilon$. The bound of the norm depends continuously on c^* and $||\tilde{\boldsymbol{f}}_t||_{L^1(I;\mathbf{L}^2(\Omega))}$.
Because c_0, c_1 and c^* can be chosen not to depend on the domain Ω for small $W^{1,\infty}$ variations of Ω_{ref} we conclude that the bounds of $||\tilde{\boldsymbol{v}}_t||_{L^\infty(I;\mathbf{L}^2(\Omega))}$ and $||\tilde{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega))}$ depend continuously on the norms $||\tilde{\boldsymbol{f}}_t||_{L^1(I;\mathbf{L}^2(\Omega))}, ||\tilde{\boldsymbol{f}}(0)||_{\mathbf{L}^2(\Omega)}$ and $||\tilde{\boldsymbol{v}}_0||_{\mathbf{H}^2(\Omega)}$. Using Lemma 4.9 we obtain the velocity part of (4.15) in the same way as in the 2d case. □

4.2.1.2 Boundedness of the pressure To derive regularity estimates for the pressure we need to analyze the properties of the Bogovskii operator $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ defined via div $(Bf) = f$. For this we will use a result of Geissert, Hieber and Heck [21] that we will also need for the differentiability results later.
We start with a result describing the topology of domains under transformations.

Lemma 4.12. *Let $\bar{\Omega}$ be a bounded Lipschitz domain. Then there exists an open cover G_j, $j = 1, \ldots, m$ of $\bar{\Omega}$, such that $\Omega_j = G_j \cap \Omega$ are star shaped with respect* *to some ball with radius $r_j > 0$. Moreover, there exists $\epsilon > 0$ such that for all $\tau \in \mathbf{W}^{1,\infty}(\Omega)$ with $\|\tau - id\|_{\mathbf{W}^{1,\infty}} < \epsilon$ the sets $\tilde{\Omega}_j := \tau(\Omega_j)$ are star shaped with respect to some ball with radius $r_j/32$.*

The technical proof of it was given by Stefan Ulbrich [64].
At several places we need the following result. The first part is the main result of [21, Theorem 2.5]. The second part was again shown by Stefan Ulbrich [64] where Lemma 4.12 is used.

Lemma 4.13. *Let Ω be a bounded Lipschitz domain.*

i) Then there exists a continuous linear operator $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ such that $B : H_0^s(\Omega) \to \mathbf{H}_0^{s+1}(\Omega)$ is continuous and linear for $-1 \leq s < 0$ and $div(Bf) = f$ for all $f \in L_0^2(\Omega)$. Here, for $s > 0$ we have $H_0^{-s}(\Omega) = H^s(\Omega)^*$.

ii) There exists a bounded linear operator $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ with $div(Bf) = f$ for all $f \in L_0^2(\Omega)$ such that

$$\|B\|_{L(L_0^2(\Omega),\mathbf{H}_0^1(\Omega))} \leq c(\Omega),$$

where $c(\Omega)$ is locally uniform for $W^{1,\infty}$-transformations of Ω close to identity.

Lemma 4.14. *Let $\boldsymbol{g} \in \mathbf{H}^{-1}(\Omega)$ with $(\boldsymbol{g}, \boldsymbol{v}) = 0$ for all $\boldsymbol{v} \in V(\Omega)$. Then there exists $p \in L_0^2(\Omega)$ such that $\nabla p = \boldsymbol{g}$ and with the operator $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ of Lemma 4.13 ii)*

$$\|p\|_{L_0^2(\Omega)} \leq \|B\|_{L(L_0^2(\Omega),\mathbf{H}_0^1(\Omega))} \|\boldsymbol{g}\|_{\mathbf{H}^{-1}(\Omega)}.$$

Note that $\|B\|_{L(L_0^2(\Omega),\mathbf{H}_0^1(\Omega))}$ is locally uniformly bounded for $W^{1,\infty}$-transformations of Ω close to identity.

Proof. The existence of $p \in L_0^2(\Omega)$ follows by Prop. I.1.2, (ii) in [59]. Now let $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ be the operator of Lemma 4.13 ii). Then $\boldsymbol{v} = Bp \in \mathbf{H}_0^1(\Omega)$ and

$$\begin{aligned}\langle Bp, \boldsymbol{g}\rangle_{\mathbf{H}_0^1(\Omega),\mathbf{H}^{-1}(\Omega)} &= \langle \boldsymbol{v}, \boldsymbol{g}\rangle_{\mathbf{H}_0^1(\Omega),\mathbf{H}^{-1}(\Omega)} = \langle \boldsymbol{v}, \nabla p\rangle_{\mathbf{H}_0^1(\Omega),\mathbf{H}^{-1}(\Omega)} \\ &= (\text{div } \boldsymbol{v}, p)_{L^2(\Omega)} = (p, p)_{L^2(\Omega)} = \|p\|^2_{L_0^2(\Omega)}.\end{aligned}$$

Hence,

$$\|p\|^2_{L_0^2(\Omega)} \leq \|Bp\|_{\mathbf{H}_0^1(\Omega)} \|\boldsymbol{g}\|_{\mathbf{H}^{-1}(\Omega)} \leq \|B\|_{L(L_0^2(\Omega),\mathbf{H}_0^1(\Omega))} \|p\|_{L_0^2(\Omega)} \|\boldsymbol{g}\|_{\mathbf{H}^{-1}(\Omega)}.$$

$\square$

Using Lemma 4.14 we can proof the boundedness of p:

Lemma 4.15. *Let $d \in \{2, 3\}$ and $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of (4.6) for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ the solutions for arbitrary $\tau \in T_{ad}$. Then there exists $\epsilon, C > 0$ with*

$$\begin{aligned}&||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} < \epsilon \quad \Longrightarrow \\ &||\boldsymbol{v} - \bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{ref}))} \leq C, \; ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))} \leq C, \\ &||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^\infty(I;\mathbf{L}^2(\Omega_{ref}))} \leq C, \; ||p - \bar{p}||_{L^2(I;L_0^2(\Omega_{ref}))} \leq C.\end{aligned} \tag{4.17}$$

Proof. The assertions for the velocity are already proved in Lemma 4.10 and Lemma 4.11. For the pressure estimate we use that by Lemma 3.8 for 2D and Lemma 3.11 for 3D

$$
\begin{aligned}
||\tilde{p}||_{L^\infty(I;L_0^2(\Omega))} \leq c(\Omega)(||\tilde{\boldsymbol{v}}_t||_{L^\infty(I;H(\Omega))} + \nu||\tilde{\boldsymbol{v}}||_{L^\infty(I;V(\Omega))} + \\
||\tilde{\boldsymbol{v}}||^2_{L^\infty(I;V(\Omega))} + ||\tilde{\boldsymbol{f}}||_{L^\infty(I;\mathbf{H}^{-1}(\Omega))})
\end{aligned}
\tag{4.18}
$$

with a constant $c(\Omega)$. By Lemma 4.14 $c(\Omega)$ is bounded for transformations τ near id. $\square$

4.2.2 Continuity of the Velocity

In this section we will prove the continuity of the velocity and the pressure in several steps. We will start with a continuity result for $\tau \to \boldsymbol{v}(\tau)$ in $L^\infty(I, \mathbf{L}^2(\Omega_{\text{ref}})) \cap L^2(I; \mathbf{H}_0^1(\Omega_{\text{ref}}))$. From this we will derive stability estimates for $\boldsymbol{v}_t(\tau)$ in $L^2(I; \mathbf{L}^2(\Omega_{\text{ref}}))$ and for the pressure p in $L^2(I; L_0^2(\Omega_{\text{ref}}))$. Using interpolation theory we will show that this implies continuity of $\tau \to \boldsymbol{v}(\tau) \in L^r(I; \mathbf{H}_0^1(\Omega_{\text{ref}}))$ for $r < \infty$ and of $\tau \to \boldsymbol{v}(\tau) \in L^\infty(I; \mathbf{L}^s(\Omega_{\text{ref}}))$ for $s \leq 6$.
These results will be used to show Fréchet differentiability of $\tau \mapsto \boldsymbol{v}(\tau) \in W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) + W(I; V(\Omega_{\text{ref}}))$ in $\tau = \text{id}$ in the next section.
To simplify matters we introduce functions g_1, g_2 and g_3 defined on T_{ad} to describe the τ-terms that appear through the transformation to the reference domain in (4.6). First we show that these terms are Fréchet differentiable in the correct spaces:

Lemma 4.16. *Let $\tau \in \mathcal{T}^{k,\infty}$ and*

$$g_1(\tau) := |\det \tau'|,\; g_2(\tau) := \tau'^{-1}\tau'^{-T}|\det \tau'|,\; g_3(\tau) := \tau'^{-T}|\det \tau'|. \tag{4.19}$$

Then

$$g_1 : \mathcal{V}^{k,\infty} \to W^{k-1,\infty}(\mathbb{R}^d),\; g_2, g_3 : \mathcal{V}^{k,\infty} \to W^{k-1,\infty}(\mathbb{R}^d)^{d\times d}$$

are Fréchet differentiable in τ with derivatives

$$\begin{aligned}
g_1'(\tau)\psi &= tr\,(\tau'^{-1}\psi')|\det \tau'|,\\
g_2'(\tau)\psi &= -\tau'^{-1}\psi'\tau'^{-1}\tau'^{-T}|\det \tau'| - \tau'^{-1}\tau'^{-T}\psi'^T\tau'^{-T}|\det \tau'|\\
&\quad +\tau'^{-1}\tau'^{-T}\; tr\,(\tau'^{-1}\psi')|\det \tau'|,\\
g_3'(\tau)\psi &= -\tau'^{-T}\psi'^T\tau'^{-T}|\det \tau'| + \tau'^{-T}\; tr\,(\tau'^{-1}\psi')|\det \tau'|,
\end{aligned}$$

where $\psi \in W^{k,\infty}(\mathbb{R}^d)^d$. For $\tau = \text{id}$ we have

$$\begin{aligned}
g_1'(\text{id})\psi &= tr\,(\psi'),\\
g_2'(\text{id})\psi &= -\psi' - \psi'^T + \; tr\,(\psi')I,\\
g_3'(\text{id})\psi &= -\psi'^T + \; tr\,(\psi')I.
\end{aligned}$$

Proof. Using Lemma 3.4 the assertion for g_1 follows directly. Furthermore g_2 and g_3 are a product of the $|\det \tau'|$ and τ'^{-1} operators, using also the linear transpose operator. Hence, using the product rule and Lemma 3.4 we also obtain the derivatives for g_2 and g_3. □

We show now that under the regularity assumptions (N3) on the data the mapping $\tau \in W^{2,\infty}(\Omega_{\text{ref}}) \mapsto \boldsymbol{v}(\tau)$ is continuous, where the topology on the velocity space is stronger than the usual space for weak solutions. This will be essential to prove in the next section the Fréchet differentiability of $\tau \mapsto \boldsymbol{v}(\tau) \in W(I; \mathbf{H}_0^1(\Omega_{\text{ref}})) + W(I; V(\Omega_{\text{ref}}))$ in $\tau = \text{id}$.
We start with a first continuity result:

Theorem 4.3. *Let $d \in \{2, 3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of (4.6) for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ be the solutions for arbitrary $\tau \in T_{ad}$. Writing $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ we have*

$$\begin{aligned}
||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^2(\Omega_{ref}))} \to 0 \qquad &as\; ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0, &(4.20)\\
||\nabla \boldsymbol{e}||_{L^2(I;L^2(\Omega_{ref})^{d\times d})} \to 0 \qquad &as\; ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0. &(4.21)
\end{aligned}$$

Proof. Let $e_p := p - \bar{p}$. After subtracting the equations (4.6) for $(\boldsymbol{v}, p)$ and $(\bar{\boldsymbol{v}}, \bar{p})$ from each other, rearranging yields for a.a. $t \in I$

$$
\begin{aligned}
&\int_{\Omega_{\text{ref}}} \boldsymbol{e}_t(t)^T \boldsymbol{w} \; dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla e_i(t)^T \nabla w_i \; dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{e}(t)^T \nabla \boldsymbol{v}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}(t)) \boldsymbol{w} \; dx - \int_{\Omega_{\text{ref}}} e_p(t) \text{ tr } (\nabla \boldsymbol{w}) \; dx \\
&= \int_{\Omega_{\text{ref}}} (\tilde{\boldsymbol{f}}(\tau(x), t) g_1(\tau) - \tilde{\boldsymbol{f}}(x, t) g_1(\text{id}))^T \boldsymbol{w} \; dx \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t(t)^T \boldsymbol{w} (g_1(\text{id}) - g_1(\tau)) \; dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu (\nabla v(t)_i^T (g_2(\text{id}) - g_2(\tau)) \nabla w_i \; dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{v}(t)^T (g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t)) \boldsymbol{w} \; dx \\
&- \int_{\Omega_{\text{ref}}} p(t) (\text{ tr } ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{w})) \; dx \qquad \forall \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\text{ref}}), \\
&\int_{\Omega_{\text{ref}}} q \text{ tr } (\nabla \boldsymbol{e}) \; dx = \int_{\Omega_{\text{ref}}} q (\text{ tr } ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t))) \; dx \qquad \forall q \in L_0^2(\Omega_{\text{ref}}), \\
&\boldsymbol{e}(\cdot, 0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0.
\end{aligned}
\tag{4.22}
$$

We would like to get stability estimates for $\boldsymbol{e}$. Therefore we will test (4.22) with $\boldsymbol{w} = \boldsymbol{e}(t)$ and derive an energy inequality for $\boldsymbol{e}(t)$ by estimating (4.22) term by term. In the following we will use Young's inequality (see Lemma 2.6) frequently.

Testing with $\boldsymbol{w} = \boldsymbol{e}(t)$ the first term on the left side is equal to $\frac{1}{2} \frac{d}{dt} ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}$ and the second term is the same as $\nu ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d \times d}}$.

For the trilinear form $b(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w})$ with $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\text{ref}})$ we have for $d \in \{2, 3\}$ (see Lemma 4.1):

$$
\begin{aligned}
|b(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w})| \leq & c ||\nabla \boldsymbol{u}||^{3/4}_{L^2(\Omega_{\text{ref}})^{d \times d}} ||\boldsymbol{u}||^{1/4}_{\mathbf{L}^2(\Omega_{\text{ref}})} \\
& \cdot ||\nabla \boldsymbol{v}||_{L^2(\Omega_{\text{ref}})^{d \times d}} ||\nabla \boldsymbol{w}||^{3/4}_{L^2(\Omega_{\text{ref}})^{d \times d}} ||\boldsymbol{w}||^{1/4}_{\mathbf{L}^2(\Omega_{\text{ref}})}
\end{aligned}
\tag{4.23}
$$

with a constant $c > 0$. Since $\bar{\boldsymbol{v}}(t)$ is solenoidal on Ω_{ref}, we have by integration by parts

$$
\int_{\Omega_{\text{ref}}} \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}(t) \boldsymbol{e}(t) \; dx = - \int_{\Omega_{\text{ref}}} \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}(t) \boldsymbol{e}(t) \; dx = 0.
$$

Hence for the third term on the left side of (4.22) we obtain

$$
\begin{aligned}
&\int_{\Omega_{\text{ref}}} (\boldsymbol{e}(t)^T \nabla \boldsymbol{v}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}(t)) \boldsymbol{e}(t) \; dx = \int_{\Omega_{\text{ref}}} \boldsymbol{e}(t)^T \nabla \boldsymbol{v}(t) \boldsymbol{e}(t) \; dx \\
&\geq -c ||\boldsymbol{v}(t)||_{\mathbf{H}_0^1(\Omega_{\text{ref}})} ||\nabla \boldsymbol{e}(t)||^{3/2}_{L^2(\Omega_{\text{ref}})^{d \times d}} ||\boldsymbol{e}(t)||^{1/2}_{\mathbf{L}^2(\Omega_{\text{ref}})} \\
&\geq -\frac{\nu}{4} ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d \times d}} - \frac{27 c^4}{4 \nu^3} ||\boldsymbol{v}(t)||^4_{\mathbf{H}_0^1(\Omega_{\text{ref}})} ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}
\end{aligned}
\tag{4.24}
$$

with a constant $c > 0$ where we have used (4.23) and Young's inequality (2.3) with $p = 4/3$ and $q = 4$.
From the second equation we have

$$\begin{aligned} || \text{ tr } (\nabla \boldsymbol{e}(t))||_{L^2(\Omega_{\text{ref}})} &= || \text{ tr } ((g_3(\text{id}) - g_3(\tau))\nabla \boldsymbol{v}(t))||_{L^2(\Omega_{\text{ref}})} \\ &\leq c||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{v}(t)||_{\mathbf{H}_0^1(\Omega_{\text{ref}})} \end{aligned} \tag{4.25}$$

for a constant $c > 0$. The equality follows by the fact that $||a||_{L^2(\Omega_{\text{ref}})} = \sup_{||b||_{L^2(\Omega_{\text{ref}})}=1} \int_{\Omega_{\text{ref}}} ab\ dx$ for all $a \in L^2(\Omega_{\text{ref}})$. In the last inequality we have used that for $A \in L^2(\Omega_{\text{ref}})^{d\times d}, B \in L^\infty(\Omega_{\text{ref}})^{d\times d}$ we have

$$|| \text{ tr } (B \cdot A)||_{L^2(\Omega_{\text{ref}})} \leq c||A||_{L^2(\Omega_{\text{ref}})^{d\times d}}||B||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}, \tag{4.26}$$

Therefore we get for the fourth term on the left side

$$\begin{aligned} &||e_p(t)||_{L^2(\Omega_{\text{ref}})}|| \text{ tr } (\nabla \boldsymbol{e}(t))||_{L^2(\Omega_{\text{ref}})} \leq \\ &\qquad c||e_p(t)||_{L^2(\Omega_{\text{ref}})}||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{v}(t)||_{\mathbf{H}_0^1(\Omega_{\text{ref}})}. \end{aligned} \tag{4.27}$$

We now estimate the right hand side. For the first term we obtain using Young's inequality

$$\begin{aligned} &|\int_{\Omega_{\text{ref}}} (\tilde{\boldsymbol{f}}(\tau(x), t)g_1(\tau) - \tilde{\boldsymbol{f}}(x, t)g_1(\text{id}))^T \boldsymbol{e}(t)\ dx| \\ &\leq ||\boldsymbol{e}(t)||_{\mathbf{L}^2(\Omega_{\text{ref}})}||\tilde{\boldsymbol{f}}(\tau(\cdot), t)g_1(\tau) - \tilde{\boldsymbol{f}}(\cdot, t)g_1(\text{id})||_{\mathbf{L}^2(\Omega_{\text{ref}})} \\ &\leq \frac{1}{2}||\tilde{\boldsymbol{f}}(\tau(\cdot), t) \det \tau' - \tilde{\boldsymbol{f}}(\cdot, t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + \frac{1}{2}||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}. \end{aligned} \tag{4.28}$$

For the second term we get in the same way

$$\begin{aligned} &|\int_{\Omega_{\text{ref}}} \boldsymbol{v}_t(t)^T \boldsymbol{e}(t)(g_1(\text{id}) - g_1(\tau))\ dx| \\ &\leq ||\boldsymbol{v}_t(t)||_{\mathbf{L}^2(\Omega_{\text{ref}})}||\boldsymbol{e}(t)||_{\mathbf{L}^2(\Omega_{\text{ref}})}||g_1(\text{id}) - g_1(\tau)||_{L^\infty(\Omega_{\text{ref}})} \\ &\leq \frac{1}{2}||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + \frac{1}{2}||\boldsymbol{v}_t(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}||g_1(\text{id}) - g_1(\tau)||^2_{L^\infty(\Omega_{\text{ref}})}. \end{aligned} \tag{4.29}$$

For the third term we have again with Young's inequality

$$\begin{aligned} &|\sum_{i=1}^d \int_{\Omega_{\text{ref}}} \nu \nabla v(t)_i^T (g_2(\text{id}) - g_2(\tau))\nabla e(t)_i\ dx| \\ &\leq \sum_{i=1}^d \nu||\nabla v(t)_i||_{\mathbf{L}^2(\Omega_{\text{ref}})}||g_2(\text{id}) - g_2(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\nabla e(t)_i||_{\mathbf{L}^2(\Omega_{\text{ref}})} \\ &\leq ||g_2(\text{id}) - g_2(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\nabla \boldsymbol{v}(t)||_{L^2(\Omega_{\text{ref}})^{d\times d}}||\nabla \boldsymbol{e}(t)||_{L^2(\Omega_{\text{ref}})^{d\times d}} \\ &\leq \frac{2}{\nu}||g_2(\text{id}) - g_2(\tau)||^2_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\nabla \boldsymbol{v}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} + \frac{\nu}{8}||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}}. \end{aligned} \tag{4.30}$$

Indeed we used

$$\sum_{i=1}^{d} ||\nabla \boldsymbol{v}(t)_i||_{\mathbf{L}^2(\Omega_{\text{ref}})} ||\nabla \boldsymbol{e}(t)_i||_{\mathbf{L}^2(\Omega_{\text{ref}})} \leq ||\nabla \boldsymbol{v}(t)||_{L^2(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{e}(t)||_{L^2(\Omega_{\text{ref}})^{d\times d}}$$

because $||\nabla \boldsymbol{v}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} = \sum_{i=1}^{d} ||\nabla \boldsymbol{v}(t)_i||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}$ and the Cauchy-Schwarz inequality.
For the fourth term on the right side we use Lemma 4.2 and obtain

$$\begin{aligned}
& |\int_{\Omega_{\text{ref}}} (\boldsymbol{v}(t)^T (g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t)) \boldsymbol{e}(t)\ dx| \\
\leq\ & c_1 ||\boldsymbol{e}(t)||^{1/4}_{\mathbf{L}^2(\Omega_{\text{ref}})} ||\nabla \boldsymbol{e}(t)||^{3/4}_{L^2(\Omega_{\text{ref}})^{d\times d}} ||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}} \\
& \cdot ||\boldsymbol{v}(t)||^{1/4}_{\mathbf{L}^2(\Omega_{\text{ref}})} ||\boldsymbol{v}(t)||^{7/4}_{\mathbf{H}^1_0(\Omega_{\text{ref}})} \\
\leq\ & \frac{\nu}{4} ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} \qquad (4.31)\\
& + c_2 ||\boldsymbol{e}(t)||^{2/5}_{\mathbf{L}^2(\Omega_{\text{ref}})} ||g_3(\text{id}) - g_3(\tau)||^{8/5}_{L^\infty(\Omega_{\text{ref}})^{d\times d}} ||\boldsymbol{v}(t)||^{2/5}_{\mathbf{L}^2(\Omega_{\text{ref}})} ||\boldsymbol{v}(t)||^{14/5}_{\mathbf{H}^1_0(\Omega_{\text{ref}})} \\
\leq\ & \frac{\nu}{4} ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} + c_3 ||\boldsymbol{v}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} \\
& + c_4 ||g_3(\text{id}) - g_3(\tau)||^2_{L^\infty(\Omega_{\text{ref}})^{d\times d}} ||\boldsymbol{v}(t)||^{7/2}_{\mathbf{H}^1_0(\Omega_{\text{ref}})}
\end{aligned}$$

with constants $c_1, c_2, c_3, c_4 > 0$, where we have used Young's inequality with $p = 8/3, q = 8/5$ and $p = 5, q = 5/4$, respectively.
For the fifth term on the right hand side we obtain

$$\begin{aligned}
& |\int_{\Omega_{\text{ref}}} p(t)(\ \text{tr}\ ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{e}(t)))\ dx| \\
& \leq ||p(t)||_{L^2(\Omega_{\text{ref}})} ||\ \text{tr}\ ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{e}(t))||_{L^2(\Omega_{\text{ref}})} \\
& \leq ||p(t)||_{L^2(\Omega_{\text{ref}})} ||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{e}(t)||_{L^2(\Omega_{\text{ref}})^{d\times d}} \qquad (4.32)\\
& \leq \frac{\nu}{8} ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} + \frac{2}{\nu} ||p(t)||^2_{L^2(\Omega_{\text{ref}})} ||g_3(\text{id}) - g_3(\tau)||^2_{L^\infty(\Omega_{\text{ref}})^{d\times d}}.
\end{aligned}$$

Taking all together we get for $\tau \in T_{\text{ad}}$ with $\|\tau - \text{id}\|_{W^{1,\infty}(\Omega_{\text{ref}})}$ small enough by Lemma 4.16

$$\begin{aligned}
& \frac{d}{dt} ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + \frac{\nu}{2} ||\nabla \boldsymbol{e}(t)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} \\
& \leq \tilde{c} \Big((1 + ||\boldsymbol{v}(t)||^4_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\boldsymbol{v}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})})\ ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} \\
& + ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} ||e_p(t)||_{L^2(\Omega_{\text{ref}})} ||\boldsymbol{v}(t)||_{\mathbf{H}^1_0(\Omega_{\text{ref}})} \\
& + ||\tau - \text{id}||^2_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} (||\boldsymbol{v}(t)||^{7/2}_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\boldsymbol{v}(t)||^2_{\mathbf{H}^1_0(\Omega_{\text{ref}})} \\
& + ||\boldsymbol{v}_t(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + ||p(t)||^2_{L^2(\Omega_{\text{ref}})}) \\
& + ||\tilde{\boldsymbol{f}}(\tau(\cdot), t) \det \tau' - \tilde{\boldsymbol{f}}(\cdot, t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} \Big), \\
& \boldsymbol{e}(0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0,
\end{aligned}$$

with a constant $\tilde{c} > 0$ depending on Ω_{ref} and ν.
Now we apply the Gronwall Lemma 2.4 with

$$\begin{aligned}
\eta(t) &:= ||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + \frac{\nu}{2}\int_0^t ||\nabla \boldsymbol{e}(s)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}}\, ds \\
\phi(t) &:= \tilde{c}(1 + ||\boldsymbol{v}(t)||^4_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\boldsymbol{v}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}) \\
\psi(t) &:= \tilde{c}\Big(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}||e_p(t)||_{L^2(\Omega_{\text{ref}})}||\boldsymbol{v}(t)||_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\tau - \text{id}||^2_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \\
&\qquad \cdot (||\boldsymbol{v}(t)||^{7/2}_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\boldsymbol{v}(t)||^2_{\mathbf{H}^1_0(\Omega_{\text{ref}})} + ||\boldsymbol{v}_t(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + ||p(t)||^2_{L^2(\Omega_{\text{ref}})}) \\
&\qquad + ||\tilde{\boldsymbol{f}}(\tau(\cdot), t)\det\tau' - \tilde{\boldsymbol{f}}(\cdot, t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})}\Big)
\end{aligned}$$

Since $\phi(t) > 0$, we have $\forall t \in I$ and for $\tau \in T_{\text{ad}}$ with $\|\tau - \text{id}\|_{W^{1,\infty}(\Omega_{\text{ref}})}$ small enough that $\eta'(t) \leq \phi(t)\eta(t) + \psi(t)$. Therefore there exists a constant

$$C = C(||p||_{L^2(I;L^2(\Omega_{\text{ref}}))}, ||\bar{p}||_{L^2(I;L^2(\Omega_{\text{ref}}))}, ||\boldsymbol{v}||_{L^4(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}, ||\boldsymbol{v}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}) \tag{4.33}$$

such that for $\tau \in T_{\text{ad}}$ close to identity

$$\begin{aligned}
&||\boldsymbol{e}(t)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + \frac{\nu}{2}\int_0^t ||\nabla \boldsymbol{e}(s)||^2_{L^2(\Omega_{\text{ref}})^{d\times d}}\, ds \\
&\leq C\ (||\boldsymbol{e}(0)||^2_{\mathbf{L}^2(\Omega_{\text{ref}})} + ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} + ||\tau - \text{id}||^2_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \\
&\qquad + ||\tilde{\boldsymbol{f}}(\tau(\cdot), \cdot)\det\tau' - \tilde{\boldsymbol{f}}||^2_{\mathbf{L}^2(I;L^2(\Omega_{\text{ref}}))}).
\end{aligned}$$

Now the norms $||p||_{L^2(I;L^2(\Omega_{\text{ref}}))}, ||\boldsymbol{v}||_{L^\infty(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}$ and $||\boldsymbol{v}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}$ are uniformly bounded by Lemma 4.15 for $||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0$. Furthermore $||\boldsymbol{e}(0)||_{\mathbf{L}^2(\Omega_{\text{ref}})} \to 0$ and $||\tilde{\boldsymbol{f}}(\tau(\cdot), \cdot)\det\tau' - \tilde{\boldsymbol{f}}||_{\mathbf{L}^2(I;L^2(\Omega_{\text{ref}}))} \to 0$ if we assume $||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0$. Therefore we obtain

$$\begin{aligned}
||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \to 0 &\qquad \text{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0, \\
||\nabla \boldsymbol{e}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \to 0 &\qquad \text{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0.
\end{aligned}$$

□

Remark 4.1. *For $d = 2$ the constant C in* (4.33) *can be chosen to depend only on*

$$C = C(||p||_{L^2(I;L^2(\Omega_{ref}))}, ||\bar{p}||_{L^2(I;L^2(\Omega_{ref}))}, ||\boldsymbol{v}||_{L^3(I;\mathbf{H}^1_0(\Omega_{ref}))}, ||\boldsymbol{v}_t||_{L^2(I;\mathbf{L}^2(\Omega_{ref}))}).$$

This can be derived by using the estimates for b and $\tilde{b}$ in Lemma 4.2 for $d = 2$ in (4.24) *and* (4.31).

Using again the uniform boundedness stated in Lemma 4.15 we can derive stability estimates for $\boldsymbol{e}_t$ and e_p:

Lemma 4.17. *Let $d \in \{2, 3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solution of* (4.6) *for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ be the solution for arbitrary $\tau \in T_{ad}$. Writing $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ and $e_p := p - \bar{p}$ we have*

$$||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{ref}))} \to 0 \qquad \text{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0, \tag{4.34}$$

$$||e_p||_{L^2(I;L^2_0(\Omega_{ref}))} \to 0 \qquad \text{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0, \tag{4.35}$$

$$||\nabla e_p||_{L^2(I;\mathbf{H}^{-1}(\Omega_{ref}))} \to 0 \qquad \text{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0. \tag{4.36}$$

Proof. For the time derivative we will show that all other terms in (4.22) tend to zero as functionals w.r.t. $\boldsymbol{w} \in L^2(I; \mathbf{H}_0^1(\Omega_{\text{ref}}))$. For the right hand side we have

$$
\begin{aligned}
&\left|\int_I \int_{\Omega_{\text{ref}}} (\tilde{\boldsymbol{f}}(\tau(x),t)\det\tau' - \tilde{\boldsymbol{f}}(x,t))^T \boldsymbol{w}\ dx\ dt\right| \\
&\leq ||\tilde{\boldsymbol{f}}(\tau(\cdot),\cdot)\det\tau' - \tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}, \\
&\left|\int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{w}(g_1(\text{id}) - g_1(\tau))\ dx\ dt\right| \\
&\leq ||\boldsymbol{v}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||g_1(\text{id}) - g_1(\tau)||_{L^\infty(\Omega_{\text{ref}})}.
\end{aligned}
$$

Furthermore we get

$$
\begin{aligned}
&\left|\int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^d \nu\nabla v_i^T(g_2(\text{id}) - g_2(\tau))\nabla w_i\ dx\ dt\right| \\
&\leq C||\boldsymbol{v}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||g_2(\text{id}) - g_2(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}
\end{aligned}
$$

with a constant $C > 0$, where we use that for $\boldsymbol{a}, \boldsymbol{b} \in \mathbf{L}^2(\Omega_{\text{ref}}), T \in L^\infty(\Omega_{\text{ref}})^{d\times d}$ and a constant c we have

$$
\begin{aligned}
\left|\int_\Omega \boldsymbol{a}^T T \boldsymbol{b}\ dx\right| &= \left|\int_\Omega \sum_{i,j=1}^d \boldsymbol{a}_i T_{ij} \boldsymbol{b}_j\ dx\right| \\
&\leq \sum_{i,j=1}^d ||\boldsymbol{a}_i||_{L^2(\Omega)}||T_{ij}||_{L^\infty(\Omega)}||\boldsymbol{b}_j||_{L^2(\Omega)} \\
&\leq c \cdot ||\boldsymbol{a}||_{\mathbf{L}^2(\Omega)}||T||_{L^\infty(\Omega)^{d\times d}}||\boldsymbol{b}||_{\mathbf{L}^2(\Omega)}.
\end{aligned}
$$

For the term $\int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(g_3(\text{id}) - g_3(\tau))\nabla\boldsymbol{v}\boldsymbol{w}$ we can use Lemma 4.2 and Hölder's inequality to obtain

$$
\begin{aligned}
&\left|\int_I \tilde{b}(\boldsymbol{u},\boldsymbol{v},\boldsymbol{w},T)\ dt\right| \leq \\
&C||\boldsymbol{u}||_{L^4(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||\boldsymbol{v}||_{L^4(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||T||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}
\end{aligned}
$$

with a constant $C > 0$ and therefore

$$
\begin{aligned}
&\left|\int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(g_3(\text{id}) - g_3(\tau))\nabla\boldsymbol{v}\boldsymbol{w}\ dx\ dt\right| \\
&\leq C||\boldsymbol{v}||^2_{L^4(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}.
\end{aligned}
$$

For the last term on the right hand side we have

$$
\begin{aligned}
&\left|\int_I \int_{\Omega_{\text{ref}}} p\ \text{tr}\ ((g_3(\text{id}) - g_3(\tau))\nabla\boldsymbol{w})\ dx\ dt\right| \\
&\leq ||p||_{L^2(I;L^2(\Omega_{\text{ref}}))}||g_3(\text{id}) - g_3(\tau)||_{L^\infty(\Omega_{\text{ref}})^{d\times d}}||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}.
\end{aligned}
$$

We now estimate the other terms on the left hand side. We have

$$|\int_I \int_{\Omega_{\rm ref}} \sum_{i=1}^d \nu \nabla e_i^T \nabla w_i \; dx \; dt| \leq \nu ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}$$

and

$$\begin{aligned}
&|\int_I \int_{\Omega_{\rm ref}} (\boldsymbol{e}^T \nabla \boldsymbol{v} + \bar{\boldsymbol{v}}^T \nabla \boldsymbol{e}) \boldsymbol{w} \; dx \; dt \\
&\leq \tilde{c} \Big(||\boldsymbol{v}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} \\
&\qquad + ||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} \Big)
\end{aligned}$$

with a constant $\tilde{c} > 0$.
Hence, for $\tau \in T_{\rm ad}$ with $\|\tau - {\rm id}\|_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})}$ small enough we can estimate the term with the time derivative of the velocity by

$$\begin{aligned}
|\int_I \int_{\Omega_{\rm ref}} \boldsymbol{e}_t^T \boldsymbol{w} \; dx \; dt| \leq & c ||\boldsymbol{w}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} (||\tau - {\rm id}||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}) \\
& + ||p - \bar{p}||_{L^2(I;L^2(\Omega_{\rm ref}))} || \text{ tr } (\nabla \boldsymbol{w})||_{L^2(I;L^2(\Omega_{\rm ref}))} \\
& + ||\tilde{\boldsymbol{f}}(\tau(\cdot), \cdot) \det \tau' - \tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))} ||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))}
\end{aligned} \tag{4.37}$$

where

$$\begin{aligned}
c := c(&||\boldsymbol{v}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}, ||\boldsymbol{v}||^2_{L^4(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}, ||p||_{L^2(I;L^2(\Omega_{\rm ref}))}, \\
&||\boldsymbol{v}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))}, ||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\rm ref}))})
\end{aligned}$$

is a constant.
Because of Lemma 4.15 we know that $\boldsymbol{e}_t \in L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref})) \cap L^\infty(I;\mathbf{L}^2(\Omega_{\rm ref}))$ is uniformly bounded for $||\tau - {\rm id}||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})} \to 0$. Moreover, we have from the incompressibility condition

$$\text{tr } (\nabla \boldsymbol{e}) = \text{ tr } ((g_3({\rm id}) - g_3(\tau)) \nabla \boldsymbol{v})$$

and therefore with a constant $\bar{c}$

$$\begin{aligned}
|| \text{ tr } (\nabla \boldsymbol{e}_t)||_{L^2(I;L^2(\Omega_{\rm ref}))} &\leq || \text{ tr } ((g_3({\rm id}) - g_3(\tau)) \nabla \boldsymbol{v}_t)||_{L^2(I;L^2(\Omega_{\rm ref}))} \\
&\leq \bar{c} ||\boldsymbol{v}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||g_3({\rm id}) - g_3(\tau)||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})}.
\end{aligned}$$

Testing (4.37) with $\boldsymbol{w} = \boldsymbol{e}_t$ we arrive for $\tau \in T_{\rm ad}$ close to identity at

$$\begin{aligned}
||\boldsymbol{e}_t||^2_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))} \leq & c ||\boldsymbol{v}_t - \bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} (||\tau - {\rm id}||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}) \\
& + \bar{c} ||p - \bar{p}||_{L^2(I;L^2(\Omega_{\rm ref}))} ||\boldsymbol{v}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))} ||\tau - {\rm id}||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})} \\
& + ||\tilde{\boldsymbol{f}}(\tau(\cdot), \cdot) \det \tau' - \tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))} ||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))}
\end{aligned}$$

and thus

$$\begin{aligned}
&||\boldsymbol{e}_t||^2_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))} \\
\leq & \tilde{C} (||\tau - {\rm id}||_{\mathbf{W}^{1,\infty}(\Omega_{\rm ref})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\rm ref}))}) + ||\tilde{\boldsymbol{f}}(\tau(\cdot), \cdot) \det \tau' - \tilde{\boldsymbol{f}}||^2_{L^2(I;\mathbf{L}^2(\Omega_{\rm ref}))}
\end{aligned}$$

with another constant $\tilde{C} > 0$ depending on

$$\tilde{C}(\;||\boldsymbol{v}||_{L^\infty(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}, ||\boldsymbol{v}||^2_{L^4(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}, ||p||_{L^2(I;L^2(\Omega_{\text{ref}}))}, ||\bar{p}||_{L^2(I;L^2(\Omega_{\text{ref}}))},$$
$$||\boldsymbol{v}_t||_{L^2(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}, ||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}, ||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}).$$

Here, we have used that

$$\begin{aligned}&||\tilde{\boldsymbol{f}}(\tau(\cdot),\cdot)\det\tau' - \tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}\\ \leq&\frac{1}{2}||\tilde{\boldsymbol{f}}(\tau(\cdot),\cdot)\det\tau' - \tilde{\boldsymbol{f}}||^2_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))} + \frac{1}{2}||\boldsymbol{e}_t||^2_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}.\end{aligned}$$

Using the uniform boundedness of Lemma 4.15 we finally have shown

$$||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \to 0 \text{ as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0.$$

For the pressure term we get exactly as in (4.37) for $\tau \in T_{\text{ad}}$ close to identity and all $\boldsymbol{w} \in L^2(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))$

$$\begin{aligned}&|\int_I\int_{\Omega_{\text{ref}}} (p-\bar{p}) \text{ tr } (\nabla\boldsymbol{w})\; dx\; dt| = |\int_I\int_{\Omega_{\text{ref}}} -\nabla(p-\bar{p})^T\boldsymbol{w}\; dx\; dt|\\ &\leq c||\boldsymbol{w}||_{L^2(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))}(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}^1_0(\Omega_{\text{ref}}))})\\ &+ ||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}\\ &+ ||\tilde{\boldsymbol{f}}(\tau(\cdot),\cdot)\det\tau' - \tilde{\boldsymbol{f}}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}||\boldsymbol{w}||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))}.\end{aligned} \tag{4.38}$$

This shows

$$||\nabla e_p||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} \to 0 \text{ as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0.$$

By Proposition I.1.2 in [59] we have for all $t \in I$:

$$||e_p(t)||_{L^2_0(\Omega_{\text{ref}})} \leq c(\Omega_{\text{ref}})||\nabla e_p(t)||_{\mathbf{H}^{-1}(\Omega_{\text{ref}})}.$$

Hence we conclude that

$$||e_p||_{L^2(I;L^2_0(\Omega_{\text{ref}}))} \to 0 \text{ as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0.$$

□

Finally we can use interpolation theory to obtain the following lemma.

Lemma 4.18. *Let $d \in \{2,3\}$. Let $(\bar{\boldsymbol{v}},\bar{p})$ be the solution of (4.6) for $\tau = \text{id}$ and $(\boldsymbol{v},p)$ be the solution for arbitrary $\tau \in T_{ad}$. Writing $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ and $e_p := p - \bar{p}$ we have $\forall r \in [2,\infty), \forall s \in [2,6)$:*

$$||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^s(\Omega_{ref}))} \to 0 \qquad \textit{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0, \tag{4.39}$$
$$||\nabla\boldsymbol{e}||_{L^r(I;L^2(\Omega_{ref})^{d\times d})} \to 0 \qquad \textit{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0, \tag{4.40}$$
$$||\boldsymbol{e}||_{L^r(I;\mathbf{H}^1_0(\Omega_{ref}))} \to 0 \qquad \textit{as } ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0. \tag{4.41}$$

Proof. By Theorem 4.3 we know that we have $||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \to 0$ and $||\nabla \boldsymbol{e}||_{L^2(I;L^2(\Omega_{\text{ref}})^{d\times d})} \to 0$ for $||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0$. Moreover $||\boldsymbol{e}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}$ and $||\nabla \boldsymbol{e}||_{L^\infty(I;L^2(\Omega_{\text{ref}})^{d\times d})}$ are uniformly bounded for $||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0$ by Lemma 4.15.
Since $\mathbf{H}_0^1(\Omega_{\text{ref}}) \hookrightarrow \mathbf{L}^s(\Omega_{\text{ref}})$ for $d \in \{2,3\}$ and all $s \leq 6$ the first assertion follows by interpolation: In fact because $\mathbf{H}_0^1(\Omega_{\text{ref}}) \hookrightarrow \mathbf{L}^s(\Omega_{\text{ref}})$ we know that $||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^s(\Omega_{\text{ref}}))}$ is uniformly bounded for $||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})} \to 0$. Now for $s \in [2,6)$ define $\theta := \frac{6-s}{2s}$. Then obviously $\theta \in (0,1)$ and $\frac{1}{s} = \frac{\theta}{2} + \frac{1-\theta}{6}$. Now standard complex interpolation theory (see e.g. [60, Section 1.18]) yields the interpolation space $L^s(\Omega_{\text{ref}}) = [L^2(\Omega_{\text{ref}}), L^6(\Omega_{\text{ref}})]_\theta$ and for all $\boldsymbol{v} \in \mathbf{L}^6(\Omega_{\text{ref}})$ we have

$$||\boldsymbol{v}||_{\mathbf{L}^s(\Omega_{\text{ref}})} \leq C_\theta ||\boldsymbol{v}||^{1-\theta}_{\mathbf{L}^6(\Omega_{\text{ref}})} ||\boldsymbol{v}||^{\theta}_{\mathbf{L}^2(\Omega_{\text{ref}})}$$

with a constant C_θ. From this we directly obtain (4.39).
For the second assertion we again use interpoation. In detail let $r \in [2,\infty)$. We define $\theta := \frac{1}{r}, p_0 := 2, p_1 := 2r-2$. Then $\frac{1}{r} = \frac{\theta}{p_0} + \frac{1-\theta}{p_1}$. Using the complex interpolation method we obtain the interpolation space

$$L^r(I;L^2(\Omega_{\text{ref}})^{d\times d}) = [L^{p_0}(I;L^2(\Omega_{\text{ref}})^{d\times d}), L^{p_1}(I;L^2(\Omega_{\text{ref}})^{d\times d})]_\theta$$

and the estimate

$$\begin{aligned} ||\nabla \boldsymbol{e}||_{L^r(I;L^2(\Omega_{\text{ref}})^{d\times d})} &\leq c_1 ||\nabla \boldsymbol{e}||^{\theta}_{L^2(I;L^2(\Omega_{\text{ref}})^{d\times d})} ||\nabla \boldsymbol{e}||^{1-\theta}_{L^{2r-2}(I;L^2(\Omega_{\text{ref}})^{d\times d})} \\ &\leq c_2 ||\nabla \boldsymbol{e}||^{\theta}_{L^2(I;L^2(\Omega_{\text{ref}})^{d\times d})} ||\nabla \boldsymbol{e}||^{1-\theta}_{L^\infty(I;L^2(\Omega_{\text{ref}})^{d\times d})} \end{aligned}$$

with constants c_1, c_2. From this we obtain (4.40) and the last assertion (4.41) is a direct consequence. □

4.2.3 The Linearized Equation

Using the continuity results of the last section, we will now show the differentiability of $\tau \mapsto \boldsymbol{v}(\tau) \in W(I;\mathbf{H}_0^1(\Omega_{\text{ref}})) + W(I;V(\Omega_{\text{ref}}))$.
For this we will first show the solvability of the linearized equation and analyze the stability for the velocity part $\bar{\boldsymbol{e}}$ of this solution. This is done by eliminating the pressure terms and splitting $\bar{\boldsymbol{e}}$ into a solenoidal part and a remaining term. After transforming the state equation in a similar way in the following section, we will show that $\bar{\boldsymbol{e}}$ is the derivative $\boldsymbol{v}_\tau(\text{id})(\tau - \text{id})$ by estimating the residual terms. In context of shape optimization problems $v_\tau(\text{id})$ is called the material derivative (c.f. Section 3.1.3).
We consider the linearization of (4.6) about $(\bar{\boldsymbol{v}}, \bar{p}, \bar{\tau}) := (\boldsymbol{v}(\text{id}), p(\text{id}), \text{id})$ in

direction $(\hat{\boldsymbol{e}}, \hat{e}_p, \tau - \mathrm{id})$ for a.a. $t \in I$:

$$
\begin{aligned}
&\int_{\Omega_{\mathrm{ref}}} \hat{\boldsymbol{e}}_t(t)^T \boldsymbol{w}\, dx + \sum_{i=1}^{d} \int_{\Omega_{\mathrm{ref}}} \nu \nabla \hat{e}_i(t)^T \nabla w_i\, dx \\
&+ \int_{\Omega_{\mathrm{ref}}} (\hat{\boldsymbol{e}}(t)^T \nabla \bar{\boldsymbol{v}}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \hat{\boldsymbol{e}}(t)) \boldsymbol{w}\, dx - \int_{\Omega_{\mathrm{ref}}} \hat{e}_p(t) \text{ tr } (\nabla \boldsymbol{w})\, dx \\
&= - \int_{\Omega_{\mathrm{ref}}} \bar{\boldsymbol{v}}_t(t)^T \boldsymbol{w} g_1'(\mathrm{id})(\tau - \mathrm{id})\, dx - \sum_{i=1}^{d} \int_{\Omega_{\mathrm{ref}}} \nu \nabla \bar{v}_i(t)^T g_2'(\mathrm{id})(\tau - \mathrm{id}) \nabla w_i\, dx \\
&- \int_{\Omega_{\mathrm{ref}}} (\bar{\boldsymbol{v}}(t)^T g_3'(\mathrm{id})(\tau - \mathrm{id}) \nabla \bar{\boldsymbol{v}}(t)) \boldsymbol{w}\, dx + \int_{\Omega_{\mathrm{ref}}} \bar{p}(t) \text{ tr } (g_3'(\mathrm{id})(\tau - \mathrm{id}) \nabla \boldsymbol{w})\, dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{d}{d\tau} (\tilde{\boldsymbol{f}}(\tau(x), t)^T \det \tau')|_{\tau = \mathrm{id}} (\tau - \mathrm{id}) \boldsymbol{w}\, dx \quad \forall \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\mathrm{ref}}) \\
&\int_{\Omega_{\mathrm{ref}}} q \text{ tr } (\nabla \hat{\boldsymbol{e}}(t))\, dx = \int_{\Omega_{\mathrm{ref}}} q \text{ tr } (-g_3'(\mathrm{id})(\tau - \mathrm{id}) \nabla \bar{\boldsymbol{v}}(t))\, dx \quad \forall q \in L_0^2(\Omega_{\mathrm{ref}}), \\
&\hat{\boldsymbol{e}}(\cdot, 0) = \frac{d}{d\tau} (\tilde{\boldsymbol{v}}_0(\tau(\cdot)))|_{\tau = \mathrm{id}} (\tau - \mathrm{id}).
\end{aligned}
\tag{4.42}
$$

We show now that for $\tau \in T_{\mathrm{ad}}$ this equation has a solution $(\hat{\boldsymbol{e}}, \hat{e}_p)$ and we derive some regularity results for the velocity part $\hat{\boldsymbol{e}}$. To this end we use a splitting $\hat{\boldsymbol{e}} = \hat{\boldsymbol{e}}_0 + \hat{\boldsymbol{e}}_1$, where $\hat{\boldsymbol{e}}_1$ is divergence free on Ω_{ref}, and estimate $\hat{\boldsymbol{e}}_0$ and $\hat{\boldsymbol{e}}_1$ individually.
In a first step we will construct an $\hat{\boldsymbol{e}}_0$ such that $\hat{\boldsymbol{e}}_1 := \hat{\boldsymbol{e}} - \hat{\boldsymbol{e}}_0$ is solenoidal in Ω_{ref} and $\hat{\boldsymbol{e}}_0$ has good stability properties. For estimating $\hat{\boldsymbol{e}}_0$ we use again Lemma 4.13.

Lemma 4.19. *Let $d \in \{2, 3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solution of the Navier-Stokes equations* (3.44) *for $\Omega = \Omega_{ref}$. Furthermore let $\tau \in T_{ad}$. Then with the operator B defined in Lemma 4.13 and*

$$
\hat{\boldsymbol{e}}_0 := B(\ tr\ (-g_3'(\mathrm{id})(\tau - \mathrm{id}) \nabla \bar{\boldsymbol{v}})) \tag{4.43}
$$

we have

$$
\hat{\boldsymbol{e}}_0 \in C(I; \mathbf{H}_0^1(\Omega_{ref})), (\hat{\boldsymbol{e}}_0)_t \in L^2(I; \mathbf{L}^2(\Omega_{ref}))
$$

and there exists a constant $C > 0$ with

$$
\begin{aligned}
||\hat{\boldsymbol{e}}_0||_{L^2(I; \mathbf{H}_0^1(\Omega_{ref}))} &\le C ||\bar{\boldsymbol{v}}||_{L^2(I; \mathbf{H}_0^1(\Omega_{ref}))} ||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}, \\
||\hat{\boldsymbol{e}}_0||_{C(I; \mathbf{H}_0^1(\Omega_{ref}))} &\le C ||\bar{\boldsymbol{v}}||_{C(I; \mathbf{H}_0^1(\Omega_{ref}))} ||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}, \\
||(\hat{\boldsymbol{e}}_0)_t||_{L^2(I; \mathbf{L}^2(\Omega_{ref}))} &\le C ||\bar{\boldsymbol{v}}_t||_{L^2(I; \mathbf{H}_0^1(\Omega_{ref}))} ||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}.
\end{aligned}
$$

Proof. As $\bar{\boldsymbol{v}}$ vanishes on the boundary, we have by the definition of g_3

$$
\text{tr } (g_3(\mathrm{id}) \nabla \bar{\boldsymbol{v}}(t)) = \text{ tr } (\nabla \bar{\boldsymbol{v}}(t)) \in L_0^2(\Omega_{\mathrm{ref}})
$$

for all $t \in I$. Furthermore because of Lemma 3.12 for every $\tau \in T_{\text{ad}}$ we have $\bar{\boldsymbol{v}}(\tau^{-1}(\cdot), t) \in \mathbf{H}_0^1(\tau(\Omega_{\text{ref}}))$. Using the notation $\tilde{x} = \tau(x)$ we obtain for all $t \in I$

$$\begin{aligned}
\int_{\Omega_{\text{ref}}} \operatorname{tr}\,(g_3(\tau)\nabla_x \bar{\boldsymbol{v}}(x,t))\; dx &= \int_{\Omega_{\text{ref}}} \operatorname{tr}\,(\tau'^{-T}\nabla_x \bar{\boldsymbol{v}}(\tau^{-1}(\tau(x)),t)) \det \tau'\; dx \\
&= \int_{\tau(\Omega_{\text{ref}})} \operatorname{tr}\,(\tau'^{-T}\nabla_x \bar{\boldsymbol{v}}(\tau^{-1}(\tilde{x}),t)) \det(\tau^{-1})' \det \tau'\; d\tilde{x} \\
&= \int_{\tau(\Omega_{\text{ref}})} \operatorname{tr}\,(\nabla_{\tilde{x}} \bar{\boldsymbol{v}}(\tau^{-1}(\tilde{x}),t))\; d\tilde{x} \\
&= \int_{\partial\tau(\Omega_{\text{ref}})} \bar{\boldsymbol{v}}(\tau^{-1}(\tilde{x}),t)^T \tilde{n}\; d\tilde{S} = 0,
\end{aligned}$$

where we used $(\tau^{-1})' = \tau'^{-1}$ and $D_{\tilde{x}}\bar{\boldsymbol{v}}(\tau^{-1}(\tilde{x})) = D_x\bar{\boldsymbol{v}}(\tau^{-1}(\tilde{x}))(\tau^{-1})'$.
So we conclude that for a.a. $t \in I$ we have $\operatorname{tr}\,(g_3(\tau)\nabla\bar{\boldsymbol{v}}(t)) \in L_0^2(\Omega_{\text{ref}})$. Then because $\operatorname{tr}\,(g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}(t))$ is the limit of the corresponding difference quotients we also have $\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}(t)) \in L_0^2(\Omega_{\text{ref}})$.
Therefore by Lemma 4.13 there exists a unique $\hat{\boldsymbol{e}}_0 = B(\operatorname{tr}\,(-g_3'(\text{id})(\tau-\text{id})\nabla\bar{\boldsymbol{v}})) \in C(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))$. This is true because $B : L_0^2(\Omega) \to \mathbf{H}_0^1(\Omega)$ is linear and bounded and

$$||\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}})||_{C(I;L_0^2(\Omega_{\text{ref}}))} \le c_1||\bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}$$

for a constant $c_1 > 0$.
For the time derivative we know $\bar{\boldsymbol{v}}_t \in L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))$ and therefore

$$||\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}_t)||_{L^2(I;L^2(\Omega_{\text{ref}}))} \le C||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}.$$

Since bounded linear operators and integration are commutable we have

$$(B(\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}})))_t = B((\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}))_t).$$

In detail let $A : X \to Y$ be linear and bounded and $g_t \in L^p(I;X)$. By definition of the weak derivatives we have for all $\phi \in C_0^\infty(I;\mathbb{R})$

$$\int_I g_t(t)\phi(t)\; dt = -\int_I g(t)\phi'(t)\; dt$$

and because bounded linear operators and integration are commutable

$$\begin{aligned}
\int_I Ag_t(t)\phi(t)\; dt = A\left(\int_I g_t(t)\phi(t)\; dt\right) &= -A\left(\int_I g(t)\phi'(t)\; dt\right) \\
&= -\int_I Ag(t)\phi'(t)\; dt.
\end{aligned}$$

This shows $(Ag)_t = Ag_t \in L^p(I;Y)$. Therefore because B is a bounded linear operator from $L^2(\Omega_{\text{ref}}) \subset H^1(\Omega_{\text{ref}})^* = H_0^{-1}(\Omega_{\text{ref}})$ to $\mathbf{L}^2(\Omega_{\text{ref}})$ we have $B(\operatorname{tr}\,(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}_t)) \in L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))$ and

$$||(\hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))} \le C_2||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}$$

for a constant $C_2 > 0$. $\square$

Now let $\hat{\boldsymbol{e}}_1 := \hat{\boldsymbol{e}} - \hat{\boldsymbol{e}}_0$. By construction $\hat{\boldsymbol{e}}_1$ is solenoidal on Ω_{ref} because $\text{tr }(\nabla \hat{\boldsymbol{e}}_1) = \text{tr }(\nabla \hat{\boldsymbol{e}}) - \text{tr }(\nabla \hat{\boldsymbol{e}}_0) = 0$. To analyze the solvability of (4.42) we consider the resulting equation for $\hat{\boldsymbol{e}}_1$

$$\begin{aligned}
&\int_{\Omega_{\text{ref}}} (\hat{\boldsymbol{e}}_1(t))_t^T \boldsymbol{w}\, dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla (\hat{e}_1(t))_i^T \nabla w_i\, dx \\
&+ \int_{\Omega_{\text{ref}}} (\hat{\boldsymbol{e}}_1(t)^T \nabla \bar{\boldsymbol{v}}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \hat{\boldsymbol{e}}_1(t)) \boldsymbol{w}\, dx \\
&= \int_{\Omega_{\text{ref}}} \hat{\boldsymbol{g}}(t,x,\tau) \boldsymbol{w}\, dx - \int_{\Omega_{\text{ref}}} \bar{\boldsymbol{v}}_t(t)^T \boldsymbol{w} g_1'(\text{id})(\tau - \text{id})\, dx \\
&- \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla \bar{v}(t)_i^T g_2'(\text{id})(\tau - \text{id}) \nabla w_i\, dx \\
&- \int_{\Omega_{\text{ref}}} (\bar{\boldsymbol{v}}(t)^T g_3'(\text{id})(\tau - \text{id}) \nabla \bar{\boldsymbol{v}}(t)) \boldsymbol{w}\, dx + \int_{\Omega_{\text{ref}}} \bar{p}(t) \text{ tr } (g_3'(\text{id})(\tau - \text{id}) \nabla \boldsymbol{w})\, dx \\
&+ \int_{\Omega_{\text{ref}}} \frac{d}{d\tau} (\tilde{\boldsymbol{f}}(\tau(x),t)^T \det \tau')|_{\tau=\text{id}} (\tau - \text{id}) \boldsymbol{w}\, dx \quad \forall \boldsymbol{w} \in V(\Omega_{\text{ref}}), \\
&\int_{\Omega_{\text{ref}}} q \text{ tr } (\nabla \hat{\boldsymbol{e}}_1(t))\, dx = 0 \quad \forall q \in L_0^2(\Omega_{\text{ref}}), \\
&\hat{\boldsymbol{e}}_1(\cdot,0) = \frac{d}{d\tau} (\tilde{\boldsymbol{v}}_0(\tau(\cdot)))|_{\tau=\text{id}} (\tau - \text{id}) - \hat{\boldsymbol{e}}_0(\cdot,0)
\end{aligned} \tag{4.44}$$

for a.a. $t \in I$, where

$$\hat{\boldsymbol{g}}(t,x,\tau) := -(\hat{\boldsymbol{e}}_0)_t + \nu \Delta \hat{\boldsymbol{e}}_0 - \hat{\boldsymbol{e}}_0^T \nabla \bar{\boldsymbol{v}} - \bar{\boldsymbol{v}}^T \nabla \hat{\boldsymbol{e}}_0 \in L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}})). \tag{4.45}$$

The fact that $\hat{\boldsymbol{g}}(t,x,\tau) \in L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}}))$ follows from Lemma 4.19.
This equation has the form of the classical linearized Navier-Stokes equations, so we can use standard theory to show existence and regularity results for the solution $\hat{\boldsymbol{e}}_1$. From this and the regularity of $\hat{\boldsymbol{e}}_0$ we obtain regularity results for $\hat{\boldsymbol{e}}$.

Theorem 4.4. *Let $d \in \{2,3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solution of the Navier-Stokes equations* (3.44) *for $\Omega = \Omega_{ref}$ and $\tau \in T_{ad}$. Then the linearized equation* (4.42) *has for given $\tau \in T_{ad}$ a unique solution $\hat{\mathbf{e}}$ with*

$$||\hat{\boldsymbol{e}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))} + ||\hat{\boldsymbol{e}}||_{C(I;\mathbf{L}^2(\Omega_{ref}))} + ||\hat{\boldsymbol{e}}_t||_{L^2(I;V(\Omega_{ref})^*)} \le c||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})},$$

where $c > 0$ is a constant. Furthermore $\hat{\boldsymbol{e}} = \hat{\boldsymbol{e}}_0 + \hat{\boldsymbol{e}}_1$ and

$$\begin{aligned}
&||\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))} + ||(\hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{ref}))} = O(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}), \\
&||\hat{\boldsymbol{e}}_1||_{W(I;V(\Omega_{ref}))} = O(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}).
\end{aligned}$$

$\hat{e}_p$ can be introduced as a distribution on $\Omega_{ref} \times I$.

Proof. The right hand side of (4.44) can be written as $\langle \boldsymbol{h}(t), \boldsymbol{w} \rangle_{\mathbf{H}^{-1}(\Omega_{\text{ref}}), \mathbf{H}_0^1(\Omega_{\text{ref}})}$ with

$$||\boldsymbol{h}||_{L^2(I;H^{-1}(\Omega_{\text{ref}}))} \le c||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}$$

with $c = c(||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}, ||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}, ||\bar{p}||_{L^2(I;L_0^2(\Omega_{\text{ref}}))}) > 0$.
This is true because of Lemma 4.19 and Lemmas 4.16, 4.2.
Now standard theory on the linearized Navier-Stokes equations can be applied and yields a unique $\hat{\boldsymbol{e}}_1 \in W(I;V(\Omega_{\text{ref}}))$ with

$$||\hat{\boldsymbol{e}}_1||_{W(I;V(\Omega_{\text{ref}}))} \le c_1 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}$$

with a constant $c_1 > 0$. Using $W(I;V(\Omega_{\text{ref}})) \hookrightarrow C(I;H(\Omega_{\text{ref}}))$ this implies

$$\begin{aligned}
||\hat{\boldsymbol{e}}_1||_{L^2(I;V(\Omega_{\text{ref}}))} &\le c_2 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||\hat{\boldsymbol{e}}_1||_{C(I;\mathbf{L}^2(\Omega_{\text{ref}}))} &\le c_2 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||(\hat{\boldsymbol{e}}_1)_t||_{L^2(I;V(\Omega_{\text{ref}})^*)} &\le c_2 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}
\end{aligned}$$

with a constant $c_2 > 0$. Furthermore we have for $\hat{\boldsymbol{e}}_0 := B(\text{ tr }(-g_3'(\text{id})(\tau - \text{id})\nabla\bar{\boldsymbol{v}}))$ by Lemma 4.19

$$\begin{aligned}
||\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} &\le c_3 ||\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||\hat{\boldsymbol{e}}_0||_{C(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} &\le c_3 ||\bar{\boldsymbol{v}}||_{C(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||(\hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{\text{ref}}))} &\le c_3 ||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}
\end{aligned}$$

with a constant $c_3 > 0$ and since $\hat{\boldsymbol{e}} = \hat{\boldsymbol{e}}_0 + \hat{\boldsymbol{e}}_1$ we arrive at

$$\begin{aligned}
||\hat{\boldsymbol{e}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} &\le c_4 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||\hat{\boldsymbol{e}}||_{C(I;\mathbf{L}^2(\Omega_{\text{ref}}))} &\le c_4 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}, \\
||\hat{\boldsymbol{e}}_t||_{L^2(I;V(\Omega_{\text{ref}})^*)} &\le c_4 ||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}
\end{aligned}$$

with a constant $c_4 > 0$. The pressure $\hat{e}_p$ can now be introduced in a standard fashion in the sense of distributions, see e.g. [59, Section I.1.4]. □

4.2.4 Fréchet Differentiability of the Velocity

Clearly the velocity part $\hat{\boldsymbol{e}}$ of the solution of the linearized equation (4.42) is the candidate for the material derivative $\frac{d}{d\tau}\boldsymbol{v}(\tau)_{|\tau=\text{id}}$. Therefore we want to show that with

$$\boldsymbol{r} := \boldsymbol{v} - \bar{\boldsymbol{v}} - \hat{\boldsymbol{e}} \tag{4.46}$$

we have

$$||\boldsymbol{r}||_{W(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))+W(I;V(\Omega_{\text{ref}}))} = o(||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\text{ref}})}). \tag{4.47}$$

Then $\tau \mapsto v(\tau) \in W(I;\mathbf{H}_0^1(\Omega_{\text{ref}})) + W(I;V(\Omega_{\text{ref}}))$ is Fréchet differentiable in $\tau = \text{id}$. For this we will first derive an equation in terms of $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ similar as in (4.22) that has the form of the linearized equation while putting the remaining terms on the right hand side. Again we will split $\boldsymbol{e} = \boldsymbol{e}_0 + \boldsymbol{e}_1$, where $\boldsymbol{e}_1$ is solenoidal, and derive stability estimates for $\boldsymbol{e}_0$. From this we implicitly get a splitting

$$\boldsymbol{r} = \boldsymbol{r}_0 + \boldsymbol{r}_1 := \underbrace{(\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0)}_{=:r_0} + \underbrace{(\boldsymbol{e}_1 - \hat{\boldsymbol{e}}_1)}_{=:r_1}.$$

We will derive an equation that has the form of the standard linearized Navier-Stokes equations for $\boldsymbol{e}_1$ with different right hand side. Then we will subtract from this the equation (4.44) to get a linearized equation for $\boldsymbol{r}_1$. By estimating the right hand side we derive stability estimates for $\boldsymbol{r}_1$. Estimating $\boldsymbol{r}_0$ via estimating the difference $\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0$ we finally get the estimate (4.47).
Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solution of the Navier-Stokes equations on $\Omega = \Omega_{\text{ref}}$ and $(\boldsymbol{v}, p) := (\boldsymbol{v}(\tau), p(\tau))$ be the solution of (4.6) for arbitrary $\tau \in T_{\text{ad}}$. In a first step we will derive an equation for $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ by subtracting the corresponding equations (4.6) and rearranging the terms. We obtain a slightly different version of (4.22):

$$
\begin{aligned}
&\int_{\Omega_{\text{ref}}} \boldsymbol{e}_t(t)^T \boldsymbol{w}\ dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla e(t)_i^T \nabla w_i\ dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{e}(t)^T \nabla \bar{\boldsymbol{v}}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}(t)) \boldsymbol{w}\ dx - \int_{\Omega_{\text{ref}}} e_p(t) \text{ tr } (\nabla \boldsymbol{w})\ dx \\
&= \int_{\Omega_{\text{ref}}} (\tilde{\boldsymbol{f}}(\tau(x), t) \det \tau' - \tilde{\boldsymbol{f}}(x, t))^T \boldsymbol{w}\ dx \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t(t)^T \boldsymbol{w} (g_1(\text{id}) - g_1(\tau))\ dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla v(t)_i^T (g_2(\text{id}) - g_2(\tau)) \nabla w_i\ dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{v}(t)^T (g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t)) \boldsymbol{w}\ dx + \int_{\Omega_{\text{ref}}} (\boldsymbol{v} - \bar{\boldsymbol{v}})^T (\nabla \bar{\boldsymbol{v}} - \nabla \boldsymbol{v}) \boldsymbol{w}\ dx \\
&- \int_{\Omega_{\text{ref}}} p(t) (\text{ tr } ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{w}))\ dx \qquad \forall \boldsymbol{w} \in \mathbf{H}_0^1(\Omega_{\text{ref}}), \\
&\int_{\Omega_{\text{ref}}} q \text{ tr } (\nabla \boldsymbol{e}(t))\ dx = \int_{\Omega_{\text{ref}}} q (\text{ tr } ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t)))\ dx \qquad \forall q \in L_0^2(\Omega_{\text{ref}}), \\
&\boldsymbol{e}(\cdot, 0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0
\end{aligned}
\tag{4.48}
$$

for a.a. $t \in I$. Since $\boldsymbol{v}$ vanishes on the boundary, we have $\text{tr } (\nabla \boldsymbol{v}(t)) \in L_0^2(\Omega_{\text{ref}})$ and also

$$
\int_{\Omega_{\text{ref}}} \text{tr } (\tau'^{-T} \nabla \boldsymbol{v}(t)) \det \tau'\ dx = \int_{\tau(\Omega_{\text{ref}})} \text{tr } (\nabla_{\tilde{x}} \boldsymbol{v}(\tilde{x}, t))\ d\tilde{x} = 0
$$

and therefore in the same way as in the last subsection by Lemma 4.13 there exists a unique

$$
\begin{aligned}
\boldsymbol{e}_0 &:= B(\text{ tr } ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v})) \\
&= B(\text{ tr } (\nabla \boldsymbol{v}) - \text{ tr } (\tau'^{-T} \nabla \boldsymbol{v}) \det \tau') \in C(I; \mathbf{H}_0^1(\Omega_{\text{ref}}))
\end{aligned}
$$

with $(\boldsymbol{e}_0)_t \in L^2(I; \mathbf{L}^2(\Omega_{\text{ref}}))$.

Furthermore $\boldsymbol{e}_1 := \boldsymbol{e} - \boldsymbol{e}_0$ is divergence free on Ω_{ref} and satisfies for a.a. $t \in I$

$$
\begin{aligned}
&\int_{\Omega_{\text{ref}}} (\boldsymbol{e}_1(t))_t^T \boldsymbol{w}\ dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla e_1(t)_i^T \nabla w_i\ dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{e}_1(t)^T \nabla \bar{\boldsymbol{v}}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{e}_1(t)) \boldsymbol{w}\ dx \\
&= \int_{\Omega_{\text{ref}}} \boldsymbol{g}(t,x,\tau) \boldsymbol{w}\ dx + \int_{\Omega_{\text{ref}}} (\tilde{\boldsymbol{f}}(\tau(x),t) \det \tau' - \tilde{\boldsymbol{f}}(x,t))^T \boldsymbol{w}\ dx \\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t(t)^T \boldsymbol{w} (g_1(\text{id}) - g_1(\tau))\ dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu (\nabla v(t)_i^T (g_2(\text{id}) - g_2(\tau)) \nabla w_i\ dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{v}(t)^T (g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{v}(t)) \boldsymbol{w}\ dx + \int_{\Omega_{\text{ref}}} (\boldsymbol{v} - \bar{\boldsymbol{v}})^T (\nabla \bar{\boldsymbol{v}} - \nabla \boldsymbol{v}) \boldsymbol{w}\ dx \\
&- \int_{\Omega_{\text{ref}}} p(t) (\ \text{tr}\ ((g_3(\text{id}) - g_3(\tau)) \nabla \boldsymbol{w})\ dx \qquad \forall \boldsymbol{w} \in V(\Omega_{\text{ref}}), \\
&\int_{\Omega_{\text{ref}}} q\ \text{tr}\ (\nabla \boldsymbol{e}_1(t))\ dx = 0 \qquad \forall q \in L_0^2(\Omega_{\text{ref}}), \\
&\boldsymbol{e}_1(\cdot,0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0 - \boldsymbol{e}_0(\cdot,0)
\end{aligned}
\tag{4.49}
$$

with the additional term

$$
\boldsymbol{g}(t,x,\tau) := -(\boldsymbol{e}_0)_t + \nu \Delta \boldsymbol{e}_0 - \boldsymbol{e}_0^T \nabla \bar{\boldsymbol{v}} - \bar{\boldsymbol{v}}^T \nabla \boldsymbol{e}_0 \in L^2(I; \mathbf{H}^{-1}(\Omega_{\text{ref}})). \tag{4.50}
$$

We now have a splitting

$$
\boldsymbol{r} = \boldsymbol{r}_0 + \boldsymbol{r}_1 = (\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0) + (\boldsymbol{e}_1 - \hat{\boldsymbol{e}}_1) \tag{4.51}
$$

where $\boldsymbol{r}_1$ is solenoidal on Ω_{ref} and by subtracting (4.49) and (4.44) satisfies for a.a. $t \in I$

$$
\begin{aligned}
&\int_{\Omega_{\text{ref}}} (\boldsymbol{r}_1(t))_t^T \boldsymbol{w}\ dx + \sum_{i=1}^{d} \int_{\Omega_{\text{ref}}} \nu \nabla r_1(t)_i^T \nabla w_i\ dx \\
&+ \int_{\Omega_{\text{ref}}} (\boldsymbol{r}_1(t)^T \nabla \bar{\boldsymbol{v}}(t) + \bar{\boldsymbol{v}}(t)^T \nabla \boldsymbol{r}_1(t)) \boldsymbol{w}\ dx \\
&= \int_{\Omega_{\text{ref}}} (\boldsymbol{g}(t,x,\tau) - \hat{\boldsymbol{g}}(t,x,\tau)) \boldsymbol{w}\ dx \\
&- \int_{\Omega_{\text{ref}}} (R_1(\boldsymbol{w},t) + R_2(\boldsymbol{w},t) + R_3(\boldsymbol{w},t) + R_4(\boldsymbol{w},t) + R_5(\boldsymbol{w},t))\ dx\ \forall \boldsymbol{w} \in V(\Omega_{\text{ref}}), \\
&\int_{\Omega_{\text{ref}}} q\ \text{tr}\ (\nabla \boldsymbol{r}_1(t))\ dx = 0 \qquad \forall q \in L_0^2(\Omega_{\text{ref}}), \\
&\boldsymbol{r}_1(\cdot,0) = \tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0 + \hat{\boldsymbol{e}}_0(\cdot,0) - \boldsymbol{e}_0(\cdot,0) - \frac{d}{d\tau}(\tilde{\boldsymbol{v}}_0(\tau(\cdot)))|_{\tau=\text{id}}(\tau - \text{id}),
\end{aligned}
\tag{4.52}
$$

where

$$
\begin{aligned}
R_1(\boldsymbol{w},t) :=& -(\tilde{\boldsymbol{f}}(\tau(x),t)\det\tau' - \tilde{\boldsymbol{f}}(x,t) - (\frac{d}{d\tau}\tilde{\boldsymbol{f}}(\tau(x),t)^T\det\tau')_{|\tau=\mathrm{id}}(\tau-\mathrm{id})),\\
R_2(\boldsymbol{w},t) :=& \boldsymbol{v}_t(t)^T\boldsymbol{w}(g_1(\tau)-g_1(\mathrm{id})) - \bar{\boldsymbol{v}}_t(t)^T\boldsymbol{w}g_1'(\mathrm{id})(\tau-\mathrm{id})\\
=& \bar{\boldsymbol{v}}_t(t)^T(g_1(\tau)-g_1(\mathrm{id})-g_1'(\mathrm{id})(\tau-\mathrm{id}))\boldsymbol{w}\\
&+(\boldsymbol{v}_t(t)-\bar{\boldsymbol{v}}_t(t))^T(g_1(\tau)-1)\boldsymbol{w},\\
R_3(\boldsymbol{w},t) :=& \sum_{i=1}^d \nu\nabla v(t)_i^T(g_2(\tau)-g_2(\mathrm{id}))\nabla w_i - \sum_{i=1}^d \nu(\nabla\bar{v}(t)_i^T g_2'(\mathrm{id})(\tau-\mathrm{id})\nabla w_i\\
=& \sum_{i=1}^d \nu\nabla\bar{v}(t)_i^T(g_2(\tau)-g_2(\mathrm{id})-g_2'(\mathrm{id})(\tau-\mathrm{id}))\nabla w_i\\
&+\sum_{i=1}^d \nu(\nabla v(t)_i-\nabla\bar{v}(t)_i)^T(g_2(\tau)-g_2(\mathrm{id}))\nabla w_i,\\
R_4(\boldsymbol{w},t) :=& \big(\boldsymbol{v}(t)^T(g_3(\tau)-g_3(\mathrm{id}))\nabla\boldsymbol{v}(t) + (\bar{\boldsymbol{v}}(t)-\boldsymbol{v}(t))^T(\nabla\bar{\boldsymbol{v}}(t)-\nabla\boldsymbol{v}(t))\big)\,\boldsymbol{w}\\
&-\big(\bar{\boldsymbol{v}}(t)^T g_3'(\mathrm{id})(\tau-\mathrm{id})\nabla\bar{\boldsymbol{v}}(t)\big)\,\boldsymbol{w}\\
=& \big(\bar{\boldsymbol{v}}(t)^T(g_3(\tau)-g_3(\mathrm{id})-g_3'(\mathrm{id})(\tau-\mathrm{id}))\nabla\bar{\boldsymbol{v}}(t)\\
&+(\boldsymbol{v}(t)-\bar{\boldsymbol{v}}(t))^T(g_3(\tau)-g_3(\mathrm{id}))\nabla\bar{\boldsymbol{v}}(t)\\
&+\boldsymbol{v}(t)^T(g_3(\tau)-g_3(\mathrm{id}))(\nabla\boldsymbol{v}(t)-\nabla\bar{\boldsymbol{v}}(t))\\
&+(\bar{\boldsymbol{v}}(t)-\boldsymbol{v}(t))^T(\nabla\bar{\boldsymbol{v}}(t)-\nabla\boldsymbol{v}(t))\big)\,\boldsymbol{w},\\
R_5(\boldsymbol{w},t) :=& -p(t)(\ \mathrm{tr}\ ((g_3(\tau)-g_3(\mathrm{id}))\nabla\boldsymbol{w})) + \bar{p}(t)\ \mathrm{tr}\ (g_3'(id)(\tau-\mathrm{id})\nabla\boldsymbol{w})\\
=& -\bar{p}(t)\,\big(\ \mathrm{tr}\ (g_3(\tau)\nabla\boldsymbol{w}) -\ \mathrm{tr}\ (g_3(\mathrm{id})\nabla\boldsymbol{w}) -\ \mathrm{tr}\ (g_3'(id)(\tau-\mathrm{id})\nabla\boldsymbol{w})\big)\\
&+(\bar{p}(t)-p(t))\,(\ \mathrm{tr}\ (g_3(\tau)\nabla\boldsymbol{w}) -\ \mathrm{tr}\ (g_3(\mathrm{id})\nabla\boldsymbol{w}))\,.
\end{aligned}
\tag{4.53}
$$

First we estimate $\boldsymbol{r}_0 = \boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0$. We have

Lemma 4.20. *Let $d \in \{2,3\}$. Let $(\bar{\boldsymbol{v}},\bar{p})$ be the solutions of (4.6) for $\tau = \mathrm{id}$ and $(\boldsymbol{v},p)$ the solutions for arbitrary $\tau \in T_{ad}$. With*

$$
\begin{aligned}
\boldsymbol{e}_0 &:= B(\ tr\ ((g_3(\mathrm{id})-g_3(\tau))\nabla\boldsymbol{v})) = B(\ tr\ (\nabla\boldsymbol{v}) -\ tr\ (\tau'^{-T}\nabla\boldsymbol{v})\det\tau'),\\
\hat{\boldsymbol{e}}_0 &:= B(\ tr\ (-g_3'(\mathrm{id})(\tau-\mathrm{id})\nabla\bar{\boldsymbol{v}}))
\end{aligned}
$$

we have $\forall r \in [2,\infty)$

$$
\begin{aligned}
||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||_{L^r(I;\mathbf{H}_0^1(\Omega_{ref}))} &= o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}),\\
||(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{ref}))} &= o(||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})})
\end{aligned}
$$

for $||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})} \to 0$ and $||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})} \to 0$.

Proof. We have

$$
\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0 = B(\ \mathrm{tr}\ (\nabla\boldsymbol{v}) -\ \mathrm{tr}\ (\tau'^{-T}\nabla\boldsymbol{v})\det\tau' -\ \mathrm{tr}\ (-g_3'(\mathrm{id})(\tau-\mathrm{id})\nabla\bar{\boldsymbol{v}}))
$$

and

$$
\begin{aligned}
&||\ \mathrm{tr}\ (\nabla \boldsymbol{v}) -\ \mathrm{tr}\ (\tau'^{-T}\nabla \boldsymbol{v}) \det \tau' -\ \mathrm{tr}\ (-g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}})||_{L^r(I;L^2_0(\Omega_{\mathrm{ref}}))}\\
=&||\ \mathrm{tr}\ (g_3(\mathrm{id})\nabla \boldsymbol{v} - g_3(\tau)\nabla \boldsymbol{v} + g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}})||_{L^r(I;L^2_0(\Omega_{\mathrm{ref}}))}\\
\leq&||\ \mathrm{tr}\ (g_3(\mathrm{id})\nabla \bar{\boldsymbol{v}} - g_3(\tau)\nabla \bar{\boldsymbol{v}} + g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}})||_{L^r(I;L^2_0(\Omega_{\mathrm{ref}}))}\\
&+ ||\ \mathrm{tr}\ ((g_3(\mathrm{id}) - g_3(\tau))(\nabla \boldsymbol{v} - \nabla \bar{\boldsymbol{v}}))||_{L^r(I;L^2_0(\Omega_{\mathrm{ref}}))}\\
=&o(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})||\nabla \bar{\boldsymbol{v}}||_{L^r(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}\\
&+ ||g_3(\mathrm{id}) - g_3(\tau)||_{L^\infty(\Omega_{\mathrm{ref}})^{d\times d}}||\nabla \boldsymbol{v} - \nabla \bar{\boldsymbol{v}}||_{L^r(I;L^2(\Omega_{\mathrm{ref}})^{d\times d})}.
\end{aligned}
$$

Since $||g_3(\mathrm{id}) - g_3(\tau)||_{L^\infty(\Omega_{\mathrm{ref}})^{d\times d}} = O(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})$ and furthermore $||\nabla \boldsymbol{v} - \nabla \bar{\boldsymbol{v}}||_{L^r(I;L^2(\Omega_{\mathrm{ref}})^{d\times d})} \to 0$ for $||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})} \to 0$ by Lemma 4.18 we conclude

$$
||\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0||_{L^r(I;\mathbf{H}^1_0(\Omega_{\mathrm{ref}}))} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})
$$

For the time derivative we have

$$
(\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0)_t = B(\ \mathrm{tr}\ (\nabla \boldsymbol{v}_t) -\ \mathrm{tr}\ (\tau'^{-T}\nabla \boldsymbol{v}_t) \det \tau' -\ \mathrm{tr}\ (-g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}}_t)).
$$

Since $\boldsymbol{e}$ vanishes on the boundary of Ω_{ref}, we have for all $t \in I$

$$
\langle \boldsymbol{w}, \nabla \boldsymbol{e}_t(t)\rangle_{\mathbf{H}^1(\Omega_{\mathrm{ref}}),\mathbf{H}^1(\Omega_{\mathrm{ref}})^*} = -(\nabla \boldsymbol{w}, \boldsymbol{e}_t(t))_{\mathbf{L}^2(\Omega_{\mathrm{ref}})} \leq ||\boldsymbol{w}||_{\mathbf{H}^1(\Omega_{\mathrm{ref}})}||\boldsymbol{e}_t(t)||_{\mathbf{L}^2(\Omega_{\mathrm{ref}})} \tag{4.54}
$$

and we conclude $||\nabla \boldsymbol{e}_t||_{L^2(I;\mathbf{H}^1(\Omega_{\mathrm{ref}})^*)} \leq ||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}$. Using this, $\mathbf{L}^2(\Omega_{\mathrm{ref}}) \hookrightarrow \mathbf{H}^1(\Omega_{\mathrm{ref}})^*$ and Lemma 4.8 we obtain

$$
\begin{aligned}
&||\ \mathrm{tr}\ (\nabla \boldsymbol{v}_t) -\ \mathrm{tr}\ (\tau'^{-T}\nabla \boldsymbol{v}_t) \det \tau' -\ \mathrm{tr}\ (-g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}}_t)||_{L^2(I;H^1(\Omega_{\mathrm{ref}})^*)}\\
=&||\ \mathrm{tr}\ (g_3(\mathrm{id})\nabla \bar{\boldsymbol{v}}_t - g_3(\tau)\nabla \bar{\boldsymbol{v}}_t + g_3'(\mathrm{id})(\tau - \mathrm{id})\nabla \bar{\boldsymbol{v}}_t + (g_3(\mathrm{id}) - g_3(\tau))\nabla \boldsymbol{e}_t)||_{L^2(I;H^1(\Omega_{\mathrm{ref}})^*)}\\
=&o(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{H}^1_0(\Omega_{\mathrm{ref}}))}\\
&+ ||g_3(\mathrm{id}) - g_3(\tau)||_{W^{1,\infty}(\Omega_{\mathrm{ref}})^{d\times d}}||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}\\
=&o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})})
\end{aligned} \tag{4.55}
$$

for $||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})} \to 0$ where we used Lemma 4.17 in the last step. By Lemma 4.17 and Lemma 4.13 we obtain

$$
||(\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})}).
$$

□

Now we have to estimate $\int_{\Omega_{\mathrm{ref}}}(\boldsymbol{g}(t,x,\tau) - \hat{\boldsymbol{g}}(t,x,\tau))\boldsymbol{w}\ dx$ and the remainder terms $R_1(\boldsymbol{w},t), \ldots, R_5(\boldsymbol{w},t)$ defined in (4.53).

Lemma 4.21. *Let $d \in \{2,3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of* (4.6) *for $\tau = \mathrm{id}$ and $(\boldsymbol{v}, p)$ the solutions for arbitrary $\tau \in T_{ad}$. Let $\mathbf{e}_0$ and $\hat{\mathbf{e}}_0$ be as in Lemma 4.20. With*

$$
\begin{aligned}
\boldsymbol{g}(t,x,\tau) &:= -(\boldsymbol{e}_0)_t + \nu\Delta \boldsymbol{e}_0 - \boldsymbol{e}_0^T\nabla \bar{\boldsymbol{v}} - \bar{\boldsymbol{v}}^T\nabla \boldsymbol{e}_0,\\
\hat{\boldsymbol{g}}(t,x,\tau) &:= -(\hat{\boldsymbol{e}}_0)_t + \nu\Delta \hat{\boldsymbol{e}}_0 - \hat{\boldsymbol{e}}_0^T\nabla \bar{\boldsymbol{v}} - \bar{\boldsymbol{v}}^T\nabla \hat{\boldsymbol{e}}_0
\end{aligned}
$$

we have

$$||\boldsymbol{g}(t,x,\tau)-\hat{\boldsymbol{g}}(t,x,\tau)||_{L^2(I;\mathbf{H}^{-1}(\Omega_{ref}))}=o(||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})})$$

for $||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})}\to 0$

Proof. We have

$$\boldsymbol{g}(t,x,\tau)-\hat{\boldsymbol{g}}(t,x,\tau)=-(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)_t+\nu\Delta(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)-(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)^T\nabla\bar{\boldsymbol{v}}-\bar{\boldsymbol{v}}^T\nabla(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0). \tag{4.56}$$

We estimate each term individually. For the first term we get

$$||(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}=o(||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})})$$

directly because $\mathbf{L}^2(\Omega_{\mathrm{ref}})\hookrightarrow\mathbf{H}^{-1}(\Omega_{\mathrm{ref}})$ and Lemma 4.20. For the second term we have

$$\begin{aligned}||\nu\Delta(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}&=||\nu\nabla(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0):\nabla(\cdot)||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}\\&\le\nu||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}\end{aligned}$$

and use again Lemma 4.20. For the third term we have

$$\begin{aligned}||(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)^T\nabla\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}&\le c_1||(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)^T\nabla\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{L}^{4/3}(\Omega_{\mathrm{ref}}))}\\&=\left(c_1\int_I||(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)^T\nabla\bar{\boldsymbol{v}}||^2_{\mathbf{L}^{4/3}(\Omega_{\mathrm{ref}})}\,dt\right)^{1/2}\\&\le\left(c_2\int_I||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||^2_{\mathbf{L}^4(\Omega_{\mathrm{ref}})}||\nabla\bar{\boldsymbol{v}}||^2_{L^2(\Omega_{\mathrm{ref}})^{d\times d}}\,dt\right)^{1/2}\\&\le c_3||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{L}^4(\Omega_{\mathrm{ref}}))}||\nabla\bar{\boldsymbol{v}}||_{L^\infty(I;L^2(\Omega_{\mathrm{ref}})^{d\times d})}\\&\le c_4||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}\\&=o(||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})})\end{aligned}$$

with constants $c_1,\dots,c_4>0$ because $\mathbf{H}_0^1(\Omega_{\mathrm{ref}})\hookrightarrow\mathbf{L}^4(\Omega_{\mathrm{ref}})$ and therefore $\mathbf{L}^{4/3}(\Omega_{\mathrm{ref}})=\mathbf{L}^4(\Omega_{\mathrm{ref}})^*\hookrightarrow\mathbf{H}^{-1}(\Omega_{\mathrm{ref}})$. Finally we have used again Lemma 4.20. For the last term we have in a similar way

$$\begin{aligned}||\bar{\boldsymbol{v}}^T\nabla(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}&\le c_5||\bar{\boldsymbol{v}}^T\nabla(\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0)||_{L^2(I;\mathbf{L}^{4/3}(\Omega_{\mathrm{ref}}))}\\&\le c_6||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}||\boldsymbol{e}_0-\hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}\\&=o(||\tau-\mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})})\end{aligned}$$

with constants $c_5,c_6>0$. □

Finally we estimate the norms of the remainder terms $R_1(\boldsymbol{w},t),\dots,R_5(\boldsymbol{w},t)$.

Lemma 4.22. *Let* $d\in\{2,3\}$. *Let* $(\bar{\boldsymbol{v}},\bar{p})$ *be the solutions of* (4.6) *for* $\tau=\mathrm{id}$ *and* $(\boldsymbol{v},p)$ *the solutions for arbitrary* $\tau\in T_{ad}$. *Then*

$$\sum_{i=1}^5 R_i(\boldsymbol{w},t)=o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}+||\boldsymbol{v}-\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))})$$

for $||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{ref})}+||\boldsymbol{v}-\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{ref}))}\to 0$ *with* $R_i(\boldsymbol{w},t)$ *as defined in* (4.53).

Proof. Let again $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ and $e_p := p - \bar{p}$. For R_1 we have

$$\begin{aligned}&||R_1||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\=&||\tilde{\boldsymbol{f}}(\tau(x),t)\det\tau' - \tilde{\boldsymbol{f}}(x,t) - (\frac{d}{d\tau}\tilde{\boldsymbol{f}}(\tau(x),t)^T\det\tau')_{|\tau=\mathrm{id}}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}.\end{aligned}$$

Because of the regularity of $\tilde{\boldsymbol{f}}$ in (N3) we have

$$\begin{aligned}&||\tilde{\boldsymbol{f}}(\tau(x),t)\det\tau' - \tilde{\boldsymbol{f}}(x,t) - (\frac{d}{d\tau}\tilde{\boldsymbol{f}}(\tau(x),t)^T\det\tau')_{|\tau=\mathrm{id}}(\tau-\mathrm{id})||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\=&o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})}).\end{aligned}$$

For R_2 we obtain

$$\begin{aligned}&||R_2||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\=&||\bar{\boldsymbol{v}}_t(g_1(\tau)-g_1(\mathrm{id})-g_1'(\mathrm{id})(\tau-\mathrm{id})) + (\boldsymbol{v}_t-\bar{\boldsymbol{v}}_t)(g_1(\tau)-1)||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\\le&||\bar{\boldsymbol{v}}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\\&+||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))}O(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})}) = o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\end{aligned}$$

where we used that $||\boldsymbol{e}_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))} \to 0$ for $||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})} \to 0$ by Lemma 4.17. For R_3 we have

$$\begin{aligned}&||R_3||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\\le&||\sum_{i=1}^{d}\nu\nabla\bar{v}(t)_i^T(g_2(\tau)-g_2(\mathrm{id})-g_2'(\mathrm{id})(\tau-\mathrm{id}))\nabla(\cdot)_i||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\+&||\sum_{i=1}^{d}\nu(\nabla v(t)_i-\nabla\bar{v}(t)_i)^T(g_2(\tau)-g_2(\mathrm{id}))\nabla(\cdot)_i||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\\le&||\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})}) + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}O(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\\=&o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\end{aligned}$$

where $||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))} \to 0$ for $||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})} \to 0$ by Lemma 4.18. For R_4 we have

$$\begin{aligned}||R_4||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))} \le\ & ||\bar{\boldsymbol{v}}^T(g_3(\tau)-g_3(\mathrm{id})-g_3'(\mathrm{id})(\tau-\mathrm{id}))\nabla\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\&+||(\boldsymbol{v}-\bar{\boldsymbol{v}})^T(g_3(\tau)-g_3(\mathrm{id}))\nabla\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\&+||\boldsymbol{v}^T(g_3(\tau)-g_3(\mathrm{id}))(\nabla\boldsymbol{v}-\nabla\bar{\boldsymbol{v}})||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\&+||(\boldsymbol{v}-\bar{\boldsymbol{v}})^T(\nabla\boldsymbol{v}-\nabla\bar{\boldsymbol{v}})||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\mathrm{ref}}))}\\\le\ & ||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}||\bar{\boldsymbol{v}}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\\&+||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}||\bar{\boldsymbol{v}}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}O(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\\&+||\boldsymbol{v}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}O(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})\\&+||\boldsymbol{e}||_{L^\infty(I;\mathbf{L}^4(\Omega_{\mathrm{ref}}))}||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}\\=&o(||\tau-\mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))})\end{aligned}$$

where we used that for $\boldsymbol{a} \in L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}})), \boldsymbol{b} \in L^\infty(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))$ and $C \in L^\infty(\Omega_{\text{ref}})^{d\times d}$ we have

$$\begin{aligned}
||\boldsymbol{a}^T C\nabla \boldsymbol{b}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} &= \left(c_1 \int_I ||\boldsymbol{a}^T C\nabla \boldsymbol{b}||^2_{\mathbf{L}^{4/3}(\Omega_{\text{ref}})} \, dt\right)^{\frac{1}{2}} \\
&\leq \left(c_2 \int_I ||\boldsymbol{a}||^2_{\mathbf{L}^4(\Omega_{\text{ref}})} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{b}||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} \, dt\right)^{\frac{1}{2}} \\
&\leq c_3 ||\boldsymbol{a}||_{L^2(I;\mathbf{L}^4(\Omega_{\text{ref}}))} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{b}||_{L^\infty(I;L^2(\Omega_{\text{ref}})^{d\times d})} \\
&\leq c_4 ||\boldsymbol{a}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\boldsymbol{b}||_{L^\infty(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}
\end{aligned}$$

or in a similar way for $\boldsymbol{a} \in L^\infty(I;\mathbf{L}^4(\Omega_{\text{ref}})), \boldsymbol{b} \in L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))$ and $C \in L^\infty(\Omega_{\text{ref}})^{d\times d}$

$$\begin{aligned}
||\boldsymbol{a}^T C\nabla \boldsymbol{b}||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} &= \left(c_1 \int_I ||\boldsymbol{a}^T C\nabla \boldsymbol{b}||^2_{\mathbf{L}^{4/3}(\Omega_{\text{ref}})} \, dt\right)^{\frac{1}{2}} \\
&\leq \left(c_2 \int_I ||\boldsymbol{a}||^2_{\mathbf{L}^4(\Omega_{\text{ref}})} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{b}||^2_{L^2(\Omega_{\text{ref}})^{d\times d}} \, dt\right)^{\frac{1}{2}} \\
&\leq c_3 ||\boldsymbol{a}||_{L^\infty(I;\mathbf{L}^4(\Omega_{\text{ref}}))} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\nabla \boldsymbol{b}||_{L^2(I;L^2(\Omega_{\text{ref}})^{d\times d})} \\
&\leq c_4 ||\boldsymbol{a}||_{L^\infty(I;\mathbf{L}^4(\Omega_{\text{ref}}))} ||C||_{\mathbf{L}^\infty(\Omega_{\text{ref}})^{d\times d}} ||\boldsymbol{b}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\text{ref}}))}
\end{aligned}$$

with appropriate constants $c_1, \ldots, c_4 > 0$ respectively. In both estimates we used that $H_0^1(\Omega_{\text{ref}}) \hookrightarrow L^4(\Omega_{\text{ref}})$ for $d \in \{2, 3\}$. For R_5 we obtain

$$\begin{aligned}
&||R_5||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} \\
\leq &|| -\bar{p}(t)(\text{ tr } (g_3(\tau)\nabla(\cdot)) - \text{ tr } (g_3(\text{id})\nabla(\cdot)) - \text{ tr } (g_3'(id)(\tau - \text{id})\nabla(\cdot)))||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} \\
&+ ||(\bar{p}(t) - p(t))(\text{ tr } (g_3(\tau)\nabla(\cdot)) - \text{ tr } (g_3(\text{id})\nabla(\cdot)))||_{L^2(I;\mathbf{H}^{-1}(\Omega_{\text{ref}}))} \\
\leq &||\bar{p}||_{L^2(I;L^2(\Omega_{\text{ref}}))} o(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}) + ||e_p||_{L^2(I;L^2(\Omega_{\text{ref}}))} O(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}) \\
= &o(||\tau - \text{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\text{ref}})}).
\end{aligned}$$

□

Now we can proof the following theorem which is a main result of this thesis.

Theorem 4.5. *Let $d \in \{2, 3\}$. Let $(\bar{\boldsymbol{v}}, \bar{p})$ be the solutions of* (4.6) *for $\tau = \text{id}$ and $(\boldsymbol{v}, p)$ the solutions for arbitrary $\tau \in T_{ad}$. Let $\boldsymbol{e} := \boldsymbol{v} - \bar{\boldsymbol{v}}$ and $\hat{\boldsymbol{e}}$ be the solution of* (4.42). *Then*

$$\begin{aligned}
&||\boldsymbol{r}||_{W(I;\mathbf{H}_0^1(\Omega_{ref}))+W(I;V(\Omega_{ref}))} = \\
&||\boldsymbol{e} - \hat{\boldsymbol{e}}||_{W(I;\mathbf{H}_0^1(\Omega_{ref}))+W(I;V(\Omega_{ref}))} = o(||\tau - \text{id}||_{\mathbf{W}^{2,\infty}(\Omega_{ref})}).
\end{aligned}$$

This shows that $\tau \mapsto \boldsymbol{v}(\tau) \in W(I;\mathbf{H}_0^1(\Omega_{ref})) + W(I;V(\Omega_{ref}))$ is Fréchet differentiable at $\tau = \text{id}$.

Proof. Let $\boldsymbol{r} = \boldsymbol{e} - \hat{\boldsymbol{e}} = (\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0) + (\boldsymbol{e}_1 - \hat{\boldsymbol{e}}_1)$ as before. Using Lemma 4.20 we have

$$\begin{aligned} ||\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))} &= o(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})}), \\ ||(\boldsymbol{e}_0 - \hat{\boldsymbol{e}}_0)_t||_{L^2(I;\mathbf{L}^2(\Omega_{\mathrm{ref}}))} &= o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})}). \end{aligned}$$

Because of Lemma 4.21 and 4.22 the right hand side h of (4.52) can be estimated as

$$||h||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})} + ||\boldsymbol{e}||_{L^2(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))}).$$

Furthermore for the initial value $\boldsymbol{r}_1(\cdot, 0)$ we have

$$\begin{aligned} &||\boldsymbol{r}_1(\cdot,0)||_{\mathbf{H}_0^1(\Omega_{\mathrm{ref}})} \\ &= ||\tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0 + \hat{\boldsymbol{e}}_0(\cdot,0) - \boldsymbol{e}_0(\cdot,0) - \frac{d}{d\tau}(\tilde{\boldsymbol{v}}_0(\tau(\cdot)))|_{\tau=\mathrm{id}}(\tau - \mathrm{id})||_{\mathbf{H}_0^1(\Omega_{\mathrm{ref}})} \\ &= o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})}). \end{aligned}$$

In fact by the regularity of $\tilde{\boldsymbol{v}}_0$ we have

$$||\tilde{\boldsymbol{v}}_0(\tau(\cdot)) - \tilde{\boldsymbol{v}}_0 - \frac{d}{d\tau}(\tilde{\boldsymbol{v}}_0(\tau(\cdot)))|_{\tau=\mathrm{id}}(\tau - \mathrm{id})||_{\mathbf{H}_0^1(\Omega_{\mathrm{ref}})} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{1,\infty}(\Omega_{\mathrm{ref}})})$$

and we can also show that

$$||\hat{\boldsymbol{e}}_0(\cdot,0) - \boldsymbol{e}_0(\cdot,0)||_{\mathbf{H}_0^1(\Omega_{\mathrm{ref}})} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})})$$

where we use nearly the same proof as in Lemma 4.20 but for $t = 0$.
Therefore by the theory of the standard linearized Navier-Stokes equations we obtain

$$\begin{aligned} ||\boldsymbol{e}_1 - \hat{\boldsymbol{e}}_1||_{L^2(I;V(\Omega_{\mathrm{ref}}))} &= o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})} + ||\boldsymbol{e}||_{L^2(I;V(\Omega_{\mathrm{ref}}))}), \\ ||(\boldsymbol{e}_1 - \hat{\boldsymbol{e}}_1)_t||_{L^2(I;V(\Omega_{\mathrm{ref}})^*)} &= o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})} + ||\boldsymbol{e}||_{L^2(I;V(\Omega_{\mathrm{ref}}))}). \end{aligned}$$

Taking both results together we have

$$||\boldsymbol{e} - \hat{\boldsymbol{e}}||_{W(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))+W(I;V(\Omega_{\mathrm{ref}}))} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})} + ||\boldsymbol{e}||_{L^2(I;V(\Omega_{\mathrm{ref}}))}).$$

From this we directly obtain

$$||\boldsymbol{e} - \hat{\boldsymbol{e}}||_{W(I;\mathbf{H}_0^1(\Omega_{\mathrm{ref}}))+W(I;V(\Omega_{\mathrm{ref}}))} = o(||\tau - \mathrm{id}||_{\mathbf{W}^{2,\infty}(\Omega_{\mathrm{ref}})}).$$

$\square$

5 Design Parametrization and Implementation Aspects

In this section we describe different design parametrizations and link them to the shape derivative calculation approach developed in Section 3.3. Furthermore, we show how shape derivatives with respect to shape parameters can be evaluated efficiently using an adjoint elasticity approach. Finally, we discuss relevant implementation aspects such as mesh deformation and the discretization of the Navier-Stokes equations which we use for the numerical results in Chapter 6.

5.1 Design Parametrization

The shape optimization approach of Chapter 3 gives us a large amount of flexibility in modelling the design space. Usually the boundary design of one or more objects B is modeled by a parametrization of the admissible shapes. We distinguish two basic parametrizations of the object boundary Γ_B:

- Class $\mathcal{A}$: Direct Parametrization of the boundary curve/surface
- Class $\mathcal{B}$: Indirect parametrization of the boundary (e.g. via forces on the boundary)

Many parametrizations fit into one of these two categories, with the majority of them falling into the first class $\mathcal{A}$, e.g.

- Use of boundary nodal coordinates as parameters
- Use of polynomials to describe/approximate the boundary design (e.g. B-spline curves/surfaces, Bezier curves)

In the shape optimization approach in function spaces (see Chapter 3) a design is represented by a domain vector field as a deformation of a reference domain Ω_{ref}. To use this framework we have to show how the parametrization classes can be linked to the shape optimization approach.
Note that introducing parametrizations of the design and introducing a shape parameter space U could also ensure more regularity for the associated transformations. Furthermore, if U is a Hilbert space, we can also introduce a shape gradient on U such that we can use optimization steps of the type

$$u^{k+1} = u^k + \alpha \nabla \bar{j}(u) \in U$$

or Quasi-Newton steps based on the gradient.

5.1.1 Obtaining the Domain Vector Field for a Parametrization

As already described in Section 3.3.3, the shape derivative for a current design can be calculated on the physical domain $\Omega = \tau(\Omega_{\text{ref}})$. For this approach the Navier-Stokes equations and the adjoint Navier-Stokes system are computed on Ω. Finally the shape derivative $\langle j'(\tau), V \rangle_{S^*,S}$ in direction of a displacement vector field $V \in S$ is evaluated. Here, for the state and adjoint solve the concrete representation of $\tau \in T_{\text{ad}}$ is not needed, since the solves are done on the physical domain. However, for the evaluation of $j'(\tau)$ we need the concrete relation between U and S, i.e. the map

$$u \in U \mapsto V \in S.$$

5.1.1.1 Obtaining the domain vector field for the parametization class $\mathcal{A}$. In the first category above the parametrization provides a description of the boundary curve (in 2D) or boundary surface (in 3D) of the design object in a natural way. If we use the boundary nodal coordinates as parameters, we obtain directly the points on the object boundary. In the case of polynomials, that describe (parts of) the boundary, we often get the boundary points in a simple map, usually using a curve or a surface parameter. To obtain a domain vector field as a displacement of the reference domain we can first calculate a boundary vector field (or a discretization of it): In 2D a boundary vector field is calculated by subtracting the boundary curve of the actual object from the boundary curve of the reference object. In 3D we can do the same by subtracting the corresponding boundary points. Here the curve or surface parameter plays an important role. Finally we get a (discrete) boundary vector field on the boundary $\Gamma_B \subset \partial\Omega_{\text{ref}}$, where Γ_B is the boundary of the reference object B_{ref}. Furthermore, for many parametrizations the map from the design space to the boundary curve is linear or affine such that the map

$$u \in U \xrightarrow{A} V_{\text{bdry}} \in S(\Gamma_B) \tag{5.1}$$

is also linear or affine (e.g. B-Spline curves/surfaces and Bezier curves/surfaces where the coefficients of the polynomials are the design variables). Here $u \in U_{\text{ad}} \subset U \subset \mathbb{R}^n$ is a design vector and $V_{\text{bdry}} \in S(\Gamma_B)$ is a boundary vector field with respect to the boundary of a reference object.
Finally we transport the boundary displacement to the whole domain Ω_{ref} by using a linear elliptic PDE as described in Section 3.1.12. In our numerical tests we will use a linear elasticity equation (see Section 5.3 for details). Finally we arrive at the following chain

$$u \in U \xrightarrow{A} V_{\text{bdry}} \in S(\Gamma_B) \xrightarrow{B} V \in S \tag{5.2}$$

where S describes the space of domain vector fields defined on the reference domain.

5.1.1.2 Obtaining the domain vector field for the parametization class $\mathcal{B}$. The second parametrization category is structural different from the other parametrizations. Instead of a direct parametrization of the boundary, we have an indirect influence on the boundary curve/surface. For example in the *pseudo-solid approach*, that will be described in detail in Section 5.1.3, forces on the boundary of a reference object are used to describe other designs. This means that we do not have a direct map (5.1) as in many parametrizations of category $\mathcal{A}$. For example, in the pseudo-solid approach the domain displacement is calculated in one step by solving a linear elasticity equation, i.e. we have a map

$$u \in U \xrightarrow{C} V \in S.$$

From this we obtain the boundary vector field $V_{\text{bdry}} = V_{|\Gamma_B}$ and the boundary curve/surface directly. However, in the pseudo-solid approach the map $u \mapsto V_{\text{bdry}}$ involves the solution of a partial differential equation to map the boundary forces to a boundary displacement. On the other hand no additional PDE is needed to transport the domain vector field into the domain.
For 2D problems, another parametrization that fits into class $\mathcal{B}$ is to use the curvature of the boundary curve as parameters. One advantage of this approach is that usually no big boundary oscillations occur during the shape optimization process. For details of this approach see e.g. [33]. However, there is again no simple evaluation of the boundary curve.
One disadvantage of these parametrizations is that usually the constraints in the optimization depend on the boundary curve of the object. In this case additional nonlinearities can be introduced and the evaluation of the constraints and constraint derivatives with respect to changes in the design space U can be more difficult (for the pseudo-solid approach C includes the solution of a PDE).
In the case of a linear, simple evaluation of the map (5.1) and its derivatives, the constraints and constraint derivatives can often be calculated faster.
In the following sections we will discuss the choice of the parametrization in 2D, i.e. the design space U and how the map A can be realized there.

5.1.2 Direct Parametrizations of the Boundary Curve

In parts of our numerical results we use B-splines to parametrize the boundary curve in 2D. Typical other parametrizations with polynomials in 2D are *four-point curves*, *Bezier curves* or *spline curves*. The advantages of using polynomials for the design parametrization are on the one hand the smaller number of design variables and on the other hand the guarantee for smooth boundaries and smooth boundary displacements. To avoid oscillating boundaries higher-order polynomials are usually avoided to desribe the boundary. In contrast a spline is a composition of low-order polynomial segments to maximize the smoothness of the boundaries. A good overview about these parametrizations can be found in [12, Chapter 12] and [42].
In this work we will focus on B-spline parametrizations in 2D and describe how typical constraints in shape optimization problems can be evaluated efficiently. These concepts can be extended to the other parametrizations.

5.1.2.1 B-Spline parametrization in 2D. In our application in Chapter 6 the object in the flow can be interpreted as a closed curve. We analyze two concrete possibilities of modeling this closed curve using B-Splines.
The first one is to use a closed B-Spline curve. Given n_{cp} B-spline control points $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{n_{cp}-1}$ we obtain n_{cp} B-spline segments and using for each segment a cubic polynomial we arrive at the following formula for a parametrization of

the segments (see also [42, Section 5.4]):

$$\begin{aligned}\boldsymbol{q}_i(t) =& \frac{1}{6}(t^3\ t^2\ t\ 1)\begin{pmatrix} -1 & 3 & -3 & 1 \\ 3 & -6 & 3 & 0 \\ -3 & 0 & 3 & 0 \\ 1 & 4 & 1 & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{p}_{(i-1) \bmod n_{cp}} \\ \boldsymbol{p}_{i \bmod n_{cp}} \\ \boldsymbol{p}_{(i+1) \bmod n_{cp}} \\ \boldsymbol{p}_{(i+2) \bmod n_{cp}} \end{pmatrix} \\ =& \frac{1}{6}(\ \ t^3(-\boldsymbol{p}_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}_{i \bmod n_{cp}} - 3\boldsymbol{p}_{(i+1) \bmod n_{cp}} + \boldsymbol{p}_{(i+2) \bmod n_{cp}}) \\ & + t^2(3\boldsymbol{p}_{(i-1) \bmod n_{cp}} - 6\boldsymbol{p}_{i \bmod n_{cp}} + 3\boldsymbol{p}_{(i+1) \bmod n_{cp}}) \\ & + t(-3\boldsymbol{p}_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}_{(i+1) \bmod n_{cp}}) \\ & + (\boldsymbol{p}_{(i-1) \bmod n_{cp}} + 4\boldsymbol{p}_{i \bmod n_{cp}} + \boldsymbol{p}_{(i+1) \bmod n_{cp}}))\end{aligned}$$

for $i = 1, \dots, n_{cp}$. We use here a short notation for the matrix product: The last vector is interpreted as a (4×1)-matrix, such that with $\boldsymbol{p}_i \in \mathbb{R}^d$ we also have $\boldsymbol{q}_i(t) \in \mathbb{R}^d$.
Here $\boldsymbol{q}_i(t)$ describes the B-Spline curve in segement i and parametrizes the curve by a parameter $t \in [0, 1]$. We have $\boldsymbol{q}_i(1) = \boldsymbol{q}_{i+1}(0)$ for $i = 1, \dots, n_{cp} - 1$ and $\boldsymbol{q}_{n_{cp}}(1) = \boldsymbol{q}_0(0)$ such that we have a closed B-Spline curve.
This parametrization also allows self-intersecting curves which can be avoided by introducing constraints on the B-spline control points.
One important characteristic of the cubic B-spline curves is that $\mathcal{C}^2$ continuity across the curve is naturally reached, without any artificial design variable linking. On the other hand the closed B-spline curve thus cannot represent apices at the front or the end. This is a strong limitation of the design space. In theory one can model apices by choosing two or more identical B-spline control points. For a piecewise cubic curve, a double control point defines a joint point with curvature discontinuity. A corner point in the curve is obtained by a triple control point. In the latter case the segments at each side of the joint point are straight lines [42, Section 5.1]. If two or more (nearly) identical control points are used the corresponding spline segment shrinks to one point. Depending on the discretization of the spline segments this may induce irregular domain discretizations and has to be considered in the model.
An alternative is to use a connection of two or more B-splines to model the object. This is the approach that we will use in the following. For example we can use one upper and one lower B-spline curve which are bonded at the front and the end of the object. This allows also for corner points at the end or front. For the B-spline we use the following parametrization of piecewise cubic polynomials: Given n_{cp} B-spline control points $\boldsymbol{p}_0, \dots, \boldsymbol{p}_{n_{cp}-1}$ we obtain $(n_{cp} - 3)$ B-spline segments parametrized by

$$\begin{aligned}\boldsymbol{q}_i(t) =& \frac{1}{6}(t^3\ t^2\ t\ 1)\begin{pmatrix} -1 & 3 & -3 & 1 \\ 3 & -6 & 3 & 0 \\ -3 & 0 & 3 & 0 \\ 1 & 4 & 1 & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{p}_{i-1} \\ \boldsymbol{p}_{i} \\ \boldsymbol{p}_{i+1} \\ \boldsymbol{p}_{i+2} \end{pmatrix} \\ =& \frac{1}{6}(\ \ t^3(-\boldsymbol{p}_{i-1} + 3\boldsymbol{p}_i - 3\boldsymbol{p}_{i+1} + \boldsymbol{p}_{i+2}) + t^2(3\boldsymbol{p}_{i-1} - 6\boldsymbol{p}_i + 3\boldsymbol{p}_{i+1}) \\ & + t(-3\boldsymbol{p}_{i-1} + 3\boldsymbol{p}_{i+1}) + (\boldsymbol{p}_{i-1} + 4\boldsymbol{p}_i + \boldsymbol{p}_{i+1}))\end{aligned}$$

for $i = 1, \ldots, n_{cp} - 3$. Again $\boldsymbol{q}_i(t)$ describes the B-Spline curve in segment i and is parametrized by a parameter $t \in [0, 1]$.
In practice for the discretization of the boundary curve we consider a partition $\mathcal{T} := \{t_1 = 0, t_2, \ldots, t_m = 1\}$ of the interval $[0, 1]$ and take the discrete points $\boldsymbol{q}_i(t_1), \ldots, \boldsymbol{q}_i(t_m)$ for each B-spline segment i as boundary nodes.
In the setting of the parametrization chain (5.2) we split up the operator A into two operators A_1 and A_2. Introducing the set of admissible B-spline control points P we have

$$u \in U \xrightarrow{A_1} \{\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{n_{cp}-1}\} \in P \xrightarrow{A_2} V_{\text{bdry}} \in S(\Gamma_B). \tag{5.3}$$

Often the B-spline control points depend linearly on a set of design variables. In this case A_1 is an affine function. As the functions $\boldsymbol{q}_i$ depend linearly on the B-spline control points (for both the closed and non-closed B-spline curves) the corresponding boundary vector field depends also linearly on the control points such that A_2 is affine, too.
Another advantage of the B-spline parametrization is that local control of the curve shape is possible since changes in control point locations do not cause global shape changes. The control points influence only a few of the nearby curve segments. In contrast in classical Hermite or Bézier curve parametrizations a global propagation of local change appears, i.e. that local changes tend to strongly propagate throughout the entire curve.

5.1.2.2 Boundary nodal coordinates as parameters This parametrization approach is very simple and easy to use. The design space U consists of the coordinates of the boundary nodal points which describe a discretization of the boundary Γ_B of an object B. The discrete version of map A in (5.2) is thus easily defined as $A^d : u \mapsto V^d_{\text{bdry}}$ where $A^d(u) : (u_{\text{ref}}) \mapsto (u - u_{\text{ref}}) \in \mathbb{R}^{n_d}$. Here u_{ref} is the discretization of the boundary Γ_B, i.e. the boundary nodal coordinates of the reference object. More precisely $A^d(u)$ is the displacement field defined on the discretization u_{ref} of Γ_B, i.e. a discretization of V_{bdry}.
Furthermore, it allows very flexible transformations of the design object without many restrictions on the model.
On the other hand, the number of design variables tends to become very large. In this context it is important that the adjoint approach for calculating the shape derivatives in function space described in Section 3.1.12 is extended to the parametrization process. It is not reasonable to calculate the shape sensitivities for each design parameter individually by calculating the corresponding domain vector field and using formula (3.63). For a detailed description of the calculation of derivatives with respect to design variables see Section 5.4. Using this approach the large number of design variables is no drawback in the calculation of the derivatives. However, the number of optimization variables increases and the corresponding optimization problems could be more difficult to solve.
The main drawback is that the first derivative of the design boundary is not smooth across the boundary. The shape derivative cannot be interpreted as a gradient with respect to the standard euclidian inner product. This often

results in huge oscillations of the boundary curve and computational difficulties if no smoothing of the derivative or regularization is used. Another possibility to overcome this problem is to apply the correct inner product using the so called *symbol* of the Navier-Stokes operator. For details of this approach we refer, e.g., to [52].

5.1.3 Indirect Parametrizations: The Pseudo-solid Approach

The pseudo-solid approach goes back to Lynch and coworkers [38]. The idea is to use boundary forces on a reference boundary object to describe different designs. Usually the boundary forces at a boundary point $x \in \Gamma_B$ are given by $c(x)n(x)$, where $c(x)$ is a real number and $n(x)$ denotes the unit outer normal vector to the boundary curve. c can be interpreted as a control such that a push or a pull is applied to the reference boundary point x. The domain displacement field for a given boundary force $c : \Gamma_B \to \mathbb{R}$ is given by

$$\begin{aligned} \text{div } \sigma(V) &= 0 && \text{in } \Omega_{\text{ref}}, \\ \partial_n V &= c && \text{on } \Gamma_B, \\ V &= 0 && \text{on } \partial\Omega_{\text{ref}} \setminus \Gamma_B, \end{aligned} \tag{5.4}$$

where $\sigma : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is the Cauchy stress tensor

$$\sigma(\boldsymbol{u}) := \lambda \text{ tr } (\varepsilon(\boldsymbol{u}))I + 2\mu\varepsilon(\boldsymbol{u}),$$

and where $\lambda \in \mathbb{R}$ and $\mu \in \mathbb{R}$ are the Lamé constants, I is the identity matrix and $\varepsilon : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is the strain tensor

$$\varepsilon(\boldsymbol{u}) := \frac{1}{2}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T).$$

Another equivalent formulation of the first equation in (5.4) is

$$(\lambda + \mu)(\nabla \text{ div } u)^T + \mu\Delta u = 0. \tag{5.5}$$

The domain displacement field V includes the boundary displacement field $V_{\text{bdry}} = V_{|\Gamma_B}$.
However, depending on the reference object, sometimes the normal field n on the reference boundary may not be available or difficult to calculate. In this case one could also take the ansatz of a free vector field for the boundary forces. However, in the numerical tests we made the experience that a free vector field also allows for more flexibility in the object design. As we have more degrees of freedom in this case a regularization could be needed.

5.2 Constraints

As in many shape optimization problems we have constraints on the object, e.g. a volume constraint or design constraints, we also have to analyze how to calculate them using the concrete design parametrization. We investigate the cases where the parametrizations are given by B-Splines or a polygon approximating the boundary. Furthermore, we discuss the special case when the parametrization is given by the pseudo-solid approach.

However, if we use a triangulation of the domain to discretize the PDE, the boundary of the object B is finally a polygon. Therefore all parametrizations that give us a discretization of the boundary curve, can be interpreted as parametrizations of a polygon.
We now discuss some common constraints in shape optimization. In this section we assume that the shape of only one object B is optimized. Of course, in the case of two or more objects, the constraints can be applied for each object individually.

5.2.1 Volume

The area of a closed curve can be calculated via the Leibnitz' sector formula (see e.g. [34, Section 12.5]). In fact let $\gamma : [a,b] \to \mathbb{R}^2$ be a piecewise continuously differentiable closed curve without intersections. Then the oriented area volume A can be calculated via

$$V = \frac{1}{2}\int_a^b (\gamma_x(t)\gamma_y'(t) - \gamma_y(t)\gamma_x'(t))\; dt \tag{5.6}$$

where γ_x' and γ_y' are piecewise continuous functions such that γ_x and γ_y are a primitive of them.
In case of a closed B-spline the area can be calculated via

$$V = \frac{1}{2}\sum_{i=1}^{n_{cp}}\int_0^1 (\boldsymbol{q}_i^x(t)(\boldsymbol{q}_i')^y(t) - \boldsymbol{q}_i^y(t)(\boldsymbol{q}_i')^x(t)\; dt$$

where $\boldsymbol{q}_i^x$ and $\boldsymbol{q}_i^y$ denote the x- and y-component of $\boldsymbol{q}_i$. We define (c.f. Section 5.1.2.1):

$$\begin{aligned}
\alpha_3^i &:= (-\boldsymbol{p}^x_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}^x_{i \bmod n_{cp}} - 3\boldsymbol{p}^x_{(i+1) \bmod n_{cp}} + \boldsymbol{p}^x_{(i+2) \bmod n_{cp}}),\\
\alpha_2^i &:= (3\boldsymbol{p}^x_{(i-1) \bmod n_{cp}} - 6\boldsymbol{p}^x_{i \bmod n_{cp}} + 3\boldsymbol{p}^x_{(i+1) \bmod n_{cp}}),\\
\alpha_1^i &:= (-3\boldsymbol{p}^x_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}^x_{(i+1) \bmod n_{cp}}),\\
\alpha_0^i &:= (\boldsymbol{p}^x_{(i-1) \bmod n_{cp}} + 4\boldsymbol{p}^x_{i \bmod n_{cp}} + \boldsymbol{p}^x_{(i+1) \bmod n_{cp}}),\\
\beta_3^i &:= (-\boldsymbol{p}^y_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}^y_{i \bmod n_{cp}} - 3\boldsymbol{p}^y_{(i+1) \bmod n_{cp}} + \boldsymbol{p}^y_{(i+2) \bmod n_{cp}}),\\
\beta_2^i &:= (3\boldsymbol{p}^y_{(i-1) \bmod n_{cp}} - 6\boldsymbol{p}^y_{i \bmod n_{cp}} + 3\boldsymbol{p}^y_{(i+1) \bmod n_{cp}}),\\
\beta_1^i &:= (-3\boldsymbol{p}^y_{(i-1) \bmod n_{cp}} + 3\boldsymbol{p}^y_{(i+1) \bmod n_{cp}}),\\
\beta_0^i &:= (\boldsymbol{p}^y_{(i-1) \bmod n_{cp}} + 4\boldsymbol{p}^y_{i \bmod n_{cp}} + \boldsymbol{p}^y_{(i+1) \bmod n_{cp}}).
\end{aligned} \tag{5.7}$$

Using this notation we can give an explicit formula for V depending only on the control points:

$$\begin{aligned}
V = \frac{1}{72}\sum_{i=1}^{n_{cp}}\Big(&\frac{1}{5}(\alpha_2^i\beta_3^i - \beta_2^i\alpha_3^i) + \frac{1}{2}(\alpha_1^i\beta_3^i - \beta_1^i\alpha_3^i) + \frac{1}{3}(\alpha_1^i\beta_2^i - \beta_1^i\alpha_2^i)\\
&+ (\alpha_0^i\beta_3^i - \beta_0^i\alpha_3^i) + (\alpha_0^i\beta_2^i - \beta_0^i\alpha_2^i) + (\alpha_0^i\beta_1^i - \beta_0^i\alpha_1^i)\Big).
\end{aligned}$$

If the object is parametrized by two B-splines that are linked together at the front and end, we can use a similar formula. Let $\bar{\boldsymbol{p}}_0, \ldots, \bar{\boldsymbol{p}}_{\bar{n}_{cp}-1}$ denote the $\bar{n}_{cp}$ control points for the first B-spline and $\tilde{\boldsymbol{p}}_0, \ldots, \tilde{\boldsymbol{p}}_{\tilde{n}_{cp}-1}$ the $\tilde{n}_{cp}$ control points for the second B-spline. Furthermore, the rank order of the control points should guarantee that the last B-spline segment $\bar{\boldsymbol{q}}_{\bar{n}_{cp}-3}$ of the first B-spline is followed by the first segment $\tilde{\boldsymbol{q}}_1$ of the second one such that $\bar{\boldsymbol{q}}_{\bar{n}_{cp}-3}(1) = \tilde{\boldsymbol{q}}_1(0)$. Then we can use the Leibnitz' sector formula (5.6): If we define for each B-spline $\bar{\alpha}_i^j, \tilde{\alpha}_i^j, \bar{\beta}_i^j$ and $\tilde{\beta}_i^j$ in the same way as α_i^j, β_i^j above and omit the 'mod n_{cp}'-terms in the indices we obtain:

$$
\begin{aligned}
V = \frac{1}{72} \sum_{i=1}^{n_{cp}^1-3} \Big(& \frac{1}{5}(\bar{\alpha}_2^i \bar{\beta}_3^i - \bar{\beta}_2^i \bar{\alpha}_3^i) + \frac{1}{2}(\bar{\alpha}_1^i \bar{\beta}_3^i - \bar{\beta}_1^i \bar{\alpha}_3^i) + \frac{1}{3}(\bar{\alpha}_1^i \bar{\beta}_2^i - \bar{\beta}_1^i \bar{\alpha}_2^i) \\
& + (\bar{\alpha}_0^i \bar{\beta}_3^i - \bar{\beta}_0^i \bar{\alpha}_3^i) + (\bar{\alpha}_0^i \bar{\beta}_2^i - \bar{\beta}_0^i \bar{\alpha}_2^i) + (\bar{\alpha}_0^i \bar{\beta}_1^i - \bar{\beta}_0^i \bar{\alpha}_1^i) \Big) \\
+ \frac{1}{72} \sum_{i=1}^{n_{cp}^i-3} \Big(& \frac{1}{5}(\tilde{\alpha}_2^i \tilde{\beta}_3^i - \tilde{\beta}_2^i \tilde{\alpha}_3^i) + \frac{1}{2}(\tilde{\alpha}_1^i \tilde{\beta}_3^i - \tilde{\beta}_1^i \tilde{\alpha}_3^i) + \frac{1}{3}(\tilde{\alpha}_1^i \tilde{\beta}_2^i - \tilde{\beta}_1^i \tilde{\alpha}_2^i) \\
& + (\tilde{\alpha}_0^i \tilde{\beta}_3^i - \tilde{\beta}_0^i \tilde{\alpha}_3^i) + (\tilde{\alpha}_0^i \tilde{\beta}_2^i - \tilde{\beta}_0^i \tilde{\alpha}_2^i) + (\tilde{\alpha}_0^i \tilde{\beta}_1^i - \tilde{\beta}_0^i \tilde{\alpha}_1^i) \Big).
\end{aligned}
\tag{5.8}
$$

This approach can be extended directly to more than two connected B-splines. We remark that the volume formulas do not depend linearly on the control points. Hence, for calculating derivatives of V with respect to the control points, we have to differentiate (5.8) with respect to $\boldsymbol{p}_i$ using the formulas in (5.7).

Alternatively, we could calculate the area of the discretized object using the polygon defined by the boundary nodes. Again one can use (5.6) to calculate the volume by introducing a parametrization of each section between two boundary points $\boldsymbol{p}_i$ and $\boldsymbol{p}_{i+1}$ like $\boldsymbol{q}_i(t) := (1-t)\boldsymbol{p}_i + t\boldsymbol{p}_{i+1}$. Another approach would be to sum the oriented sector areas between the vectors $\boldsymbol{p}_i$ and $\boldsymbol{p}_{i+1}$. Both approaches yield the following result: Let $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{n_b-1}$ be the n_b boundary points of the object. Then the area of the induced polygon is

$$
V = \frac{1}{2} \left(\sum_{i=0}^{n_b-2} (\boldsymbol{p}_{i+1}^y \boldsymbol{p}_i^x - \boldsymbol{p}_{i+1}^x \boldsymbol{p}_i^y) + (\boldsymbol{p}_0^y \boldsymbol{p}_{n_b-1}^x - \boldsymbol{p}_0^x \boldsymbol{p}_{n_b-1}^y) \right). \tag{5.9}
$$

The last approach can also be used for all parametrizations where the boundary nodes are explicitly known. Again the derivatives with respect to $\boldsymbol{p}_i$ are obtained easily.

5.2.2 Center of Mass

Another common constraint in shape optimization problems is to fix the center of mass of the object.

The center of mass $x \in \mathbb{R}^d$ of a set M with positive volume V in dimension d is given by [34]:

$$
x_i^M := \frac{1}{V} \int_M x_i \, dx, \quad i = 1, \ldots, d.
$$

Using Green's theorem x_i^M can also be calculated as a curve integral over the boundary curve. In fact, for $\boldsymbol{w}(x_1, x_2) := (0, \frac{1}{2}x_1^2)$ we have

$$x_1^M := \frac{1}{V}\int_M x_1 \, dx = \frac{1}{V}\int_M \partial_1 w_2 - \partial_2 w_1 \, dx = \int_\gamma \boldsymbol{w} \cdot \, dx,$$

where γ is the closed boundary curve. A similar formula can be derived for x_2^M if we set $\boldsymbol{w}(x_1, x_2) := (\frac{1}{2}x_2^2, 0)$.
For a polygon the formula can be further simplified. This can be done by evaluating the formula for the boundary curve segments $\boldsymbol{q}_i(t)$ as defined in the last subsection. In fact, let $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{n_b-1}$ be the n_b boundary points of the object and $\mathcal{P}$ be the corresponding, closed, non-intersecting polygon. Then the center of mass $(c_x, c_y)^T \in \mathbb{R}^2$ of $\mathcal{P}$ is given by

$$c_x = \frac{1}{6A}\left(\sum_{i=0}^{n_b-2}(\boldsymbol{p}_i^x + \boldsymbol{p}_{i+1}^x)(\boldsymbol{p}_i^x\boldsymbol{p}_{i+1}^y - \boldsymbol{p}_{i+1}^x\boldsymbol{p}_i^y) + (\boldsymbol{p}_{n_b-1}^x + \boldsymbol{p}_0^x)(\boldsymbol{p}_{n_b-1}^x\boldsymbol{p}_0^y - \boldsymbol{p}_0^x\boldsymbol{p}_{n_b-1}^y)\right)$$
$$c_y = \frac{1}{6A}\left(\sum_{i=0}^{n_b-2}(\boldsymbol{p}_i^y + \boldsymbol{p}_{i+1}^y)(\boldsymbol{p}_i^x\boldsymbol{p}_{i+1}^y - \boldsymbol{p}_{i+1}^x\boldsymbol{p}_i^y) + (\boldsymbol{p}_{n_b-1}^y + \boldsymbol{p}_0^y)(\boldsymbol{p}_{n_b-1}^x\boldsymbol{p}_0^y - \boldsymbol{p}_0^x\boldsymbol{p}_{n_b-1}^y)\right)$$

where A is the area volume defined in (5.9). This formula can again be used for all parametrizations, where the concrete boundary curve or its discretization is given. The center of mass constraint is not linear, but the derivatives can be easily obtained.

5.2.3 Constraints on the Parametrization

Often there are also constraints for the design parameters directly. For example it is reasonable to impose constraints to avoid self-intersecting boundary curves or restrict the boundary curves into a prescribed domain. Often this can be done through box constraints or simple linear constraints on the parameters $u \in U$.

5.2.4 Evaluating Constraints for the Pseudo-solid Approach

Usually most of the constraints in shape optimization depend on the boundary curve or a discretization of it. Using the pseudo-solid approach we need to solve the elasticity equation (5.4) first to get the boundary curve and then evaluate the constraint. We have the following chain

$$u \in U \xrightarrow{A} V_{\text{bdry}} \in S(\Gamma_B) \xrightarrow{D} \mathbb{R}^m \tag{5.10}$$

where A includes the solution of the PDE (5.4) and D maps the boundary curve displacement to the constraint image space.
Given the boundary displacement we have the (discrete) boundary curve of the actual object and can evaluate constraints like volume, center of mass, etc. as described in the previous section. The derivatives with respect to the control, i.e. $c(x)$, are more complicated since A has to be differentiated. However, since we use a linear elasticity equation, we could also use sensitivities

to evaluate the constraints. This approach is efficient, if the sensitivities are only computed once offline, and the number of controls is not very big compared to the number of constraints and optimization iterations. Alternatively, an adjoint approach can be used to compute the derivatives, similar to the adjoint approach introduced in Section 5.4.

5.3 Transport of Boundary Displacements into the Domain

As described in Section 5.1.1, for parametrizations of class $\mathcal{A}$, we use for the extension of the boundary velocity field V_{bdry} to the whole domain a linear elasticity approach. Given $V_{\text{bdry}} \in S(\Gamma_B)$ we solve a linear elasticity equation without source term on the right side:

$$\begin{aligned} \text{div } \sigma(V) = 0 \qquad & \text{in } \Omega_{\text{ref}} \\ V = V_{\text{bdry}} \qquad & \text{on } \Gamma_B \\ V = 0 \qquad & \text{on } \partial\Omega_{\text{ref}} \setminus \Gamma_B \end{aligned} \tag{5.11}$$

where $\sigma : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ is the Cauchy stress tensor

$$\sigma(u) := \lambda \text{ tr } (\varepsilon(u))I + 2\mu\varepsilon(u)$$

with Lamé constants $\lambda \in \mathbb{R}$ and $\mu \in \mathbb{R}$ and $\varepsilon(\boldsymbol{u}) := \frac{1}{2}(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$.
Due to the Dirichlet boundary conditions V is fixed to $V = 0$ on the boundary $\partial\Omega_{\text{ref}} \setminus \Gamma_B$ while V is set to V_{bdry} on the object boundary Γ_B. The solution V is a domain displacement field $V \in S$ as required in the shape optimization ansatz using domain displacements/transformations to represent different designs.
The choice of the Lamé constants is not so important, since we only need a continuous extension of the boundary displacement into the domain. In numerical tests we used

$$\lambda := \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu := \frac{E}{2(1+\nu)} \tag{5.12}$$

where E is Young's modulus and ν is the Poisson ratio which we set to $E := 10$ and $\nu := 0.3$.
The elasticity equation (5.11) plays the role of the operator B in (5.2).

5.4 Calculation of Derivatives with respect to Shape Parameters

We will now apply the setting described in Section 3.1.12 to calculate the derivatives with respect to shape parameters. We will derive the derivatives directly on the discrete level.
The elasticity equation (5.11) on the discrete level can be expressed as

$$\begin{aligned} A^d V^d &= 0 \\ B^d V^d &= V_\Gamma^d \end{aligned} \tag{5.13}$$

where A^d is the stiffness matrix and V^d is the vector containing the nodal variables associated with V in (5.11). V_Γ^d is the discrete version of the boundary

nodal values, corresponding to V_{bdry} on Γ_B and to 0 on the exterior boundary. The matrix B^d is the mass matrix of the boundary values, extracting the boundary nodes of V^d.
We now define an extended system of (5.13) [3, Section 7] by introducing the equivalent optimization problem

$$\min_{V^d} (V^d)^T A^d V^d \quad \text{s.t. } B^d V^d = V_\Gamma^d.$$

As we only have equality constraints, the first order optimality system is

$$h(V^d, \Lambda^d, V_\Gamma^d) := \begin{pmatrix} A^d V^d + (B^d)^T \Lambda^d \\ B^d V^d - V_\Gamma^d \end{pmatrix} = 0 \tag{5.14}$$

where Λ^d is a Lagrange multiplier. We will call (5.14) the extended version of (5.13) which is equivalent.
Now the discretized version of the reduced optimization problem (3.21) is

$$\min_{V^d} j^d(V^d) \quad \text{s.t. } h(V^d, \Lambda^d, V_\Gamma^d(u)) = 0, u \in U_{\text{ad}}$$

where j^d is the discrete version of the usual objective functional j. To avoid technical difficulties, we use here an objective functional defined on a discretization of the displacement space S (and not T_{ref}). Furthermore we have the map

$$u \mapsto V_\Gamma^d(u) \mapsto V^d(V_\Gamma^d(u)),$$

describing how the design $u \in U_{\text{ad}}$ affects the boundary vector field $V_\Gamma^d(u)$, from which we obtain the domain vector field $V^d(V_\Gamma^d(u))$. As for many parametrizations of class $\mathcal{A}$ the first part is easy to differentiate, we focus on an efficient evaluation of the derivate of the reduced objective functional

$$\hat{j}^d(V_\Gamma^d) := j^d(V^d(V_\Gamma^d))$$

with respect to V_Γ^d where $V^d(V_\Gamma^d)$ solves $h(V^d(V_\Gamma^d), \Lambda^d, V_\Gamma^d) = 0$.
As already done in the setting in Section 3.1.12, we introduce the Lagrangian function, but here in the discrete version and for displacements:

$$\mathcal{L}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d) := j^d(V^d) + (\theta_1^d)^T (A^d V^d + (B^d)^T \Lambda^d) + (\theta_2^d)^T (B^d V^d - V_\Gamma^d)$$

We have $\mathcal{L}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d) = j^d(V^d)$ for all admissible $(V^d, \Lambda^d, V_\Gamma^d)$ satisfying $h(V^d, \Lambda^d, V_\Gamma^d) = 0$. Therefore we can use the identity

$$\frac{d}{dV_\Gamma^d} j^d(V^d) = \frac{d}{dV_\Gamma^d} \mathcal{L}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d)$$

for calculating the derivatives of $\hat{j}^d(V_\Gamma^d)$ with respect to V_Γ^d. The derivatives of $\mathcal{L}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d)$ are given by

$$\begin{aligned}
\mathcal{L}_{(\theta_1^d, \theta_2^d)}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d) &= h(V^d, \Lambda^d, V_\Gamma^d), \\
\mathcal{L}_{(V^d, \Lambda^d)}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d) &= \begin{pmatrix} j_{V^d}^d(V^d) + (A^d)^T \theta_1^d + (B^d)^T \theta_2^d \\ B^d \theta_1^d \end{pmatrix}, \\
\mathcal{L}_{V_\Gamma^d}(V^d, \Lambda^d, V_\Gamma^d, \theta_1^d, \theta_2^d) &= -(\theta_2^d)^T.
\end{aligned} \tag{5.15}$$

Now we can obtain the derivative $(\hat{j}^d)'(V_\Gamma^d)$ by the following steps

1.) Solve $\mathcal{L}_{(\theta_1^d,\theta_2^d)}(V^d,\Lambda^d,V_\Gamma^d,\theta_1^d,\theta_2^d) = 0$, which is equivalent to solving the elasticity equation (5.13).

2.) Solve $\mathcal{L}_{(V^d,\Lambda^d)}(V^d,\Lambda^d,V_\Gamma^d,\theta_1^d,\theta_2^d) = 0$, which is equivalent to solving the adjoint equation

$$\begin{pmatrix} A^d & (B^d)^T \\ B^d & 0 \end{pmatrix} \begin{pmatrix} \theta_1^d \\ \theta_2^d \end{pmatrix} = \begin{pmatrix} -j_{V^d}^d(V^d) \\ 0 \end{pmatrix}, \tag{5.16}$$

3.) Evaluate

$$(\hat{j}^d)'(V_\Gamma^d) = \mathcal{L}_{V_\Gamma^d}(V^d,\Lambda^d,V_\Gamma^d,\theta_1^d,\theta_2^d) = -(\theta_2^d)^T.$$

$(\hat{j}^d)'(V_\Gamma^d)$ is an element of the dual space of the space of discretized boundary vector fields. For a given discrete boundary vector field W the derivative in direction W can be evaluated by calculating the scalar product of the representing vectors.

Remark 5.1. *As an alternative for steps 2 and 3, one can solve the reduced adjoint system*

$$A_{BC}^d\theta_1^d = -j_{V^d}^d(V^d)_{BC}$$

where the Dirichlet boundary conditions are built into the equation. Then θ_2^d is obtained via

$$(B^d)^T\theta_2^d = -A^d\theta_1^d - j_{V^d}^d(V^d).$$

In the last step $(B^d)^T$ extracts the boundary node values of $-A^d\theta_1^d - j_{V^d}^d(V^d)$. Since the admissible domain vector fields are zero on the exterior boundary, it is sufficient to evaluate only the boundary node values of the object B.

Remark 5.2. *Note that the term $-j_{V^d}^d(V^d)$ appears in* (5.16) *on the right hand side of the linear system. Solving the adjoint system* (5.16) *is usually much cheaper than calculating all sensitivities of the reduced function j.*

5.5 Discretization of the Navier-Stokes Equations

We consider the instationary Navier-Stokes equations with Dirichlet and Neumann boundary conditions as already analyzed in Section 3.2.7.

$$\begin{aligned} \boldsymbol{v}_t - \nu\Delta\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} + \nabla p = \boldsymbol{f} &\quad \text{on } \Omega\times I \\ \operatorname{div}\boldsymbol{v} = 0 &\quad \text{on } \Omega\times I \\ \boldsymbol{v} = \boldsymbol{g} &\quad \text{on } (\Gamma_{D_{\text{ext}}}\cup\Gamma_B)\times I \\ \nu\partial_n\boldsymbol{v} - pn = 0 &\quad \text{on } \Gamma_N \\ \boldsymbol{v}(\cdot,0) = \boldsymbol{v}_0 &\quad \text{in } \Omega. \end{aligned} \tag{5.17}$$

In this section we omit the $\sim$ symbol above the variables which was used to emphasize the definition on the pysical domain Ω.

Defining the spaces

$$\begin{aligned} \hat{V} &:= \{\boldsymbol{v}\in W(I;\mathbf{H}^1(\Omega)) \mid \boldsymbol{v} = \boldsymbol{g} \text{ on } (\Gamma_{D_{\text{ext}}}\cup\Gamma_B)\times I\}, \\ \hat{W} &:= \{\boldsymbol{v}\in \mathbf{H}^1(\Omega) \mid \boldsymbol{v} = 0 \text{ on } \Gamma_{D_{\text{ext}}}\cup\Gamma_B\}, \\ \hat{P} &:= L^2(I;L^2(\Omega)), \end{aligned}$$

we obtain the weak formulation of the problem:
Find $(\boldsymbol{v}, p) \in \hat{V} \times \hat{P}$ such that

$$\begin{aligned}
&\int_\Omega \boldsymbol{v}_t(x,t)^T \boldsymbol{w}(x)\ dx + \int_\Omega \boldsymbol{v}(x,t)^T \nabla \boldsymbol{v}(x,t) \boldsymbol{w}(x)\, dx + \int_\Omega \nu \nabla \boldsymbol{v}(x,t) : \nabla \boldsymbol{w}(x)\, dx \\
&- \int_\Omega p(x,t)\ \operatorname{div}\ \boldsymbol{w}(x)\, dx = \int_\Omega \boldsymbol{f}(x,t)^T \boldsymbol{w}(x)\, dx \quad \forall\, \boldsymbol{w} \in \hat{W} \ \text{ for a.a. } t \in I \\
&\qquad \int_\Omega q(x)\ \operatorname{div}\ \boldsymbol{v}(x,t) = 0 \qquad\qquad\qquad\qquad \forall\, q \in \hat{P} \ \text{ for a.a. } t \in I \\
&\qquad\qquad\qquad \boldsymbol{v}(\cdot, 0) = \boldsymbol{v}_0.
\end{aligned} \tag{5.18}$$

The discretization builds on this weak formulation of the Navier-Stokes equations.
For time-dependent PDEs there are usually two different methods of discretizing problems with space and time variables:

- Discretize in space and time in two steps (first semidiscretize),
- Discretize in space and time simultaneously,

We will focus on the first approach. Here we distinguish on the order of the discretization. If we first discretize in space we obtain the *Method of Lines*. In contrast using the *Rothe method* we first semidiscretize in time. In the *Method of Lines* the discretization in space of (3.52) yields a system of ODEs with initial conditions. For each element of the discrete test space we obtain one ODE in time. Using the *Rothe method* yields an ODE in function space. We choose here a discretization in two steps and first discretize in space using finite elements (FE). For the mathematical theory using finite elements in the context of the Navier-Stokes equations we refer to [22]. Furthermore in [16] there is a good overview of implementation aspects in the context of FE with Navier-Stokes equations.
Let $\mathcal{T}_h$ be a triangulation of Ω consisting of simplices. For $k \in \mathbb{N}$ and any simplex $S \subset \mathcal{T}_h$ we denote by

$$P^k(S) := \{p : S \to \mathbb{R} \mid p \text{ is a polynomial of degree } \leq k\}$$

the space of polynomials of maximal degree k over S. We use the so-called $P^2 - P^1$ element, also known as Taylor-Hood element, for the spatial discretization. This element consists of globally continuous, piecewise quadratic functions in the velocity space and of globally continuous, piecewise linear functions for the pressure space. In detail we define

$$\begin{aligned}
V_h^{TH} &:= \{\boldsymbol{v} \in \mathbf{C}(\bar{\Omega}) \mid \forall S \in \mathcal{T}_h : \boldsymbol{v}_{|S} \in P^2(S)^d\} \cap \hat{W}, \\
P_h^{TH} &:= \{p \in C(\bar{\Omega}) \mid \forall S \in \mathcal{T}_h : p_{|S} \in P^1(S)\} \cap L^2(\Omega).
\end{aligned} \tag{5.19}$$

This element is *inf-sup* stable for the Navier-Stokes equations if some rather general assumptions on the triangulation $\mathcal{T}_h$ are fulfilled. The so called *inf-sup* condition guarantees that the (semi)-discrete system has a unique solution which is not naturally given for FE discretizations [22, Theorem 4.4.1].

Using the discrete spaces we arrive at the semidiscretized system: Find $(\boldsymbol{v}_h, p_h)$ such that

$$\begin{aligned}
&\int_\Omega (\boldsymbol{v}_h)_t(x,t)^T \boldsymbol{w}_h(x)\ dx + \int_\Omega \boldsymbol{v}_h(x,t)^T \nabla \boldsymbol{v}_h(x,t) \boldsymbol{w}_h(x)\, dx + \int_\Omega \nu \nabla \boldsymbol{v}_h(x,t) : \nabla \boldsymbol{w}_h(x)\, dx \\
&\quad - \int_\Omega p_h(x,t)\ \operatorname{div}\ \boldsymbol{w}_h(x)\, dx = \int_\Omega \boldsymbol{f}_h(x,t)^T \boldsymbol{w}_h(x)\, dx \quad \forall\, \boldsymbol{w}_h \in \hat{V}_h^{TH} \ \text{ for a.a. } t \in I \\
&\qquad \int_\Omega q_h(x)\ \operatorname{div}\ \boldsymbol{v}_h(x,t) = 0 \qquad \forall\, q_h \in \hat{P}_h^{TH} \ \text{ for a.a. } t \in I \\
&\qquad\qquad \boldsymbol{v}_h(\cdot, 0) = (\boldsymbol{v}_0)_h.
\end{aligned} \tag{5.20}$$

We discretize this ODE in time using the implicit Euler time discretization scheme. Let

$$\mathcal{I} := \{ I_i \mid 1 \le i \le N_T \}$$

be a partiton of the time interval $I = (0,T]$ with $I_i := (t_{i-1}, t_i]$ and a sequence of time points $0 = t_0 < t_1 < t_2 < \cdots < t_{N_T - 1} < t_{N_T} = T$. Let $k_i := t_i - t_{i-1}$ denote the length of the interval I_i and $(\boldsymbol{v}_h^i, p_h^i)$ describe the discrete velocity and pressure variable at time t_i. Then the implicit Euler time discretization yields:
For $i = 1, \ldots, N_T$ find $(\boldsymbol{v}_h^i, p_h^i)$ such that

$$\begin{aligned}
&\int_\Omega \frac{1}{k_i} (\boldsymbol{v}_h^i - \boldsymbol{v}_h^{i-1})^T \boldsymbol{w}_h(x)\ dx + \int_\Omega \boldsymbol{v}_h^i(x)^T \nabla \boldsymbol{v}_h^i(x) \boldsymbol{w}_h(x)\, dx + \int_\Omega \nu \nabla \boldsymbol{v}_h^i(x) : \nabla \boldsymbol{w}_h(x)\, dx \\
&\quad - \int_\Omega p_h^i(x)\ \operatorname{div}\ \boldsymbol{w}_h(x)\, dx = \int_\Omega \boldsymbol{f}_h^i(x)^T \boldsymbol{w}_h(x)\, dx \quad \forall\, \boldsymbol{w}_h \in \hat{V}_h^{TH} \\
&\qquad \int_\Omega q_h(x)\ \operatorname{div}\ \boldsymbol{v}_h^i(x) = 0 \qquad \forall\, q_h \in \hat{P}_h^{TH}
\end{aligned} \tag{5.21}$$

Using the discrete trial and test spaces in space we arrive at a fully discrete nonlinear system. In our numerical tests we solved this system applying Newton's method. Alternatively one could use the Picard iteration for solving the nonlinear system. For details see e.g. [16, Section 7.2.2].

5.6 Updating the Meshes

As described in Section 3.3.3 the shape derivatives can be calculated by solving the state and adjoint equations on the actual physical domain. Since the design of the object B changes in each iteration, the Navier-Stokes equations and their adjoints have to be solved on changing domains $\tau(\Omega_{\text{ref}})$.
In our numerical results the meshes are updated by a transformation of a reference mesh $\mathcal{M}_{\text{ref}}$ belonging to a reference domain Ω_{ref}. The transformation is done by using the same elasticity approach as used to transport the boundary vector field to a domain vector field (see Section 5.3). Let V be the solution of the linear elasticity equation. Then each mesh point $x \in \mathcal{M}_{\text{ref}}$ is transported to a new mesh point $x + V(x)$.
However, this approach is only possible, if the actual object design is similar to the reference object. Otherwise irregular meshes can occur like intersecting

edges of triangles. For large transformations fixing a new reference domain and remeshing is a good alternative. However, since this could have influence on the discretization error, remeshing should only be done if a large design change has occured.
In some examples of our numerical tests we used remeshing, but only if the objective value has changed significantly in the last iterations.

6 Numerical Results

In this chapter we present numerical results for the flow around one or more objects in a channel in 2D. In the first section we will discuss the implementation of the code, introducing the software package `FlowOpt` which was developed in context of this work. Furthermore, we will describe the third party packages that are used. Then numerical results for a flow setting based on a DFG benchmark are presented.

6.1 Implementation Aspects and Third Party Software

6.1.1 The `FlowOpt` Software Package

In the context of this work I developed a software package called `FlowOpt` for solving shape optimization problems where the PDE is given by the stationary or instationary Navier-Stokes equations. Furthermore it involves the following key points:

- The shape derivative computation is based on the transformation ansatz of Murat and Simon as described in chapter 3.
- The following three blocks operate independently and realizations are easily exchangeable:
  - The object representation and parametrizations (*Object Block*).
  - The PDE solvers (*Solver Block*).
  - The optimization algorithms (*Optimization Block*).

In Figure 6.1 an overview of this block framework is displayed. The *Iterate Block* is the central block that manages the interaction between the three other blocks.
`FlowOpt` was developed in C++ and the idea of an object-oriented structure was incorporated to define the blocks of Figure 6.1. In detail we have the following main abstract base classes in the *Iterate Block*, *Object Block* and *Optimization Block*:

- `Iterate`: This class manages the communication between the other blocks. In particular, it exhibits the interface for the *Optimization Block* via providing virtual methods for calculating the objective value and gradient for a given iterate. Furthermore it allows the update of the actual iterate, forwarding the calculation of the new boundary points and grid deformation to the *Object Block*. Finally, some additional features for handling iterates are included.
- `Object`: The `Object` class saves general information about the actual objects. Here it is stored how many objects are exposed to the flow and which parametrization for each object is used. It saves the actual boundary points array and provides methods to calculate common constraints and their derivatives in shape optimization. For special parametrizations the

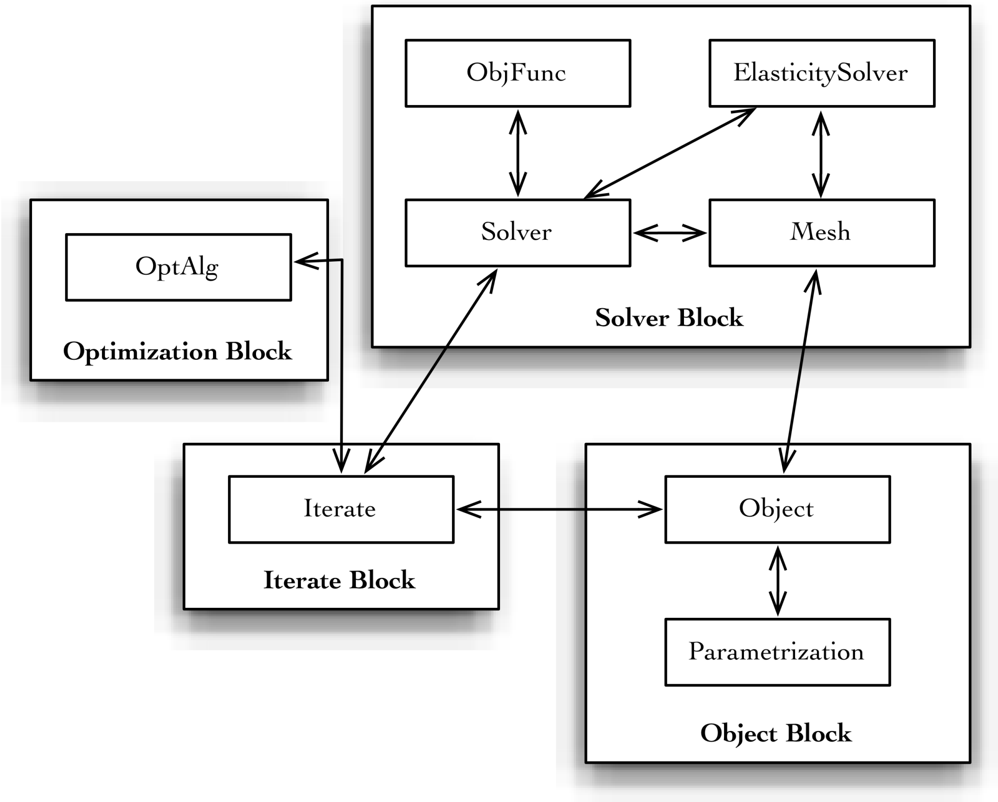

Figure 6.1: Structure of `FlowOpt`

calculation of constraints can also be forwarded to the `Parametrization` class. Furthermore it activates the grid deformation for the new object by interacting with the `Mesh` and `ElasticitySolver` classes of the *Solver Block*.

- `Parametrization`: This class is used to define the parametrization of a single object. Furthermore the calculation of constraints can be moved hither from the `Object` class.

- `OptAlg`: Here, any optimization software with C++ interface can be used. The calculation of the objective or constraints can be done by updating the control variable in the `Iterate` class and then calling the corresponding C++ functions for computing the objective value, the objective gradient, constraint values and constraint Jacobians.

Within the *Solver Block* we have the following main abstract base classes that work closely together

- `Solver`: Here the PDE solve is implemented, in our case the stationary or instationary Navier-Stokes equations. It provides the solution of state and adjoint equations and manages the evaluation of objectives.

- `Mesh`: In the `Mesh` class the mesh is stored in a for the `Solver` class suitable way. Furthermore it inherits methods for transforming meshes for a given discrete boundary vector field as provided by the `Object` class. Thus it is also linked to the `ElasticitySolver` class.

- `ObjFunc`: Here the objective function values are calculated for a given state. Furthermore derivatives are provided in a variational form such that shape derivatives can be calculated in cooperation with the `Solver` class and the `ElasticitySolver` class (for the calculation of reduced shape derivatives with respect to shape parameters the shape derivative appears on the right side of the adjoint elasticity equation, c.f. Section 3.1.12).

- `ElasticitySolver`: This class provides methods for solving the elasticity equation and its adjoint. It is used for deforming meshes and transporting boundary displacements into the domain. The adjoint is used for integrating the shape parametrization approach into the shape derivative calculation.

Note that all these classes use abstract virtual interfaces, especially between each block. In particular, the realizations of these blocks can be substituted easily.
Concrete instances of the classes are used to represent a concrete setting. For example, in one szenario we use B-Splines to represent one object. Therefore a subclass of `Parametrization` is implemented to realize this concrete parametrization. However, it also can be replaced by another parametrization without affecting the other blocks.
`FlowOpt` assumes that the parametrization of the object(s) is of class $\mathcal{A}$ as described in Section 5.1. In particular, we have a simple map of the design space

U to the object boundary gridpoints. In this case the object representation in *Object Block* does not need the solve of an elasticity equation and derivatives of the boundary gridpoints with respect to design parameters can be derived easily, c.f. Section 5.1. However, we will also use `FlowOpt` when the object is parametrized via the pseudo-solid approach (see Section 5.1.3). In this case the strict segregation of the *Solver Block* and the *Object Block* is weakened.
In all our numerical tests we used the third party package `Sundance` to realize the *Solver Block* that we discuss in the next section.

6.1.2 The State and Adjoint Solve

The main part of the computational work is the solve of the (in)stationary Navier-Stokes equations and its adjoint. As already described in section 5.5 we will use the Taylor-Hood discretization combined with an implicit Euler time stepping scheme for the instationary case. The implementation of the finite element discretization is done using the third party code `Sundance` [37] which is part of the package `Trilinos` [27]. In `Sundance` the user can formulate a partial differential equation (system) in weak form, specifying test and trial spaces, boundary conditions and other finite element parameters. Then `Sundance` automatically creates the discrete operators associated with the discrete problem. Using the `Trilinos` packages `Stratimikos`, `Teuchos` and `Thyra`, these operators can be linked to other high end tools of `Trilinos` like `Aztecoo`, `ML`, `Amesos` and `Ifpack` for solving and preconditioning the linear systems. For details about the packages, see [27] and [26].
For the instationary problem, in each time step we have to solve a nonlinear discrete system for the velocity and the pressure. A similar nonlinear system appears for the stationary Navier-Stokes equations. We solve these nonlinear systems by applying Newton's method. In each Newton step we have to solve a linear system of the type

$$\begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} v \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}. \tag{6.1}$$

In [16] there is a nice overview about some general strategies for solving and preconditioning (6.1) with iterative solvers. In the case of 2D flow, we made the experience that direct solvers are often faster than iterative solvers where we compared the direct solvers with GMRES [47] using the SIMPLEC [65] preconditioner and again preconditioned iterative solvers for the subsystems. However, in 2D, this systems can be solved very efficiently using direct factorization methods as provided by `Amesos` [51, 50]. In all our numerical results in Section 6 we used the third party software `SuperLU_Dist` [36] which is a scalable distributed-memory sparse direct solver for linear systems. The interface to `Sundance` is provided via `Stratimikos`.
For the linear algebra operations we use `Epetra` and `ACML` where `ACML` is the AMD Core Math Library which includes the basic `LAPACK` and `BLAS` routines.

6.1.3 Optimization Algorithm

For the optimization part we use IPOPT [68]. IPOPT provides a C++ interface and can easily be linked to the `FlowOpt` interface. IPOPT uses an interior point optimization algorithm and is designed to solve large-scale nonlinear optimization problems. In our numerical tests we did not use second order shape derivatives. Instead, IPOPT uses a limited memory BFGS approximation of the Hessian of the Lagrangian. This means that also the Hessians of the constraints are not calculated but approximated via the Quasi-Newton update.

6.1.4 Mesh Generation

For the mesh generation we used `Triangle` [53] that can generate high-quality triangular meshes. We generate the meshes in three steps. First, we triangulate the whole domain. For this, we discretize the whole boundary $\partial\Omega$ where the boundary points of B are exactly the boundary points saved in the `Object` class above. Then we start `Triangle` to generate a mesh for the whole domain with the constraint that no additional boundary points shall be created. In a second step we rerun `Triangle` to refine the mesh in a prescribed region around the object(s). This is done because the region around and behind the flow object plays an important role for resolving the flow charateristics. Again no additional boundary points on Γ_B are created. Finally the mesh is partitioned if parallel solvers are used. The mesh generation process is fully automatic such that remeshing can also be started during the optimization without interaction needed.

6.1.5 B-Splines Parametrization

In the forthcoming results we use the parametrization via B-splines. In Section 5.1.2 we decribed the theoretical aspects of B-splines. In our numerical results we use symmetric B-splines curves to describe an object that is symmetric with respect to the horizontal axis defined by the front point y-coordinate y_c. This means that we only model the upper part of the object using a non-closed B-spline curve. The lower part of the object is given by turning the upper curve down. For the upper curve we use a B-spline with 7 B-spline control points resulting in 4 B-spline segments.

6.2 The Benchmark Problem

My numerical tests are based on the DFG benchmark problem of a 2D flow in a channel [62]. The goal is to minimize the drag of an object B that is exposed to the flow within this channel (see Figure 6.2) by optimizing the shape of B. The flow region is a box with length $l = 2.2m$ and width $b = 0.41m$. On the left we have an inflow region $\Gamma_{\text{in}} \subset \Gamma_{D_{\text{ext}}}$ while the fluid can exit on the free outflow boundary Γ_N. In the DFG benchmark problem the object B is a fixed circle with center $x_c := (0.2m, 0.2m)$ and diameter $0.1m$. On the top and bottom we have a no-slip boundary as we have on the object boundary Γ_B. In our numerical tests we will optimize the shape of B where the volume and center of

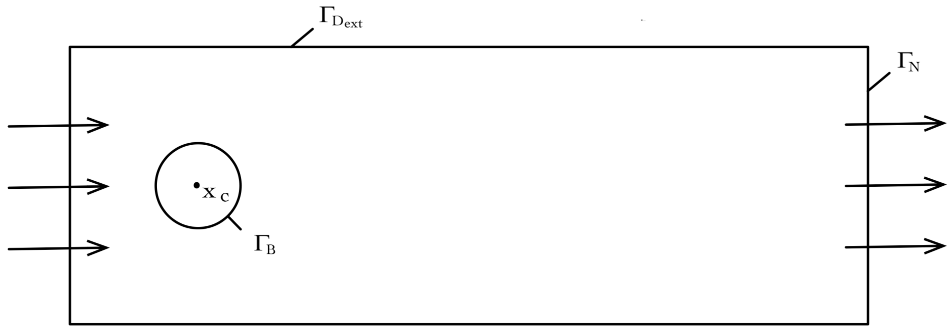

Figure 6.2: The Benchmark problem

mass x_c is fixed. In Section 6.3 we will also analyze one setting where we add another object to be shape optimized.
We consider here a stationary scenario and an instationary scenario. For the stationary case the state equation is given by (c.f. Section 3.3.6):

$$\begin{aligned} -\nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} && \text{on } \Omega, \\ \operatorname{div}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Omega, \\ \tilde{\boldsymbol{v}} &= \tilde{\boldsymbol{v}}_{D_{\text{ext}}} && \text{on } \Gamma_{D_{\text{ext}}}, \\ \tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_B, \\ \tilde{p}\,\tilde{\boldsymbol{n}} - \nu\frac{\partial}{\partial\tilde{n}}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_N. \end{aligned}$$

For the instationary scenario (c.f. Section 3.3.5) we consider:

$$\begin{aligned} \tilde{\boldsymbol{v}}_t - \nu\Delta\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} + \nabla\tilde{p} &= \tilde{\boldsymbol{f}} && \text{on } \tau(\Omega_{\text{ref}})\times I, \\ \operatorname{div}\tilde{\boldsymbol{v}} &= 0 && \text{on } \tau(\Omega_{\text{ref}})\times I, \\ \tilde{\boldsymbol{v}} &= \tilde{\boldsymbol{v}}_{D_{\text{ext}}} && \text{on } \Gamma_{D_{\text{ext}}}\times I, \\ \tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_B\times I, \\ \tilde{p}\,\tilde{\boldsymbol{n}} - \nu\frac{\partial}{\partial\tilde{n}}\tilde{\boldsymbol{v}} &= 0 && \text{on } \Gamma_N\times I, \\ \tilde{\boldsymbol{v}}(\cdot,0) &= \tilde{\boldsymbol{v}}_0 && \text{on } \tau(\Omega_{\text{ref}}). \end{aligned}$$

In both scenarios we consider a time-independent inflow on $\Gamma_{\text{in}} \subset \Gamma_{D_{\text{ext}}}$

$$\tilde{\boldsymbol{v}}_{\Gamma_{\text{in}}}(0,y) := \begin{pmatrix} 4V_m y(b-y)/b^2 \\ 0 \end{pmatrix} \tag{6.2}$$

where $V_m := 1.5$ is the characteristic velocity and $b = 0.41$ is the channel width.
We set

$$\tilde{\boldsymbol{v}}_{D_{\text{ext}}} := \begin{cases} \tilde{\boldsymbol{v}}_{\Gamma_{\text{in}}}(0,y) & \text{for } x\in\Gamma_{\text{in}} \\ 0 & \text{for } x\in\Gamma_{D_{\text{ext}}}\backslash\Gamma_{\text{in}} \end{cases}.$$

For the instationary case we start with an initial velocity $\tilde{\boldsymbol{v}}_0 = 0$. Furthermore for both scenarios we have $\tilde{\boldsymbol{f}} = 0$.

6.2.1 The Objective Function

In our numerical tests we minimize the drag of an object. The drag is usually given by

$$J(\tilde{\boldsymbol{v}},\tilde{p}) := \frac{1}{T}\int_I\int_{\Gamma_B} \tilde{n}^T\sigma(\tilde{\boldsymbol{v}},\tilde{p})\tilde{\boldsymbol{\phi}}\; d\tilde{S} \tag{6.3}$$

where $\sigma(\tilde{\boldsymbol{v}},\tilde{p})$ is the stress tensor and $\tilde{\boldsymbol{\phi}}$ is a unit vector defined on Γ_B and pointing in the mean flow direction. In the case of the flow around a cylinder as described in Section 6.2 we have $\tilde{\boldsymbol{\phi}}(x,y) = (1,0)^T$. The stress tensor is composed of the stress deviatoric $\nu(\nabla\tilde{\boldsymbol{v}}+(\nabla\tilde{\boldsymbol{v}})^T)$ with zero trace and an isotropic pressure:

$$\sigma(\tilde{\boldsymbol{v}},\tilde{p}) = \nu(\nabla\tilde{\boldsymbol{v}} + (\nabla\tilde{\boldsymbol{v}})^T) - \tilde{p}I.$$

We can derive a domain integral representation for (6.3). For this, let $\tilde{\boldsymbol{\Phi}}$ be a smooth extension of $\tilde{\boldsymbol{\phi}}$ on Ω such that $\tilde{\boldsymbol{\Phi}}_{|\Gamma_{\text{ext}}} = 0$. Here, $\Gamma_{\text{ext}} = \Gamma_{D_{\text{ext}}} \cup \Gamma_N$. Using integration by parts we obtain (see [32, Section 3.1] for details):

$$J(\tilde{\boldsymbol{v}},\tilde{p}) = \frac{1}{T}\int_I\int_\Omega \Big((\tilde{\boldsymbol{v}}_t + (\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} - \tilde{\boldsymbol{f}})^T\tilde{\boldsymbol{\Phi}} - \tilde{p}\;\text{div}\;\tilde{\boldsymbol{\Phi}} + \nu\nabla\tilde{\boldsymbol{v}} : \nabla\tilde{\boldsymbol{\Phi}}\Big)\; d\tilde{x}\; dt.$$

To derive an objective function of the type (3.50) we use integration by parts in the time variable for the time derivative term $\tilde{\boldsymbol{v}}_t^T\tilde{\boldsymbol{\Phi}}$ and arrive at

$$\begin{aligned} J(\tilde{\boldsymbol{v}},\tilde{p}) =& \frac{1}{T}\int_I\int_\Omega \Big(((\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} - \tilde{\boldsymbol{f}})^T\tilde{\boldsymbol{\Phi}} - \tilde{p}\;\text{div}\;\tilde{\boldsymbol{\Phi}} + \nu\nabla\tilde{\boldsymbol{v}} : \nabla\tilde{\boldsymbol{\Phi}}\Big)\; d\tilde{x}\; dt \\ &+ \frac{1}{T}\int_\Omega (\tilde{\boldsymbol{v}}(\tilde{x},T) - \tilde{\boldsymbol{v}}_0(\tilde{x}))^T\tilde{\boldsymbol{\Phi}}(\tilde{x})\; d\tilde{x}. \end{aligned}$$

Finally, if we choose $\tilde{\boldsymbol{\Phi}}$ as a solenoidal extension of $\tilde{\boldsymbol{\phi}}$ the pressure term drops out and we have an objective $J(\tilde{\boldsymbol{v}})$ only depending on $\tilde{\boldsymbol{v}}$ that is of type (3.50). Furthermore J can be transformed to the reference domain Ω_{ref}. Derivatives of J can be derived in the very same way as for the state equation since J contains similar terms as E.

6.3 Numerical Results

The following results were computed on a Linux cluster at TUM supported by DFG grant INST 95/919-1 FUGG. The compute cluster consists of 8 Quad-Core AMD Opteron processors 8384 with 64 GB distributed memory. As already described we use `Sundance` for the finite element implementation and solve the linear systems generated by Newton's method with the direct solver `SuperLU_Dist`.

6.3.1 Shape Optimization for the Stationary Navier-Stokes Equations

We consider here the flow around one or more objects with viscosity $\nu = 0.01$ and $\nu = 0.001$. Furthermore we compare the parametrization using B-splines with the pseudo-solid approach.

It	objective	`inf_pr`	`inf_dual`	$\lg(\mu)$
0	3.7507095e-01	1.39e-03	2.12e+00	0.0
1	2.6276890e-01	1.86e-03	3.12e+00	-1.3
2	2.6899924e-01	8.33e-05	8.72e-02	-2.3
3	2.6830761e-01	8.76e-06	7.23e-02	-3.5
4	2.6617380e-01	1.87e-04	1.32e-01	-3.8
5	2.6601381e-01	9.61e-05	1.78e-01	-4.2
6	2.6591870e-01	1.60e-05	4.71e-02	-5.2
7	2.6598410e-01	2.01e-07	3.33e-03	-6.7
8	2.6597089e-01	4.34e-07	2.01e-03	-8.2
9	2.6597044e-01	7.56e-07	3.72e-03	-9.3
10	2.6616737e-01	2.16e-08	6.15e-02	-6.0
11	2.6582121e-01	5.02e-05	8.83e-03	-6.3
12	2.6596717e-01	1.93e-07	4.62e-03	-6.3
13	2.6597404e-01	1.26e-09	1.39e-02	-7.6
14	2.6596540e-01	3.57e-07	8.98e-04	-7.7
15	2.6596599e-01	2.03e-09	9.10e-04	-8.5

Table 6.1: Convergence results for stationary flow with $\nu = 0.01$ using B-spline parametrization

6.3.1.1 Parametrization via B-Splines

We start with the case where the object is parametrized using symmetric B-splines curves as decribed in Section 6.1.5. The symmetric axis is fixed to $y_c = 0.2$ where the front and end point of B lies on.
The reference object and starting point is a circle with diameter $d = 0.1$ and origin $x_c := (0.2, 0.2)$. The initial mesh is generated by `Triangle` and consists of 245341 vertices and 732683 edges, resulting in 487342 triangles. It is especially fine in the flow region around the object. For the stationary case we do not remesh and the actual mesh is updated by solving an elasticity equation as described in Section 5.6.
We impose a volume constraint on B and demand B to have the center of mass $x_c = (0.2, 0.2)$. Furthermore we have 4 inequality constraints for the order of the spline control points in x direction to avoid a self-intersecting boundary curve. Finally we impose box constraints on the B-spline control points.
The computations are done in a parallel setting where we use 32 processes distributed on the eight Quad-cores.
For a kinematic viscosity $\nu = 0.01$, IPOPT converges in 15 iterations to a solution, see Table 6.1 for details. In the table `inf_pr` and `inf_dual` denote the primal and dual feasibilty while $\lg(\mu)$ is the logarithm of the barrier parameter μ. In the optimal solution no box constraint and no inequality constraint is active. Furthermore in each iteration only one line search step is taken such that we have in total 16 state and 16 adjoint solves. The optimal design is shown in Figure 6.3

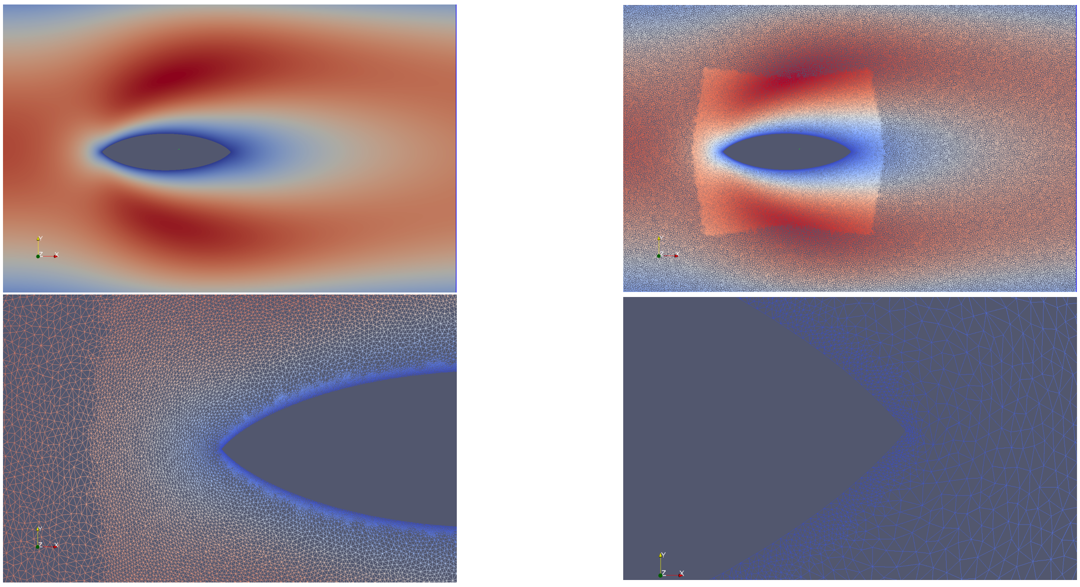

Figure 6.3: Optimal design for stationary flow with $\nu = 0.01$ using B-spline parametrization

Using the same setting, but a viscosity $\nu = 0.001$, IPOPT needs 20 iterations, see Table 6.2. In every step we use one line search step but in step 14 and 16 where IPOPT needs 4 line search steps respectively. In total we have 27 state solves and 21 adjoint solves. The optimal design is shown in Figure 6.4.

6.3.1.2 Parametrization via the Pseudo-Solid Approach

We consider a similar setting but parametrize the object via the pseudo-solid approach. In contrast to the standard pseudo-solid setting (see [38], [48]) we use a free vector field for the forces on the reference object boundary. Usually for the boundary forces the ansatz $c(x)n(x)$ is used where $n(x)$ is the unit normal vector on the boundary and $c(x) \in \mathbb{R}$ is the optimization parameter. However, the free vector field ansatz allows for more flexibility and numerical tests showed in most cases also faster convergence. Hence we use this parametrization and for n_b object boundary points we have $2n_b$ optimization variables.
The reference object and starting point is given by the circle with diameter $d = 0.08$ and origin $x_c := (0.2, 0.2)$. We use the same volume and center of mass equality constraints and an initial mesh with 108900 triangles. The object boundary Γ_B is discretized by 240 boundary points resulting in 480 optimization variables describing the boundary vector field. Furthermore we impose box constraints on the components of the pseudo-solid vector field.
We consider the viscosity $\nu = 0.01$ first. IPOPT converges in 39 iterations to the solution, see Table 6.3. The object design (see Figure 6.5) and the final objective value 0.26595424 is close to the ones determined by the B-spline parametrization. In fact, the relative difference to the objective value 0.26596599 of the

It	objective	`inf_pr`	`inf_dual`	$\lg(\mu)$
0	1.2937152e-01	1.39e-03	1.94e+00	0.0
1	6.1537524e-02	2.68e-03	2.84e+00	-1.2
2	6.4869000e-02	1.52e-04	1.50e-01	-2.0
3	6.4050037e-02	6.52e-05	7.57e-02	-3.0
4	6.1992870e-02	4.58e-04	9.86e-02	-3.5
5	6.1888368e-02	4.77e-04	1.85e-01	-3.7
6	6.1478087e-02	8.50e-05	2.53e-02	-4.1
7	6.1418091e-02	6.04e-06	5.82e-03	-5.3
8	6.1372172e-02	2.07e-06	2.51e-03	-6.6
9	6.1366230e-02	1.85e-05	1.85e-02	-6.7
10	6.1363260e-02	1.52e-05	1.27e-02	-6.4
11	6.1358088e-02	7.54e-06	2.29e-03	-6.1
12	6.1351474e-02	2.60e-06	4.86e-03	-7.4
13	6.1363230e-02	3.08e-07	1.61e-02	-7.0
14	6.1362255e-02	1.96e-06	1.07e-02	-7.4
15	6.1337944e-02	1.44e-05	1.69e-02	-7.4
16	6.1338358e-02	1.27e-05	1.48e-02	-7.5
17	6.1347527e-02	1.99e-07	2.03e-04	-6.9
18	6.1348616e-02	3.12e-09	1.61e-03	-7.8
19	6.1348179e-02	4.19e-07	3.52e-04	-9.1
20	6.1348254e-02	5.85e-08	7.38e-05	-9.2

Table 6.2: Convergence results for stationary flow with $\nu = 0.001$ using B-spline parametrization

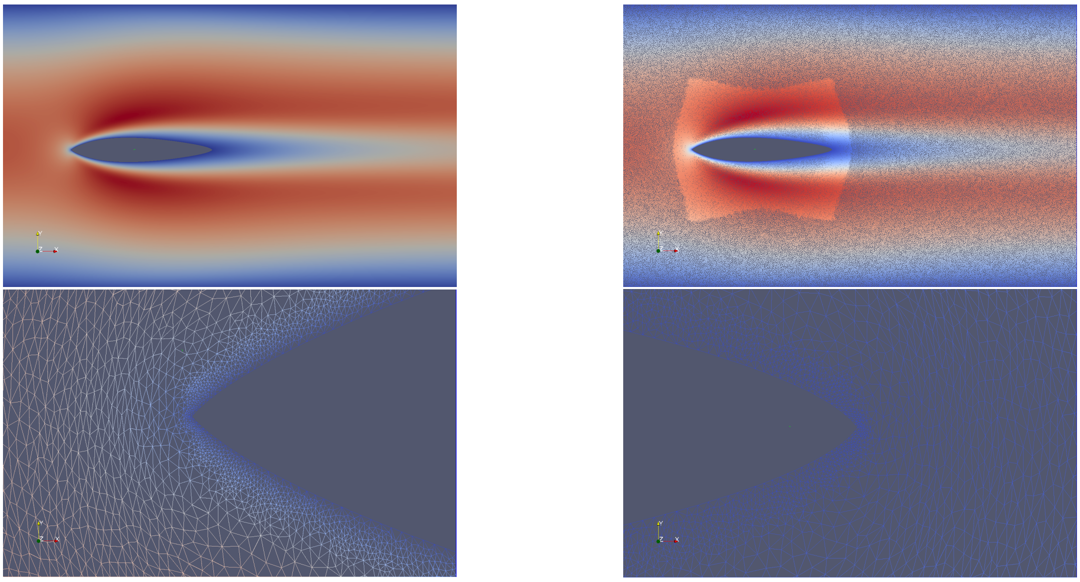

Figure 6.4: Optimal design for stationary flow with $\nu = 0.001$ using B-spline parametrization

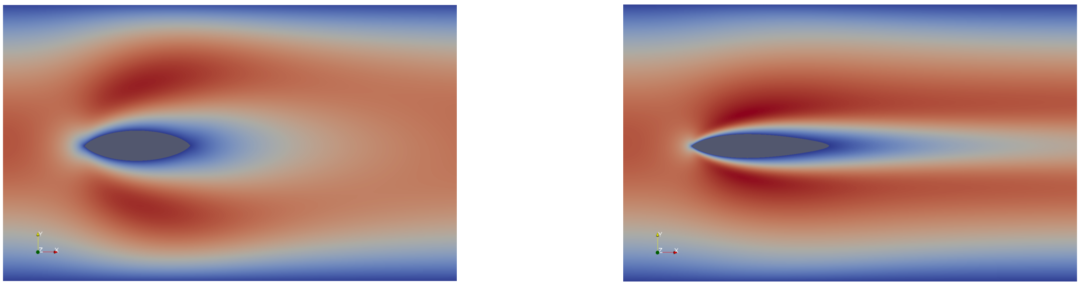

Figure 6.5: Optimal design for stationary flow with $\nu = 0.01$ (left) and $\nu = 0.001$ (right) using the pseudo solid approach

optimal B-spline object (see Figure 6.1) is about 0.004 percent. In four iterations more than one line search step is performed. However, between iteration 19 and 33 the algorithm does not make very much progress and IPOPT even enters a restoration phase.

For the viscosity $\nu = 0.001$ IPOPT needs 64 iterations to converge to the optimal solution, see Table 6.4. The optimal objective value 0.061348028 has a relative difference of about 0.00037 percent compared to the optimal value 0.061348254 for the B-spline optimization. In every iteration but the last two only one line search step is performed.

In Figure 6.6 the design of the optimal B-spline parametrization object is compared with the optimal shape of the pseudo-solid approach. The designs are very similar in the structure. However, for the B-spline parametrization we have the design space restriction of a symmetric object with symmetry axis $y = 0.2$. Since the channel has a width of 0.41 the pseudo-solid optimization generates an optimal shape where the front point is above and the back point is below the corresponding front and end point of the optimal B-spline object. However, the general structure of the objects is very similar and the orientation of the objects is only slightly different, resulting in nearly the same objective values.

In our numerical tests we saw that the convergence results of the pseudo-solid approach is not as good as for the B-spline parametrization. In fact, in many other numerical tests for the pseudo solid approach I watched convergence problems like restoration phases and no fast local convergence or even no convergence. Also the variation of starting points, fine and coarse meshes, the number of object boundary points and the introduction of regularizations did not overcome the basic problems. One reason could be that the volume and center of mass constraints depend on all 480 optimization variables and each component has a big influence on fulfilling the equality constraints.

However, one advantage of the pseudo solid approach is that no structure information about the optimal object is needed to formulate the optimization problem.

6.3.1.3 The Flow around Two Objects

We consider the flow around two objects. We use the setting described in

It	objective	`inf_pr`	`inf_dual`	lg(μ)
0	3.3173564e-01	2.60e-03	2.86e-04	0.0
1	3.3093941e-01	2.60e-03	2.34e-02	-5.0
2	3.2834301e-01	3.34e-06	2.26e-04	-2.8
3	2.7049867e-01	2.61e-03	1.27e-04	-3.7
4	2.6203030e-01	4.31e-02	7.32e-05	-5.2
5	2.7702636e-01	7.69e-03	1.24e-04	-6.0
6	2.7644937e-01	4.24e-02	7.35e-05	-5.7
7	2.6096537e-01	1.95e-02	8.60e-05	-5.7
8	2.5535575e-01	2.94e-02	5.06e-05	-5.4
9	2.6686974e-01	2.45e-02	1.09e-05	-6.4
10	2.7029254e-01	4.03e-03	3.68e-05	-6.3
11	2.6846669e-01	1.70e-02	8.50e-06	-5.8
12	2.6484932e-01	1.17e-02	4.73e-06	-6.9
13	2.6234122e-01	5.15e-03	5.22e-06	-7.0
14	2.6677662e-01	2.49e-03	3.01e-06	-8.7
15	2.6623672e-01	3.81e-03	2.00e-02	-9.3
16	2.6542607e-01	1.32e-03	2.88e-02	-11.0
17	2.6515440e-01	2.49e-03	1.36e-02	-11.0
18	2.6677551e-01	6.47e-04	5.73e-02	-9.0
19	2.6663483e-01	3.80e-03	3.05e-06	-8.2
⋮	⋮	⋮	⋮	⋮
33	2.6625130e-01	2.82e-03	1.15e-04	-6.5
34	2.6565560e-01	1.40e-03	1.63e-06	-6.6
35	2.6536104e-01	1.43e-03	1.55e-06	-6.6
36	2.6566035e-01	1.41e-03	8.45e-07	-6.6
37	2.6595458e-01	1.52e-06	1.08e-06	-6.6
38	2.6595406e-01	1.52e-06	6.60e-07	-11.0
39	2.6595424e-01	8.16e-07	5.89e-07	-11.0

Table 6.3: Convergence results for stationary flow with $\nu = 0.01$ using the pseudo-solid approach

It	objective	`inf_pr`	`inf_dual`	lg(μ)
0	1.1268029e-01	2.60e-03	2.82e-04	0.0
1	1.1238733e-01	2.60e-03	2.34e-02	-5.0
2	1.1100608e-01	3.34e-06	2.20e-04	-2.8
3	8.0484453e-02	2.60e-03	8.21e-05	-3.7
4	7.0700065e-02	2.54e-02	5.27e-05	-5.3
5	6.4963211e-02	3.19e-02	3.11e-05	-6.0
6	6.2723883e-02	1.94e-02	1.34e-05	-6.7
7	6.2104058e-02	4.20e-04	5.95e-06	-7.5
8	6.1489342e-02	6.24e-03	1.73e-05	-5.7
9	6.0811522e-02	4.75e-03	5.91e-06	-6.3
10	6.1742088e-02	4.22e-03	4.35e-06	-7.5
11	6.1493287e-02	6.98e-03	1.52e-06	-8.5
12	6.1319627e-02	2.66e-03	1.27e-06	-8.5
13	6.1194006e-02	6.83e-04	2.05e-05	-7.2
14	6.1479802e-02	1.06e-04	3.77e-06	-8.1
15	6.1436516e-02	1.96e-03	2.05e-06	-8.4
16	6.1376586e-02	1.82e-03	1.18e-06	-8.5
⋮	⋮	⋮	⋮	⋮
54	6.1353638e-02	1.95e-04	4.92e-08	-11.0
55	6.1348571e-02	1.15e-04	4.77e-08	-11.0
56	6.1343038e-02	1.13e-05	1.16e-07	-11.0
57	6.1342728e-02	1.04e-04	4.41e-07	-9.2
58	6.1353468e-02	1.29e-05	4.83e-07	-9.2
59	6.1353390e-02	1.16e-05	2.40e-07	-9.2
60	6.1350801e-02	9.92e-05	5.13e-07	-9.2
61	6.1345441e-02	4.69e-05	7.19e-08	-9.2
62	6.1343117e-02	5.36e-05	1.27e-07	-9.2
63	6.1345692e-02	4.71e-05	3.91e-08	-9.2
64	6.1348028e-02	7.23e-09	2.39e-08	-9.2

Table 6.4: Convergence results for stationary flow with $\nu = 0.001$ using the pseudo-solid approach

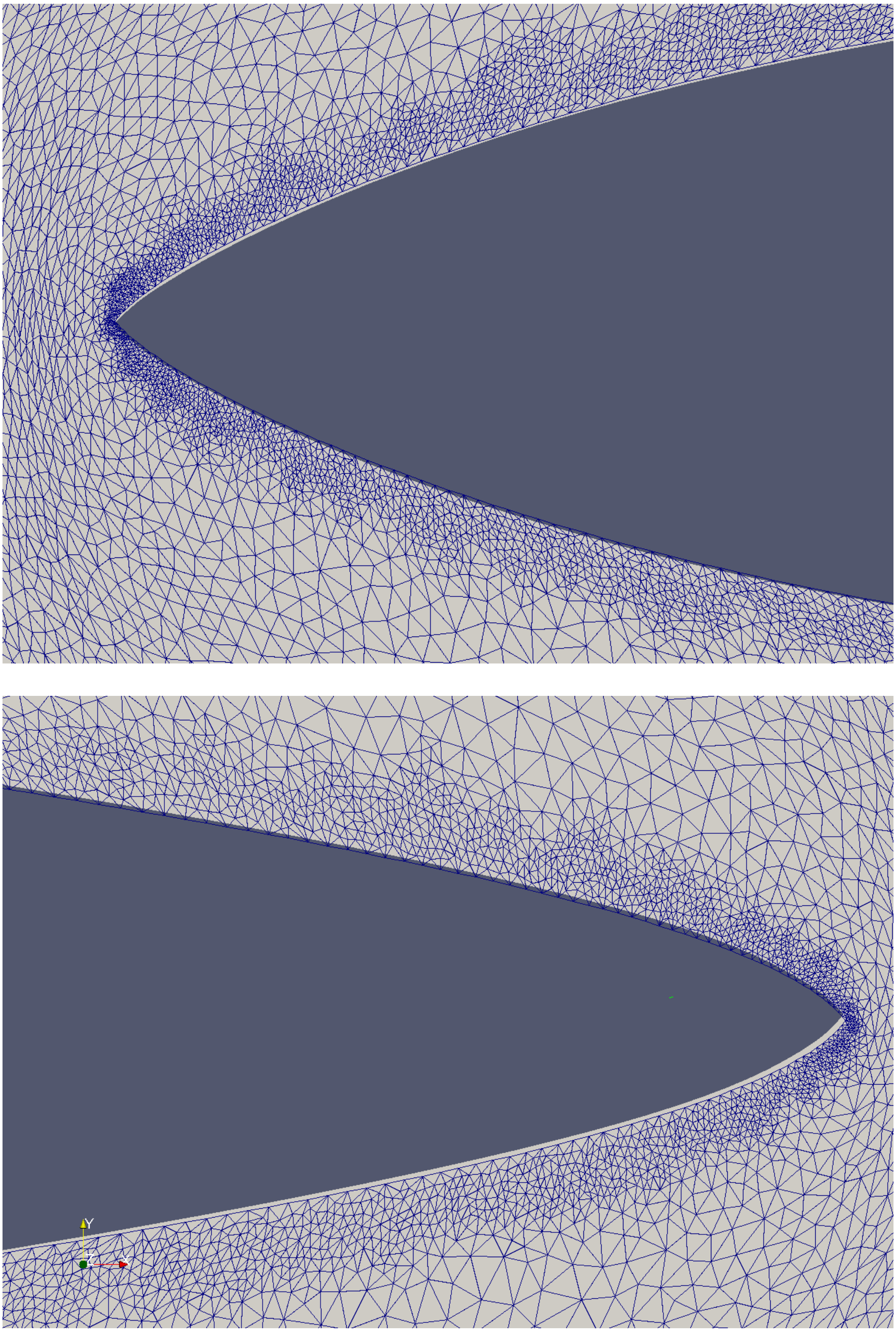

Figure 6.6: Comparison of the optimal shapes for stationary flow with $\nu = 0.001$: B-Spline parametrization (blue grid) and pseudo-solid approach (grey surface).

Section 6.2 but add a second object, see Figure 6.7.

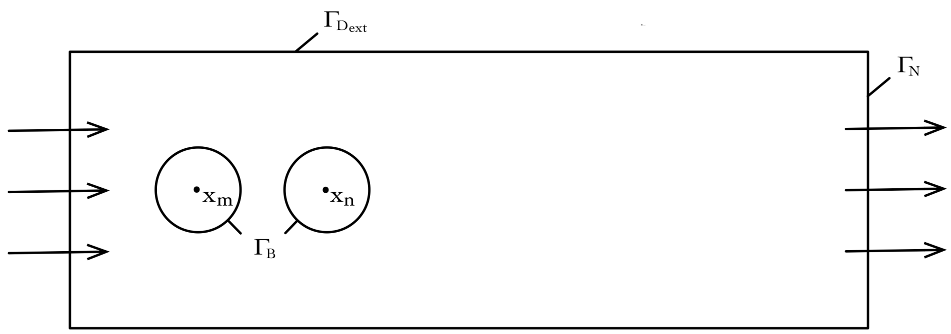

Figure 6.7: Flow around two objects in a row

The reference object is a setting with two bodies in a row, one with origin $x_m := (0.2, 0.2)$ and one with origin $x_n := (0.5, 0.2)$. For each object we have 240 boundary points such that we have 960 optimization variables. Again we fix the center of mass for both objects at the circle origins x_n and x_m and impose the same volume constraint for each object individually. Furthermore we have again box constraints.
The reference mesh has 94228 vertices which results in a grid with 185898 triangles. The fine region includes both objects. We do not use remeshing in this calculation.
For $\nu = 0.01$ IPOPT converges to the optimal solution in 48 iterations, see Table 6.5. Here only 3 iterations need more than one line search step.
In Figure 6.8 the initial shapes and the optimal shapes are shown. In the optimal design, the second object has a slightly smaller width than the first one. Furthermore the first object is wider than the optimal object for the stationary flow around one body.

6.3.2 Shape Optimization for the Instationary Navier-Stokes Equations

We consider here the flow around one object with small viscosities $\nu < 0.001$. Here, the velocity and pressure states are time-dependent and can result for small viscosities in alternating vortices behind the object. Therefore the instationary Navier-Stokes equations are used to model this scenario.
Usually the Reynolds number is used to characterize different flow regimes, such as turbulent and laminar flows. In our case it is defined by

$$Re = \frac{||\bar{v}||D}{\nu}$$

where $\bar{v}$ describes the characteristic velocity of the flow and D ist the width of the object. As described in Section 2.2 of [62] the characteristic velocity in the DFG benchmark problem is given by the mean velocity

$$\bar{v} = \frac{2}{3}\tilde{\boldsymbol{v}}(\begin{pmatrix} 0 \\ b \end{pmatrix}, 0).$$

It	objective	inf_pr	inf_dual	lg(μ)
0	5.8395197e-01	2.60e-05	2.38e-04	0.0
1	5.8243451e-01	2.60e-05	2.40e-02	-5.0
2	5.7817990e-01	3.36e-08	1.30e-04	-2.8
3	5.1048863e-01	2.61e-05	1.81e-04	-3.7
4	4.7659224e-01	2.44e-04	9.87e-05	-5.2
5	4.6717448e-01	3.19e-04	5.12e-05	-6.0
6	4.7168616e-01	1.82e-04	3.05e-05	-6.8
7	4.7675765e-01	2.04e-04	2.99e-05	-7.7
8	4.7343078e-01	5.80e-04	3.73e-05	-6.5
9	4.6351735e-01	5.43e-04	2.10e-05	-6.6
10	4.5993220e-01	1.70e-04	2.05e-05	-6.6
11	4.7125664e-01	1.23e-04	1.10e-05	-7.9
12	4.7031782e-01	2.07e-04	5.08e-05	-6.9
13	4.6377310e-01	1.57e-04	5.28e-06	-7.0
14	4.6401440e-01	1.53e-04	3.42e-06	-8.9
15	4.6347191e-01	2.81e-04	4.25e-06	-9.7
16	4.6777825e-01	1.86e-04	3.53e-06	-9.8
17	4.7002832e-01	1.59e-04	6.58e-06	-9.8
18	4.6882747e-01	8.59e-05	6.56e-06	-9.8
19	4.6657649e-01	1.62e-04	2.17e-06	-7.6
⋮	⋮	⋮	⋮	⋮
33	4.6809007e-01	9.30e-05	4.84e+02	-9.3
34	4.6830574e-01	1.07e-04	2.30e-01	-6.8
35	4.6850829e-01	5.99e-05	3.13e-03	-7.6
36	4.6849687e-01	4.63e-05	1.43e-04	-7.5
37	4.6828262e-01	1.06e-04	2.03e-06	-9.1
38	4.6808070e-01	5.99e-05	3.01e-07	-9.3
39	4.6809215e-01	4.64e-05	4.41e-07	-8.9
40	4.6849684e-01	4.62e-05	3.85e-07	-9.3
41	4.6828294e-01	1.06e-04	3.92e-07	-8.7
42	4.6808026e-01	5.98e-05	1.70e-07	-8.8
43	4.6809165e-01	4.64e-05	1.06e-07	-8.8
44	4.6821860e-01	1.87e-05	1.85e-02	-9.3
45	4.6825785e-01	5.76e-06	3.15e-08	-9.3
46	4.6836850e-01	2.43e-05	1.28e-06	-9.2
47	4.6829303e-01	2.43e-05	3.21e-07	-9.3
48	4.6821926e-01	1.04e-07	2.99e-07	-9.3

Table 6.5: Convergence results for stationary flow around two objects with $\nu = 0.01$ using the pseudo solid approach.

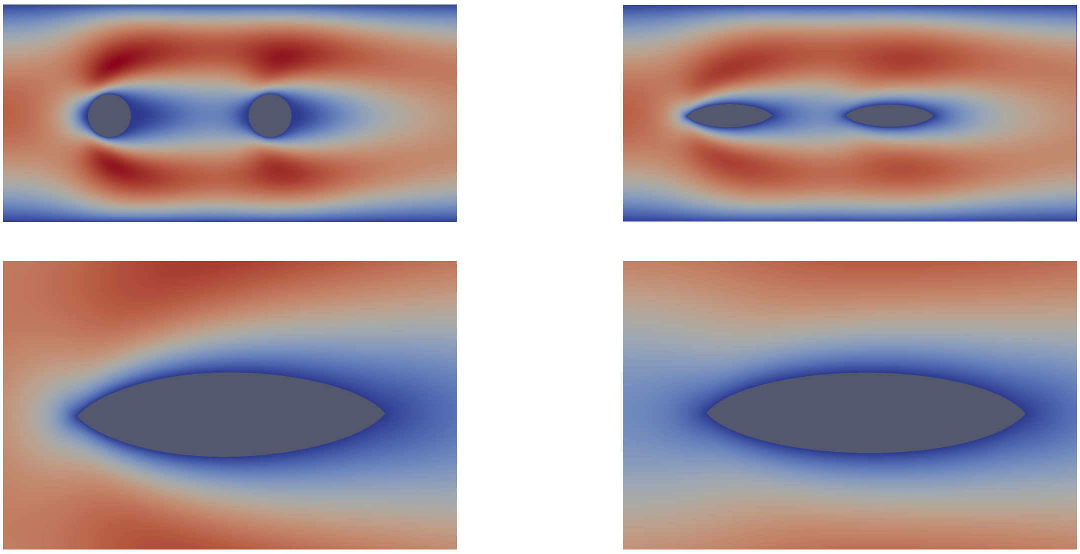

Figure 6.8: Initial and optimal design for stationary flow around two objects with $\nu = 0.01$ using the pseudo-solid approach

Given the initial condition in (6.2) we arrive at

$$\bar{v} = \frac{2}{3} \begin{pmatrix} V_m \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Thus the Reynolds number ist given by

$$Re = \frac{D}{\nu}.$$

Since a state solve for the instationary Navier-Stokes equations is more expensive than for the stationary case, a small number of optimization iterations is even more important in this case. Because the numerical results for the stationary test cases showed that the B-spline parametrization and the pseudo-solid approach generated similar optimal solutions but the pseudo-solid approach needed more iterations, we will mostly use the B-splines to model the object shape.

6.3.2.1 Parametrization via B-splines

Again we consider the case where the object is parametrized using symmetric B-splines curves with 7 B-spline control points as for stationary case. The symmetric axis is fixed to $y_c = 0.2$.
We consider a starting object where we have vortices behind the body that oscillate in time, see Figure 6.9. The width of the start object is about $0.05m$ which results to a Reynolds number of $Re \approx 200$. The volume of the starting object is even smaller than our desired volume. The initial mesh consists of 109240 triangles and is especially fine in the flow region around the object. Since

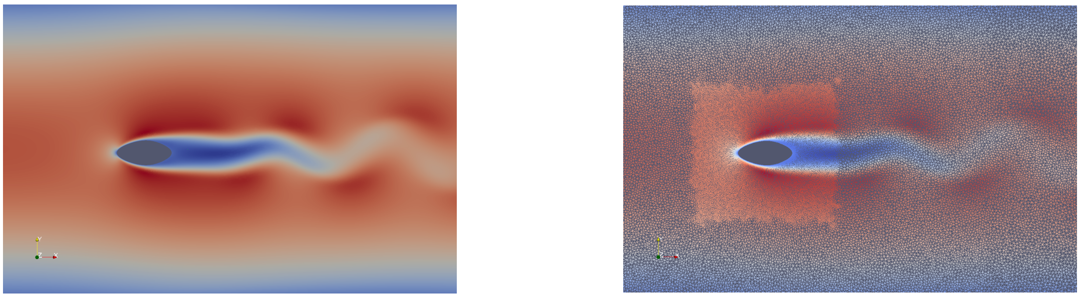

Figure 6.9: Initial design for instationary flow with ν=2.5e–04 using B-spline parametrization

for smaller viscosities the design deformations are larger than for the stationary case, we decided for remeshing if the objective values change significantly. The time interval is given by $I = [0, 1.05]$ where we use 300 time steps á 0.0035 seconds.
We impose the same constraints as in the stationary case: We have a volume constraint on B and demand B to have the center of mass $x_c = (0.2, 0.2)$. Furthermore we have 4 inequality constraints for the order of the spline control points in x direction and box constraints for the B-spline control points.
The computations are done in a parallel setting where we use 16 processes distributed on four Quad-cores.
For a kinematic viscosity ν=2.5e–04, IPOPT converges in 21 iterations to a solution, see Table 6.6 for details. In the optimal solution no box constraint and no inequality constraint is active. Furthermore in each iteration only one line search step is taken except for the iterates 14 (2 steps) and 15 (3 steps). In total 25 state and 22 adjoint solves were needed. The optimal design is shown in Figure 6.10. Remeshing was done after iteration 1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 16 and 17.
We consider now a smaller viscosity ν = 1.5e–04 which results in a Reynolds number of nearly 350. We use the same parametrization and constraints as above. However, we use a time interval of one second where we use 334 time steps of 0.003 seconds. In this scenario we use the optimal design generated by the shape optimization for the stationary problem ($\nu = 0.001$) as starting point (see Table 6.2). The initial mesh of the start object has 87088 nodes and 171776 elements. IPOPT converges in 13 iterations to the optimum where in each iterate only one line search step is performed, see Table 6.7. In the solution no box constraint is active. The optimal design is shown in Figure 6.11.
Since we used the optimal design for the stationary flow at $\nu = 0.001$ as starting design we can compare the drag reduction with respect to the stationary solution. In fact, the drag is reduced by about 2.29 percent.

6.3.2.2 Parametrization via the Pseudo-Solid Approach

We consider a similar setting as the last subsection but use the pseudo-solid approach for the designs. As for the stationary case we use a free vector field to

It	objective	`inf_pr`	`inf_dual`	lg(μ)
0	3.1693521e-02	3.19e-03	7.34e-01	0.0
1	8.1004577e-02	1.48e-03	6.99e+00	-1.6
2	3.9417936e-02	8.20e-04	4.02e+00	-0.9
3	3.7989691e-02	3.03e-05	3.05e-01	-2.2
4	3.7425804e-02	1.57e-05	6.32e-02	-3.1
5	3.6553293e-02	1.65e-04	2.54e-02	-4.1
6	3.6073307e-02	1.39e-04	3.80e-02	-5.1
7	3.5949184e-02	9.81e-05	1.71e-02	-5.7
8	3.5830011e-02	7.17e-05	4.36e-02	-5.5
9	3.5740887e-02	4.23e-06	4.81e-02	-5.3
10	3.5964354e-02	2.66e-07	8.03e-02	-5.7
11	3.5732411e-02	2.12e-05	5.66e-03	-5.2
12	3.5704308e-02	1.76e-06	6.02e-03	-6.5
13	3.5670348e-02	1.89e-06	8.34e-03	-7.6
14	3.5667175e-02	2.51e-06	9.48e-03	-7.7
15	3.5665333e-02	2.85e-06	6.48e-03	-7.1
16	3.6136347e-02	5.92e-07	1.59e-01	-8.4
17	3.5664369e-02	5.21e-07	1.64e-03	-7.5
18	3.5663452e-02	1.31e-09	2.27e-03	-7.6
19	3.5662822e-02	3.76e-08	1.58e-03	-9.0
20	3.5662515e-02	1.24e-07	1.04e-03	-10.4
21	3.5662351e-02	8.52e-08	8.76e-04	-9.7

Table 6.6: Convergence results for instationary flow with ν=2.5e–04 using B-spline parametrization

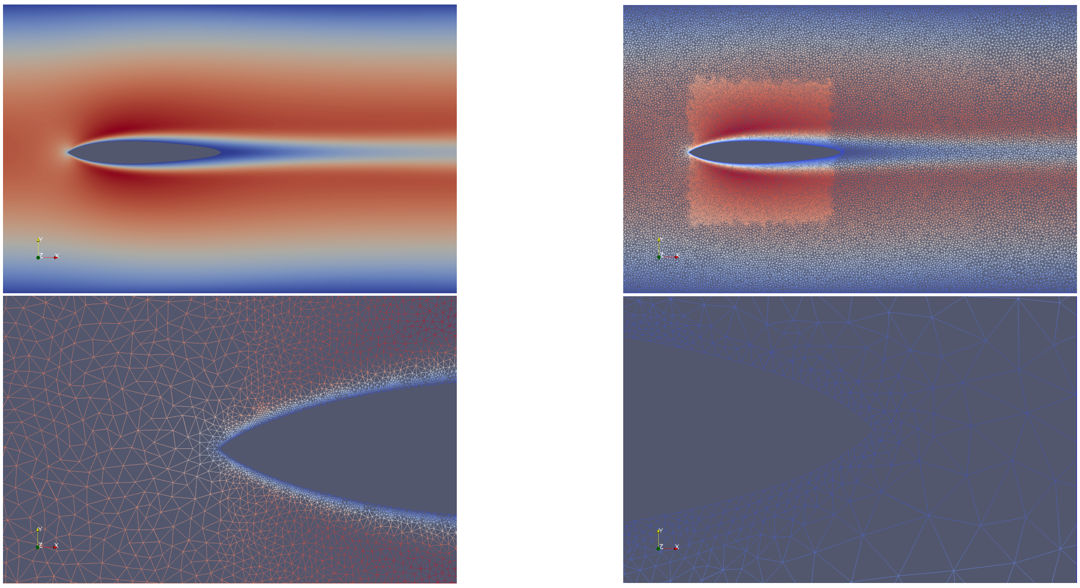

Figure 6.10: Optimal design for instationary flow with ν=2.5e–04 using B-spline parametrization

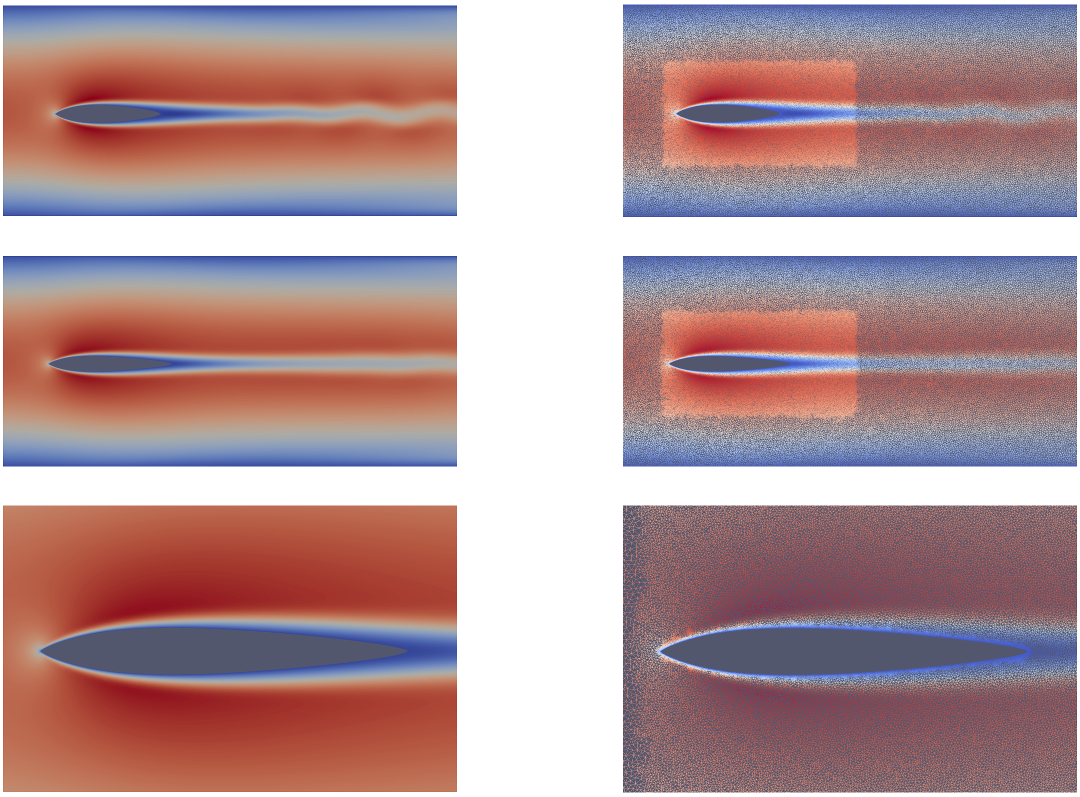

Figure 6.11: Initial design (first row) and optimal design for instationary flow with ν=1.5e–04 using B-spline parametrization

It	objective	`inf_pr`	`inf_dual`	lg(μ)
0	2.7866677e-02	1.60e-07	6.12e-01	0.0
1	2.7721688e-02	4.20e-06	3.71e-02	-3.2
2	2.7541593e-02	1.81e-05	1.11e-02	-4.2
3	2.7444523e-02	9.33e-06	2.21e-02	-5.2
4	2.7278780e-02	2.23e-05	2.99e-02	-5.4
5	2.7194185e-02	3.35e-04	2.46e-02	-5.8
6	2.7316591e-02	1.24e-05	3.33e-02	-5.0
7	2.7229945e-02	1.33e-04	7.57e-03	-4.8
8	2.7230666e-02	4.56e-06	4.87e-03	-5.7
9	2.7237123e-02	1.60e-06	1.31e-02	-6.7
10	2.7229476e-02	1.66e-05	1.36e-02	-7.3
11	2.7222232e-02	4.71e-05	5.40e-03	-5.7
12	2.7231127e-02	1.04e-05	4.54e-03	-6.9
13	2.7229643e-02	1.45e-07	9.40e-05	-7.0

Table 6.7: Convergence results for instationary flow with ν=1.5e–04 using B-spline parametrization.

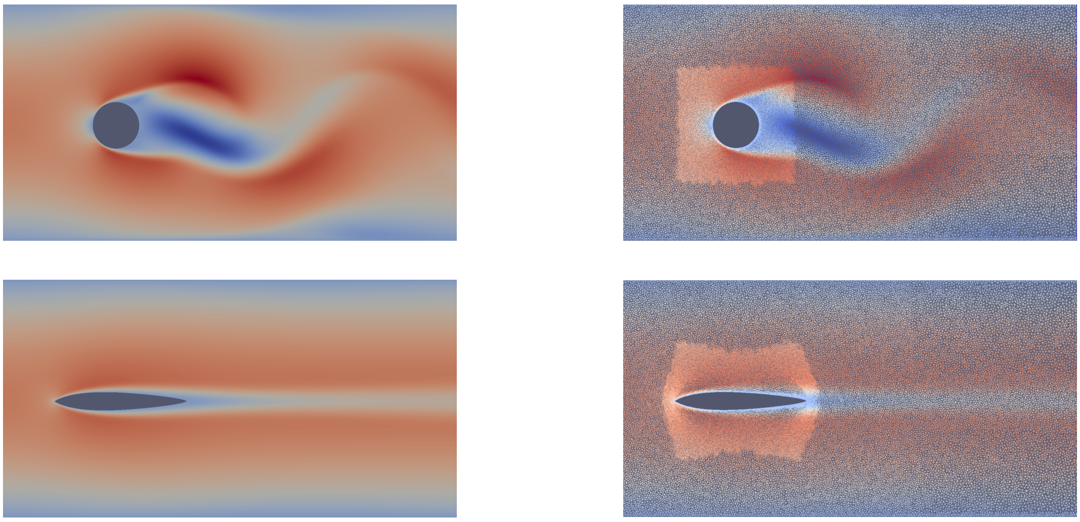

Figure 6.12: Initial design (first row) and optimal design for instationary flow with ν=2.5e–04 using the pseudo-solid approach

model the boundary forces. The same volume and center of mass constraints are are imposed as box constraints for the free vector field.
We look at a viscosity ν = 2.5e–04. The reference object and initial design is given by the circle with diameter $d = 0.08$ and origin $x_c = (0.2, 0.2)$. The time interval $I = [0, 1.05]$ is considered with 300 time steps á 0.0035 seconds. The initial mesh consists of 61641 nodes and 120962 elements. The object boundary mesh has 240 points such that we have 480 optimization variables. As in the stationary case IPOPT needs more iterations compared with B-spline parametrization. In fact 48 iterations are needed to drop under the convergence tolerance, see Table 6.8. In all but one iteration only one line search step is performed. The optimal design can be seen in Figure 6.12. Compared with the symmetric B-spline approach the optimal solution is about 0.17 percent better.

It	objective	inf_pr	inf_dual	lg(μ)
0	9.6753268e-02	2.60e-03	1.04e-03	0.0
1	9.6310373e-02	2.60e-03	2.34e-02	-5.0
2	1.1020100e-01	3.33e-06	9.58e-04	-2.8
3	1.0612561e-01	2.95e-03	1.55e-03	-4.6
4	1.0200734e-01	2.98e-03	6.47e-04	-4.5
5	6.6535030e-02	1.41e-04	5.23e-04	-4.5
6	5.3047359e-02	7.06e-03	2.26e-04	-5.1
7	4.3635338e-02	3.39e-02	1.04e-04	-5.9
8	3.9750705e-02	3.51e-02	4.49e-05	-6.8
9	3.8647792e-02	8.78e-03	2.09e-05	-7.6
10	3.7031718e-02	2.06e-02	1.25e-05	-5.4
11	3.6533612e-02	1.43e-02	2.81e-05	-5.6
12	3.4644767e-02	1.74e-02	1.21e-05	-6.3
13	3.6097598e-02	4.79e-03	5.86e-06	-6.8
14	3.6061102e-02	6.19e-03	1.54e-05	-6.1
15	3.5501343e-02	7.60e-04	2.53e-06	-6.7
16	3.5880467e-02	4.93e-04	1.75e-06	-7.0
17	3.5924926e-02	3.28e-03	5.69e-06	-6.0
18	3.5818070e-02	1.76e-04	1.68e-05	-6.1
19	3.5512842e-02	4.20e-03	3.82e-06	-6.4
20	3.5818567e-02	4.69e-04	3.16e-06	-6.5
21	3.5822887e-02	4.35e-04	1.85e-06	-6.5
22	3.5615805e-02	3.72e-03	2.64e-06	-6.5
23	3.5534352e-02	6.12e-04	7.45e-06	-6.5
24	3.5468965e-02	5.17e-03	2.15e-06	-7.1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
37	3.5575500e-02	5.83e-05	1.57e-06	-8.0
38	3.5572982e-02	5.23e-04	2.80e-07	-8.5
39	3.5602083e-02	4.84e-04	5.17e-07	-8.5
40	3.5626563e-02	3.30e-05	3.43e-07	-8.5
41	3.5601700e-02	4.12e-04	6.64e-07	-9.1
42	3.5576416e-02	3.78e-05	2.23e-07	-9.2
43	3.5619958e-02	3.69e-05	1.05e-07	-9.6
44	3.5619705e-02	3.33e-04	1.17e-07	-10.5
45	3.5613190e-02	2.96e-04	1.08e-07	-10.6
46	3.5605945e-02	1.80e-04	1.15e-07	-10.6
47	3.5601517e-02	6.30e-05	1.14e-07	-10.6
48	3.5600159e-02	6.24e-06	1.22e-07	-10.6

Table 6.8: Convergence results for instationary flow with ν=2.5e–04 using the pseudo-solid approach

A Boundary Integral Representation of the First Shape Derivative

As described in Section 3.3.3 we can show that the shape derivative (3.63) can be transformed into a boundary integral representation if the states are sufficiently smooth.
The shape derivative (3.63) on the physical domain $\Omega = \tau(\Omega_{\text{ref}})$ is given by:

$$
\begin{aligned}
\langle \tilde{j}'(\text{id}), \tilde{V} \rangle_{S^*,S} = \\
&- \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0(\tilde{x}) \tilde{\boldsymbol{\lambda}}(\tilde{x}, 0)\ d\tilde{x} \\
&+ \int_I \int_\Omega \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V}\ d\tilde{x}\ dt + \int_I \int_\Omega \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V}\ d\tilde{x}\ dt \\
&- \int_I \int_\Omega \sum_{i=1}^{d} \nu \nabla \tilde{\boldsymbol{v}}_i^T (\tilde{V}' + \tilde{V}'^T) \nabla \tilde{\boldsymbol{\lambda}}_i\ d\tilde{x}\ dt \\
&- \int_I \int_\Omega \tilde{\boldsymbol{v}}^T \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}}\ d\tilde{x}\ dt + \int_I \int_\Omega \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V}\ d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \tilde{p} \text{ tr } (\tilde{V}'^T \nabla \tilde{\boldsymbol{\lambda}})\ d\tilde{x}\ dt - \int_I \int_\Omega \tilde{p} \text{ div } \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V}\ d\tilde{x}\ dt \\
&- \int_I \int_\Omega \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V}\ d\tilde{x}\ dt - \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}}\ d\tilde{x}\ dt \\
&- \int_I \int_\Omega \tilde{\mu} \text{ tr } (\tilde{V}'^T \nabla \tilde{\boldsymbol{v}})\ d\tilde{x}\ dt + \int_I \int_\Omega \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}} \text{ div } \tilde{V}\ d\tilde{x}\ dt \\
&+ \int_I \int_\Omega f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \text{ div } \tilde{V}\ d\tilde{x}\ dt \\
&- \int_I \int_\Omega \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}}\ d\tilde{x}\ dt \\
&+ \int_I \int_\Omega \frac{\partial}{\partial \tilde{x}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\, V\ d\tilde{x}\ dt \\
&+ \int_\Omega f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \text{ div } \tilde{V}\ d\tilde{x} \\
&+ \int_\Omega \frac{\partial}{\partial \tilde{x}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}\ d\tilde{x}.
\end{aligned}
\tag{A.1}
$$

We will use integration by parts to reformulate (A.1) as a boundary integral. In a first step we state some useful identities that we will use frequently.

Useful Identities

$$\int_\Omega \tilde{u} \text{ div } \tilde{\boldsymbol{v}} \; d\tilde{x} = -\int_\Omega \nabla \tilde{u}^T \tilde{\boldsymbol{v}} \; d\tilde{x} + \int_{\partial\Omega} \tilde{u} \; \tilde{\boldsymbol{v}}^T \tilde{n} \; dS, \tag{A.2}$$

$$\begin{aligned}\int_\Omega \tilde{\boldsymbol{v}}^T \tilde{V}' \tilde{\boldsymbol{w}} d\tilde{x} = & -\int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}^T \tilde{\boldsymbol{w}} \; d\tilde{x} - \int_\Omega \tilde{V}^T \tilde{\boldsymbol{v}} \text{ div } \tilde{\boldsymbol{w}} \; d\tilde{x} \\ & + \int_{\partial\Omega} \tilde{V}^T \tilde{\boldsymbol{v}} \; \tilde{\boldsymbol{w}}^T \tilde{n} \; dS,\end{aligned} \tag{A.3}$$

$$\begin{aligned}\int_\Omega \tilde{\boldsymbol{v}}^T \tilde{V}'^T \tilde{\boldsymbol{w}} d\tilde{x} = & -\int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{v}} \; d\tilde{x} - \int_\Omega \tilde{V}^T \tilde{\boldsymbol{w}} \text{ div } v \; d\tilde{x} \\ & + \int_{\partial\Omega} \tilde{V}^T \tilde{\boldsymbol{w}} \; \tilde{\boldsymbol{v}}^T \tilde{n} \; dS,\end{aligned} \tag{A.4}$$

$$\begin{aligned}\int_\Omega \tilde{p} \text{ tr } (\tilde{V}'^T \nabla \tilde{\boldsymbol{v}}) \; d\tilde{x} = & -\int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \nabla \tilde{p} \; d\tilde{x} - \int_\Omega \tilde{p} \tilde{V}^T (\nabla \text{ div } \tilde{\boldsymbol{v}}) \; d\tilde{x} \\ & + \int_{\partial\Omega} \tilde{p} \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{n} \; dS,\end{aligned} \tag{A.5}$$

$$\begin{aligned}\int_\Omega \tilde{p} \text{ div } \tilde{\boldsymbol{v}} \text{ div } \tilde{V} \; d\tilde{x} = & -\int_\Omega \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \nabla \tilde{p} \; d\tilde{x} - \int_\Omega \tilde{p} (\nabla \text{ div } \tilde{\boldsymbol{v}})^T \tilde{V} \; d\tilde{x} \\ & + \int_{\partial\Omega} \tilde{p} \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \tilde{n} \; dS,\end{aligned} \tag{A.6}$$

$$\nabla(\tilde{\boldsymbol{v}}^T \tilde{\boldsymbol{w}}) = (\nabla \tilde{\boldsymbol{v}}) \tilde{\boldsymbol{w}} + (\nabla \tilde{\boldsymbol{w}}) \tilde{\boldsymbol{v}}, \tag{A.7}$$

$$\nabla\left((\nabla \tilde{\boldsymbol{v}}) \tilde{\boldsymbol{w}}\right) = \left(\sum_{i=1}^d \frac{\partial^2 \tilde{\boldsymbol{v}}_i}{\partial \tilde{x}_k \partial \tilde{x}_l} \tilde{\boldsymbol{w}}_i + \sum_{i=1}^d \frac{\partial \tilde{\boldsymbol{v}}_i}{\partial \tilde{x}_l} \frac{\partial \tilde{\boldsymbol{w}}_i}{\partial \tilde{x}_k} \right)_{k,l=1}^d \tag{A.8}$$

$$= \left(\sum_{i=1}^d \frac{\partial^2 \tilde{\boldsymbol{v}}_i}{\partial \tilde{x}_k \partial \tilde{x}_l} \tilde{\boldsymbol{w}}_i \right)_{k,l=1}^d + \nabla \tilde{\boldsymbol{w}} \nabla \tilde{\boldsymbol{v}}^T, \tag{A.9}$$

$$\nabla\left(\nabla \tilde{\boldsymbol{v}}^T \tilde{\boldsymbol{w}}\right) = \left(\sum_{i=1}^d \frac{\partial^2 \tilde{\boldsymbol{v}}_l}{\partial \tilde{x}_k \partial \tilde{x}_i} \tilde{\boldsymbol{w}}_i + \sum_{i=1}^d \frac{\partial \tilde{\boldsymbol{v}}_l}{\partial \tilde{x}_i} \frac{\partial \tilde{\boldsymbol{w}}_i}{\partial \tilde{x}_k} \right)_{k,l=1}^d \tag{A.10}$$

$$= \left(\sum_{i=1}^d \frac{\partial^2 \tilde{\boldsymbol{v}}_l}{\partial \tilde{x}_k \partial \tilde{x}_i} \tilde{\boldsymbol{w}}_i \right)_{k,l=1}^d + \nabla \tilde{\boldsymbol{w}} \nabla \tilde{\boldsymbol{v}}, \tag{A.11}$$

$$\text{div } (\tilde{p} \tilde{\boldsymbol{v}}) = \nabla \tilde{p}^T \tilde{\boldsymbol{v}} + \tilde{p} \text{ div } \tilde{\boldsymbol{v}}. \tag{A.12}$$

Integration by Parts

Let the terms in (A.1) be numbered ascendingly. Assuming sufficient regularity for the states we arrive at the following expressions.
For the first two terms we obtain:

$$
\begin{aligned}
&\int_I \int_\Omega \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \; d\tilde{x} \; dt - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0(\tilde{x}) \tilde{\boldsymbol{\lambda}}(\tilde{x}, 0) \; d\tilde{x} \\
&= \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{v}}_t \tilde{\boldsymbol{\lambda}} - \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{v}}_t \; d\tilde{x} \; dt + \int_I \int_{\partial\Omega} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \tilde{V}^T \tilde{n} \; dS \; dt \\
&\quad - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0(\tilde{x}) \tilde{\boldsymbol{\lambda}}(\tilde{x}, 0) \; d\tilde{x} \\
&= \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{v}}_t \; d\tilde{x} \; dt + \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}}_t \; d\tilde{x} \; dt \\
&\quad - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) \tilde{\boldsymbol{\lambda}}(\tilde{x}, T) \; d\tilde{x} + \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, 0) \tilde{\boldsymbol{\lambda}}(\tilde{x}, 0) \; d\tilde{x} \\
&\quad - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_0(\tilde{x}) \tilde{\boldsymbol{\lambda}}(\tilde{x}, 0) \; d\tilde{x} + \int_I \int_{\partial\Omega} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \tilde{V}^T \tilde{n} \; dS \; dt \\
&= \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{v}}_t \; d\tilde{x} \; dt + \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}}_t \; d\tilde{x} \; dt \\
&\quad + \int_I \int_{\partial\Omega} \tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} \tilde{V}^T \tilde{n} \; dS \; dt - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) \tilde{\boldsymbol{\lambda}}(\tilde{x}, T) \; d\tilde{x}.
\end{aligned}
$$

Using (A.2), (A.3) and (A.4) we obtain for term 3 and 4:

$$
\begin{aligned}
&\int_I \int_\Omega \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} \operatorname{div} \tilde{V} \, d\tilde{x} \, dt - \sum_{i=1}^d \int_I \int_\Omega \nu \nabla \tilde{\boldsymbol{v}}_i^T (\tilde{V}' + \tilde{V}'^T) \nabla \tilde{\boldsymbol{\lambda}}_i \, d\tilde{x} \, dt \\
&= - \int_I \int_\Omega \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}}) \, d\tilde{x} \, dt + \int_I \int_{\partial\Omega} \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} (\tilde{V}^T \tilde{n}) \, dS \, dt \\
&\quad + \sum_{i=1}^d \int_I \int_\Omega \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}}_i)^T \nabla \tilde{\boldsymbol{\lambda}}_i + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_i \operatorname{div} \nabla \tilde{\boldsymbol{\lambda}}_i \, d\tilde{x} \, dt \\
&\quad - \sum_{i=1}^d \int_I \int_{\partial\Omega} \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}}_i \nabla \tilde{\boldsymbol{\lambda}}_i^T \tilde{n} \, dS \, dt \\
&\quad + \sum_{i=1}^d \int_I \int_\Omega \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{\lambda}}_i)^T \nabla \tilde{\boldsymbol{v}}_i + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}}_i \operatorname{div} \nabla \tilde{\boldsymbol{v}}_i \, d\tilde{x} \, dt \\
&\quad - \sum_{i=1}^d \int_I \int_{\partial\Omega} \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}}_i \nabla \tilde{\boldsymbol{v}}_i^T \tilde{n} \, dS \, dt \\
&= - \int_I \int_\Omega \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}}) \, d\tilde{x} \, dt + \int_I \int_{\partial\Omega} \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} (\tilde{V}^T \tilde{n}) \, dS \, dt \\
&\quad + \int_I \int_\Omega \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \Delta \tilde{\boldsymbol{\lambda}} + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \Delta \tilde{\boldsymbol{v}} \, d\tilde{x} \, dt \\
&\quad + \sum_{i=1}^d \int_I \int_\Omega \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}}_i)^T \nabla \tilde{\boldsymbol{\lambda}}_i + \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{\lambda}}_i)^T \nabla \tilde{\boldsymbol{v}}_i \, d\tilde{x} \, dt \\
&\quad - \int_I \int_{\partial\Omega} \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \partial_n \tilde{\boldsymbol{\lambda}} - \int_I \int_{\partial\Omega} \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \partial_n \tilde{\boldsymbol{v}} \, dS \, dt \\
&= \int_I \int_\Omega \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \Delta \tilde{\boldsymbol{\lambda}} + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \Delta \tilde{\boldsymbol{v}} \, d\tilde{x} \, dt \\
&\quad + \int_I \int_{\partial\Omega} -\nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \partial_n \tilde{\boldsymbol{\lambda}} - \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \partial_n \tilde{\boldsymbol{v}} + \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} (\tilde{V}^T \tilde{n}) \, dS \, dt.
\end{aligned}
$$

Note that

$$
\nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}}) = \sum_{i=1}^d \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{v}}_i)^T \nabla \tilde{\boldsymbol{\lambda}}_i + \nu \tilde{V}^T \nabla (\nabla \tilde{\boldsymbol{\lambda}}_i)^T \nabla \tilde{\boldsymbol{v}}_i
$$

and the corresponding terms cancel out.

For the fifth and sixth term we arrive at:

$$
\begin{aligned}
&-\int_I\int_\Omega \tilde{\boldsymbol{v}}^T\tilde{V}'^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\ d\tilde{x}\ dt+\int_I\int_\Omega \tilde{\boldsymbol{v}}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\ \text{div}\ \tilde{V}\ d\tilde{x}\ dt\\
&=\int_I\int_\Omega \tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\ \text{div}\ \tilde{\boldsymbol{v}}+\tilde{V}^T(\nabla(\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}))^T\tilde{\boldsymbol{v}}\ d\tilde{x}\ dt\\
&\quad-\int_I\int_{\partial\Omega}\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\tilde{\boldsymbol{v}}^T\tilde{n}\ dS\ dt\\
&\quad-\int_I\int_\Omega(\nabla(\tilde{\boldsymbol{v}}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}))^T\tilde{V}\ d\tilde{x}\ dt+\int_I\int_{\partial\Omega}\tilde{\boldsymbol{v}}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\tilde{V}^T\tilde{n}\ dS\ dt\\
&=\int_I\int_\Omega \tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\ \text{div}\ \tilde{\boldsymbol{v}}+\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\nabla\tilde{\boldsymbol{\lambda}}^T\tilde{\boldsymbol{v}}+\tilde{V}^T\left(\sum_{i=1}^{d}\tfrac{\partial^2\tilde{\boldsymbol{v}}_i}{\partial\tilde{x}_k\partial\tilde{x}_l}\tilde{\boldsymbol{\lambda}}_i\right)_{k,l=1}^{d}\tilde{\boldsymbol{v}}\ d\tilde{x}\ dt\\
&\quad-\int_I\int_{\partial\Omega}\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\tilde{\boldsymbol{v}}^T\tilde{n}\ dS\ dt\\
&\quad-\int_I\int_\Omega \tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\nabla\tilde{\boldsymbol{v}}^T\tilde{\boldsymbol{v}}+\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}+\tilde{V}^T\left(\sum_{i=1}^{d}\tfrac{\partial^2\tilde{\boldsymbol{v}}_l}{\partial\tilde{x}_k\partial\tilde{x}_i}\tilde{\boldsymbol{v}}_i\right)_{k,l=1}^{d}\tilde{\boldsymbol{\lambda}}\ d\tilde{x}\ dt\\
&\quad+\int_I\int_{\partial\Omega}\tilde{\boldsymbol{v}}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\tilde{V}^T\tilde{n}\ dS\ dt\\
&=\int_I\int_\Omega\ \text{div}\ \tilde{\boldsymbol{v}}\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}+\tilde{V}^T\nabla\tilde{\boldsymbol{v}}(\nabla\tilde{\boldsymbol{\lambda}}^T\tilde{\boldsymbol{v}}-\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}})-\tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\nabla\tilde{\boldsymbol{v}}^T\tilde{\boldsymbol{v}}\ d\tilde{x}\ dt\\
&\quad+\int_I\int_{\partial\Omega}-\tilde{V}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}(\tilde{\boldsymbol{v}}^T\tilde{n})+\tilde{\boldsymbol{v}}^T\nabla\tilde{\boldsymbol{v}}\tilde{\boldsymbol{\lambda}}\tilde{V}^T\tilde{n}\ dS\ dt,
\end{aligned}
$$

where we used (A.2) and (A.4). Furthermore we used div $\tilde{\boldsymbol{v}}=0$ and that the terms $\left(\sum_{i=1}^{d}\frac{\partial^2\tilde{\boldsymbol{v}}_i}{\partial\tilde{x}_k\partial\tilde{x}_l}\tilde{\boldsymbol{\lambda}}_i\right)_{k,l=1}^{d}\tilde{\boldsymbol{v}}$ and $-\left(\sum_{i=1}^{d}\frac{\partial^2\tilde{\boldsymbol{v}}_l}{\partial\tilde{x}_k\partial\tilde{x}_i}\tilde{\boldsymbol{v}}_i\right)_{k,l=1}^{d}\tilde{\boldsymbol{\lambda}}$ cancel out.
For the terms 7 and 8 we use (A.5) and (A.6) and get:

$$
\begin{aligned}
&\int_I\int_\Omega\tilde{p}\ \text{tr}\ (\tilde{V}'^T\nabla\tilde{\boldsymbol{\lambda}})\ d\tilde{x}\ dt-\int_I\int_\Omega\tilde{p}\ \text{div}\ \tilde{\boldsymbol{\lambda}}\ \text{div}\ \tilde{V}\ d\tilde{x}\ dt\\
&=-\int_I\int_\Omega\tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\nabla\tilde{p}+\tilde{p}\tilde{V}^T(\nabla\ \text{div}\ \tilde{\boldsymbol{\lambda}})\ d\tilde{x}\ dt+\int_I\int_{\partial\Omega}\tilde{p}\tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\tilde{n}\ dS\ dt\\
&\quad+\int_I\int_\Omega\ \text{div}\ \tilde{\boldsymbol{\lambda}}\tilde{V}^T\nabla\tilde{p}+\tilde{p}(\nabla\ \text{div}\ \tilde{\boldsymbol{\lambda}})^T\tilde{V}\ d\tilde{x}\ dt-\int_I\int_{\partial\Omega}\tilde{p}\ \text{div}\ \tilde{\boldsymbol{\lambda}}\tilde{V}^T\tilde{n}\ dS\ dt\\
&=\int_I\int_\Omega-\tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\nabla\tilde{p}+\ \text{div}\ \tilde{\boldsymbol{\lambda}}\nabla\tilde{p}^T\tilde{V}\ d\tilde{x}\ dt\\
&\quad+\int_I\int_{\partial\Omega}\tilde{p}\tilde{V}^T\nabla\tilde{\boldsymbol{\lambda}}\tilde{n}-\tilde{p}\ \text{div}\ \tilde{\boldsymbol{\lambda}}\tilde{V}^T\tilde{n}\ dS\ dt,
\end{aligned}
$$

while for term 9 and 10 we obtain:

$$
\begin{aligned}
&- \int_I \int_\Omega \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \text{ div } \tilde{V} \; d\tilde{x} \; dt - \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x} \; dt \\
&= \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}} + \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{f}} \; d\tilde{x} \; dt - \int_I \int_{\partial\Omega} \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \tilde{V}^T \tilde{n} \; dS \; dt \\
&\quad - \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{f}} \tilde{\boldsymbol{\lambda}} \; d\tilde{x} \; dt \\
&= \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{f}} \; d\tilde{x} \; dt - \int_I \int_{\partial\Omega} \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} \tilde{V}^T \tilde{n} \; dS \; dt
\end{aligned}
$$

where we used (A.2).
With (A.5) and (A.6) we get for term 11 and 12 :

$$
\begin{aligned}
&- \int_I \int_\Omega \tilde{\mu} \text{ tr } (\tilde{V}'^T \nabla \tilde{\boldsymbol{v}}) \; d\tilde{x} \; dt + \int_I \int_\Omega \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}} \text{ div } \tilde{V} \; d\tilde{x} \; dt \\
&= \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \nabla \tilde{\mu} + \tilde{\mu} \tilde{V}^T (\nabla \text{ div } \tilde{\boldsymbol{v}}) \; d\tilde{x} \; dt - \int_I \int_{\partial\Omega} \tilde{\mu} \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{n} \; dS \; dt \\
&\quad - \int_I \int_\Omega \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \nabla \tilde{\mu} + \tilde{\mu} (\nabla \text{ div } \tilde{\boldsymbol{v}})^T \tilde{V} \; d\tilde{x} \; dt + \int_I \int_{\partial\Omega} \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \tilde{n} \; dS \; dt \\
&= \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \nabla \tilde{\mu} - \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \nabla \tilde{\mu} \; d\tilde{x} \; dt \\
&\quad + \int_I \int_{\partial\Omega} -\tilde{\mu} \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{n} + \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \tilde{n} \; dS \; dt.
\end{aligned}
$$

For the terms 13 to 15 we arrive at:

$$
\begin{aligned}
&\int_I \int_\Omega f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \text{ div } \tilde{V} \; d\tilde{x} \; dt + \int_I \int_\Omega \frac{\partial}{\partial \tilde{x}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, V \; d\tilde{x} \; dt \\
&- \int_I \int_\Omega \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \; d\tilde{x} \; dt \\
&= \int_I \int_\Omega -\tilde{V}^T \Big(\frac{\partial}{\partial \tilde{x}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\Big)^T - \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \Big(\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\Big)^T \; d\tilde{x} \; dt \\
&\quad + \int_I \int_\Omega - \left(\frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \right) \sum_{j=1}^d \frac{\partial \nabla \tilde{\boldsymbol{v}}}{\partial \tilde{x}_j} \tilde{V}_j \\
&\quad + \int_I \int_{\partial\Omega} f_1(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, t), \nabla \tilde{\boldsymbol{v}}(\tilde{x}, t)) \tilde{V}^T \tilde{n} \; dS \; dt \\
&\quad + \int_I \int_\Omega \frac{\partial}{\partial \tilde{x}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, \tilde{V} \; d\tilde{x} \; dt - \int_I \int_\Omega \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \, \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \; d\tilde{x} \; dt \\
&= - \int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \Big(\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}})\Big)^T \; d\tilde{x} \; dt \\
&\quad - \int_I \int_\Omega \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \left(\sum_{j=1}^d \frac{\partial \nabla \tilde{\boldsymbol{v}}}{\partial \tilde{x}_j} \tilde{V}_j + \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} \right) \; d\tilde{x} \; dt \\
&\quad + \int_I \int_{\partial\Omega} f_1(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, t), \nabla \tilde{\boldsymbol{v}}(\tilde{x}, t)) \tilde{V}^T \tilde{n} \; dS \; dt,
\end{aligned}
$$

where

$$\sum_{j=1}^{d} \frac{\partial \nabla \tilde{\boldsymbol{v}}}{\partial \tilde{x}_j} \tilde{V}_j + \tilde{V}'^T \nabla \tilde{\boldsymbol{v}} = \nabla(\tilde{V}^T \nabla \tilde{\boldsymbol{v}}).$$

Finally for terms 16 and 17 we obtain:

$$\begin{aligned}
&\int_\Omega f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \text{ div } \tilde{V} \ d\tilde{x} + \int_\Omega \frac{\partial}{\partial \tilde{x}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V} \ d\tilde{x} \\
&= \int_\Omega -\tilde{V}^T (\frac{\partial}{\partial \tilde{x}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)))^T \ d\tilde{x} + \int_\Omega \frac{\partial}{\partial \tilde{x}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V} \ d\tilde{x} \\
&\quad - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) (\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)))^T \ d\tilde{x} + \int_{\partial\Omega} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}^T \tilde{n} \ dS \\
&= - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) (\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)))^T \ d\tilde{x} + \int_{\partial\Omega} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}^T \tilde{n} \ dS.
\end{aligned}$$

Derivation of the Boundary Integral Representation

Grouping the expressions of the last subsection and using the state and adjoint equations we can eliminate the domain integrals. For this we test the state and adjoint equations with appropriate test functions.
Testing the state equation with $(\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}}, \tilde{V}^T \nabla \tilde{\mu})$ we have:

$$\begin{aligned}
&\int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{v}}_t + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \Delta \tilde{\boldsymbol{v}} - \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \nabla \tilde{\boldsymbol{v}}^T \tilde{\boldsymbol{v}} - \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \nabla \tilde{p} \\
&\qquad + \tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \tilde{\boldsymbol{f}} - \text{ div } \tilde{\boldsymbol{v}} \tilde{V}^T \nabla \tilde{\mu} \ d\tilde{x} \ dt \\
&= \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \left(\tilde{\boldsymbol{v}}_t - \nu \Delta \tilde{\boldsymbol{v}} + \nabla \tilde{\boldsymbol{v}}^T \tilde{\boldsymbol{v}} + \nabla \tilde{p} - \tilde{\boldsymbol{f}} \right) - \tilde{V}^T \nabla \tilde{\mu} \text{ div } \tilde{\boldsymbol{v}} \ d\tilde{x} \ dt = 0.
\end{aligned}$$

The adjoint equation, tested with $(\tilde{V}^T \nabla \tilde{\boldsymbol{v}}, \tilde{V}^T \nabla \tilde{p})$, looks like:

$$\begin{aligned}
&\int_I \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}}_t + \nu \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \Delta \tilde{\boldsymbol{\lambda}} + \tilde{V}^T \nabla \tilde{\boldsymbol{v}} (\nabla \tilde{\boldsymbol{\lambda}}^T \tilde{\boldsymbol{v}} - \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}}) \\
&\quad + \text{ div } \tilde{\boldsymbol{\lambda}} \nabla \tilde{p}^T \tilde{V} + \tilde{V}^T \nabla \tilde{\boldsymbol{v}} \nabla \tilde{\mu} - \tilde{V}^T \nabla \tilde{\boldsymbol{v}} (\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}))^T \\
&\quad - \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \nabla (\tilde{V}^T \nabla \tilde{\boldsymbol{v}}) \ d\tilde{x} \ dt \\
&= \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{v}} \left(-\tilde{\boldsymbol{\lambda}}_t - \nu \Delta \tilde{\boldsymbol{\lambda}} - \nabla \tilde{\boldsymbol{\lambda}}^T \tilde{\boldsymbol{v}} + \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} - \nabla \tilde{\mu} \right) \ d\tilde{x} \ dt \\
&\quad + \int_I \int_\Omega -\tilde{V}^T \nabla \tilde{\boldsymbol{v}} (\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}))^T - \frac{\partial}{\partial (\nabla \tilde{\boldsymbol{v}})} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \nabla (\tilde{V}^T \nabla \tilde{\boldsymbol{v}}) \ d\tilde{x} \ dt \\
&\quad + \int_I \int_\Omega + \tilde{V}^T \nabla \tilde{p} \text{ div } \tilde{\boldsymbol{\lambda}} \ d\tilde{x} \ dt = 0.
\end{aligned}$$

We test the adjoint initial state equation with $\tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\cdot, T)$ and arrive at:

$$- \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) \tilde{\boldsymbol{\lambda}}(\tilde{x}, T) \ d\tilde{x} - \int_\Omega \tilde{V}^T \nabla \tilde{\boldsymbol{v}}(\tilde{x}, T) (\frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)))^T \ d\tilde{x} = 0.$$

Thus all domain integrals cancel out and we are left over with the boundary integrals:

$$
\begin{aligned}
&\langle \tilde{j}'(\mathrm{id}), \tilde{V}\rangle_{S^*,S} = \\
&\int_I \int_{\partial\Omega} \tilde{V}^T \tilde{n} \left(\tilde{\boldsymbol{v}}_t^T \tilde{\boldsymbol{\lambda}} + \nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{v}}^T \nabla \tilde{\boldsymbol{v}} \tilde{\boldsymbol{\lambda}} - \tilde{p} \operatorname{div} \tilde{\boldsymbol{\lambda}} - \tilde{\boldsymbol{f}}^T \tilde{\boldsymbol{\lambda}} + \tilde{\mu} \operatorname{div} \tilde{\boldsymbol{v}} \right) \, dS \, dt \\
&+ \int_I \int_{\partial\Omega} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}) \tilde{V}^T \tilde{n} \, dS \, dt + \int_{\partial\Omega} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}^T \tilde{n} \, dS \\
&+ \int_I \int_{\partial\Omega} -\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} \left(\nu \partial_n \tilde{\boldsymbol{v}} - \tilde{p} \tilde{n} \right) \, dS \, dt \\
&+ \int_I \int_{\partial\Omega} -\tilde{V}^T \nabla \tilde{\boldsymbol{v}} \left(\nu \partial_n \tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{\lambda}} (\tilde{\boldsymbol{v}}^T \tilde{n}) + \tilde{\mu} \tilde{n} \right) \, dS \, dt.
\end{aligned}
$$

We note that $\tilde{V} = 0$ by (3.43) on the exterior boundary, so we only have to integrate over the object boundary Γ_B. For the last two terms it is not obvious that the boundary integrals depend only on the normal part of $\tilde{V}$ as desired for a Hadamard representation of the shape derivative. However, we can see this by the following observation.

Because $\tilde{\boldsymbol{v}} = 0$ and $\tilde{\boldsymbol{\lambda}} = 0$ on Γ_B we have $\partial_w \tilde{\boldsymbol{v}} = 0$ and $\partial_w \tilde{\boldsymbol{\lambda}} = 0$ for all $w \in < \tilde{n}(\tilde{x}) >^T$ on Γ_B. Hence, if the columns of $T(\tilde{x})$ from an orthonormal basis of the tangent space $< \tilde{n}(\tilde{x}) >^T$ of Γ_B, then $\nabla \tilde{\boldsymbol{v}}^T (T, \tilde{n}) = (0^T, \partial_{\tilde{n}} \tilde{\boldsymbol{v}})$ and $\nabla \tilde{\boldsymbol{\lambda}}^T (T, \tilde{n}) = (0^T, \partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}})$. Thus for all vectors $\boldsymbol{s}$ we have $\nabla \tilde{\boldsymbol{v}}^T \boldsymbol{s} = \nabla \boldsymbol{v}^T (T, \tilde{n})(T, \tilde{n})^T \boldsymbol{s} = \partial_{\tilde{n}} \tilde{\boldsymbol{v}} \; \tilde{n}^T \boldsymbol{s}$ and $\nabla \tilde{\boldsymbol{\lambda}}^T \boldsymbol{s} = \nabla \tilde{\boldsymbol{\lambda}}^T (T, \tilde{n})(T, \tilde{n})^T \boldsymbol{s} = \partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}} \; \tilde{n}^T \boldsymbol{s}$. Especially we have

$$
\begin{aligned}
\tilde{V}^T \nabla \tilde{\boldsymbol{v}} &= (\nabla \tilde{\boldsymbol{v}}^T \tilde{V})^T = (\partial_{\tilde{n}} \tilde{\boldsymbol{v}} \; \tilde{n}^T V)^T = \tilde{V}^T \tilde{n} (\partial_{\tilde{n}} \tilde{\boldsymbol{v}})^T, \\
\tilde{V}^T \nabla \tilde{\boldsymbol{\lambda}} &= (\nabla \tilde{\boldsymbol{\lambda}}^T \tilde{V})^T = (\partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}} \tilde{n}^T V)^T = \tilde{V}^T \tilde{n} (\partial_{\tilde{n}} \tilde{\boldsymbol{\lambda}})^T.
\end{aligned}
$$

on Γ_B.

Thus, we can write the shape derivative as an integral over the object boundary Γ_B and obtain the Hadamard representation:

$$
\begin{aligned}
&\langle \tilde{j}'(\mathrm{id}), \tilde{V}\rangle_{S^*,S} = \\
&\int_I \int_{\Gamma_B} \tilde{V}^T \tilde{n} \left(\nu \nabla \tilde{\boldsymbol{v}} : \nabla \tilde{\boldsymbol{\lambda}} - \tilde{p} \operatorname{div} \tilde{\boldsymbol{\lambda}} + \tilde{\mu} \operatorname{div} \tilde{\boldsymbol{v}} \right) \, dS \, dt \\
&+ \int_I \int_{\Gamma_B} f_1(\tilde{x}, \tilde{\boldsymbol{v}}, \nabla \tilde{\boldsymbol{v}}, \tilde{p}) \tilde{V}^T \tilde{n} \, dS \, dt + \int_{\Gamma_B} f_2(\tilde{x}, \tilde{\boldsymbol{v}}(\tilde{x}, T)) \tilde{V}^T \tilde{n} \, dS \\
&- \int_I \int_{\Gamma_B} (\partial_n \tilde{\boldsymbol{\lambda}})^T \left(\nu \partial_n \tilde{\boldsymbol{v}} - \tilde{p} \tilde{n} \right) \tilde{V}^T n \, dS \, dt \\
&- \int_I \int_{\Gamma_B} (\partial_n \tilde{\boldsymbol{v}})^T \left(\nu \partial_n \tilde{\boldsymbol{\lambda}} + \tilde{\boldsymbol{\lambda}} (\tilde{\boldsymbol{v}}^T \tilde{n}) + \tilde{\mu} \tilde{n} \right) \tilde{V}^T n \, dS \, dt.
\end{aligned}
$$

B Second Derivatives

In the following we calculate the second derivatives of the instationary Navier-Stokes equations operator E and an abstract objective functional J.

B.1 Second Derivatives of E

We will use the following definitions in formula (3.54) of E_τ to document the derivation of the second derivatives $E_{\tau,\tau}$ and $E_{\tau,(v,p)}$:

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu),E_\tau((\boldsymbol{v},p),\tau)V\rangle_{Z_{\mathrm{ref}}{}^*,Z_{\mathrm{ref}}}\\
&=\underbrace{\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}_t^T\boldsymbol{\lambda}\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx}_{=:A}\ dt\\
&\underbrace{+\int_I\int_{\Omega_{\mathrm{ref}}}\sum_{i=1}^d\nu\nabla\boldsymbol{v}_i^T\tau'^{-1}(\ \mathrm{tr}\ (\tau'^{-1}V')I-V'\tau'^{-1}-\tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{\lambda}_i\det\tau'\ dx\ dt}_{=:B}\\
&\underbrace{+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^T(\ \mathrm{tr}\ (\tau'^{-1}V')I-\tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\det\tau'\ dx\ dt}_{=:C}\\
&\underbrace{+\int_I\int_{\Omega_{\mathrm{ref}}}p\left(\ \mathrm{tr}\ (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{\lambda})-\ \mathrm{tr}\ (\tau'^{-T}\nabla\boldsymbol{\lambda})\ \mathrm{tr}\ (\tau'^{-1}V')\right)\det\tau'\ dx\ dt}_{=:D}\\
&\underbrace{-\int_I\int_{\Omega_{\mathrm{ref}}}\left(\tilde{\boldsymbol{f}}(\tau(x),t)^T\ \mathrm{tr}\ (\tau'^{-1}V')+V^T\nabla\tilde{\boldsymbol{f}}(\tau(x),t)\right)\boldsymbol{\lambda}\det\tau'\ dx\ dt}_{=:E}\\
&\underbrace{+\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}(\cdot,0)^T\boldsymbol{\lambda}_0\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx}_{=:F}\\
&\underbrace{-\int_{\Omega_{\mathrm{ref}}}\tilde{\boldsymbol{v}}_0(\tau)^T\boldsymbol{\lambda}_0\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx-\int_{\Omega_{\mathrm{ref}}}V^T\nabla\tilde{\boldsymbol{v}}_0(\tau)\boldsymbol{\lambda}_0\det\tau'\ dx}_{=:G}\\
&\underbrace{-\int_I\int_{\Omega_{\mathrm{ref}}}\mu\left(\ \mathrm{tr}\ (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v})-\ \mathrm{tr}\ (\tau'^{-T}\nabla\boldsymbol{v})\ \mathrm{tr}\ (\tau'^{-1}V')\right)\det\tau'\ dx\ dt}_{=:H}.
\end{aligned}
$$

B.1.1 The second derivative $E_{\tau\tau}$

Let $((\boldsymbol{v},p),\tau) \in Y_{\text{ref}} \times T_{\text{ad}}$, $(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu) \in {Z_{\text{ref}}}^*$ and $V,W \in S$. Then we have

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu), E_{\tau\tau}((\boldsymbol{v},p),\tau)(V)(W)\rangle_{{Z_{\text{ref}}}^*,Z_{\text{ref}}}\\
&= \int_I\int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T\boldsymbol{\lambda}(\text{ tr }(\tau'^{-1}V')\text{ tr }(\tau'^{-1}W') + \text{ tr }(-\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} \sum_{i=1}^d \nu\nabla\boldsymbol{v}_i^T\tau'^{-1}(-W'\tau'^{-1}\kappa + D\kappa + \kappa(\text{ tr }(\tau'^{-1}W')I - \tau'^{-T}W'^T))\tau'^{-T}\nabla\boldsymbol{\lambda}_i\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(-\text{ tr }(\tau'^{-1}W'\tau'^{-1}V')\;I + \tau'^{-T}W'^T\tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(-\text{ tr }(\tau'^{-1}V')\;I + \tau'^{-T}V'^T)\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} \boldsymbol{v}^T(\text{ tr }(\tau'^{-1}V')\;I - \tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\text{ tr }(\tau'^{-1}W')\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} p(\text{ tr }(\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{\lambda}) - \text{ tr }(\tau'^{-T}\nabla\boldsymbol{\lambda})\text{ tr }(\tau'^{-1}V'))\text{ tr }(\tau'^{-1}W')\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} p(-\text{ tr }(\tau'^{-T}W'^T\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{\lambda}) - \text{ tr }(\tau'^{-T}V'^T\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{\lambda})\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} p(\text{ tr }(\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{\lambda})\text{ tr }(\tau'^{-1}V') + \text{ tr }(\tau'^{-T}\nabla\boldsymbol{\lambda})\text{ tr }(\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} W^T\nabla\tilde{\boldsymbol{f}}(\tau(x),t)\boldsymbol{\lambda}\text{ tr }(\tau'^{-1}V')\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(\tau(x),t)^T\boldsymbol{\lambda}(\text{ tr }(\tau'^{-1}V')\text{ tr }(\tau'^{-1}W') + \text{ tr }(-\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\,dt\\
&+ \int_I\int_{\Omega_{\text{ref}}} V^T(\sum_{i=1}^d \nabla^2\tilde{f}_i(\tau(x),t)W\lambda_i + \nabla\tilde{\boldsymbol{f}}(\tau(x),t)\boldsymbol{\lambda}\text{ tr }(\tau'^{-1}W'))\det\tau'\,dx\,dt\\
&+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}(\cdot,0)^T\boldsymbol{\lambda}_0(\text{ tr }(\tau'^{-1}V')\text{ tr }(\tau'^{-1}W') + \text{ tr }(-\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\\
&+ \int_{\Omega_{\text{ref}}} W^T\nabla\tilde{\boldsymbol{v}}_0(\tau)\boldsymbol{\lambda}_0\text{ tr }(\tau'^{-1}V')\det\tau'\,dx\\
&+ \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{v}}_0(\tau)^T\boldsymbol{\lambda}_0(\text{ tr }(\tau'^{-1}V')\text{ tr }(\tau'^{-1}W') + \text{ tr }(-\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\\
&+ \int_{\Omega_{\text{ref}}} V^T(\sum_{i=1}^d \nabla^2(\tilde{v}_0)_i(\tau)W(\lambda_0)_i + \nabla\tilde{\boldsymbol{v}}_0(\tau)\boldsymbol{\lambda}_0\text{ tr }(\tau'^{-1}W'))\det\tau'\,dx\\
&- \int_I\int_{\Omega_{\text{ref}}} \mu(\text{ tr }(\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v}) - \text{ tr }(\tau'^{-T}\nabla\boldsymbol{v})\text{ tr }(\tau'^{-1}V'))\text{ tr }(\tau'^{-1}W')\det\tau'\,dx\,dt\\
&- \int_I\int_{\Omega_{\text{ref}}} \mu(-\text{ tr }(\tau'^{-T}W'^T\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v}) - \text{ tr }(\tau'^{-T}V'^T\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v}))\det\tau'\,dx\,dt\\
&- \int_I\int_{\Omega_{\text{ref}}} \mu(\text{ tr }(\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v})\text{ tr }(\tau'^{-1}V') + \text{ tr }(\tau'^{-T}\nabla\boldsymbol{v})\text{ tr }(\tau'^{-1}W'\tau'^{-1}V'))\det\tau'\,dx\,dt
\end{aligned}
$$

with $\kappa := \text{ tr }(\tau'^{-1}V')I - V'\tau'^{-1} - \tau'^{-T}V'^T$
and $D\kappa = \text{ tr }(-\tau'^{-1}W'\tau'^{-1}V')I + V'\tau'^{-1}W'\tau'^{-1} + \tau'^{-T}W'^T\tau'^{-T}V'^T$ in the second integral.
The first integral comes from part A, the second integral from part B, integrals 3-5 from part C, integrals 6-8 from part D, integrals 9-11 from part E, integral 12 from part F, integrals 13-15 from part G and integrals 16-18 from part H. In 2D the parts C, D and H have no contribution to this derivative, which means that the sum of the integrals 3-8 and 16-18 is zero. Hence, in 2D we can

simplify this further and obtain:

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau\tau}((\boldsymbol{v}, p), \tau)(V)(W)\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda} \ \mathrm{tr}\ (V'^{-1} W') \det V' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \tau'^{-1} (-W' \tau'^{-1} \kappa + D\kappa + \kappa(\ \mathrm{tr}\ (\tau'^{-1} W') I - \tau'^{-T} W'^{T})) \tau'^{-T} \nabla \boldsymbol{\lambda}_i \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} W^T \nabla \tilde{\boldsymbol{f}}(\tau(x), t) \boldsymbol{\lambda} \ \mathrm{tr}\ (\tau'^{-1} V') \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \tilde{\boldsymbol{f}}(\tau(x), t)^T \boldsymbol{\lambda} \ \mathrm{tr}\ (V'^{-1} W') \det V' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} V^T (\sum_{i=1}^{d} \nabla^2 \tilde{\boldsymbol{f}}_i(\tau(x), t) W \boldsymbol{\lambda}_i + \nabla \tilde{\boldsymbol{f}}(\tau(x), t) \boldsymbol{\lambda} \ \mathrm{tr}\ (\tau'^{-1} W')) \det \tau' \ dx \ dt \\
&\quad + \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}(\cdot, 0)^T \boldsymbol{\lambda}_0 \ \mathrm{tr}\ (V'^{-1} W') \det V' \ dx \\
&\quad + \int_{\Omega_{\mathrm{ref}}} W^T \nabla \tilde{v}_0(\tau) \boldsymbol{\lambda}_0 \ \mathrm{tr}\ (\tau'^{-1} V') \det \tau' \ dx + \int_{\Omega_{\mathrm{ref}}} \tilde{\boldsymbol{v}}_0(\tau)^T \boldsymbol{\lambda}_0 \ \mathrm{tr}\ (V'^{-1} W') \det V' \ dx \\
&\quad + \int_{\Omega_{\mathrm{ref}}} V^T (\sum_{i=1}^{d} \nabla^2 (\tilde{\boldsymbol{v}}_0)_i(\tau) W (\boldsymbol{\lambda}_0)_i + \nabla \tilde{\boldsymbol{v}}_0(\tau) \boldsymbol{\lambda}_0 \ \mathrm{tr}\ (\tau'^{-1} W')) \det \tau' \ dx
\end{aligned}
$$

B.1.2 Second derivative $E_{\tau\tau}$ at $\tau = \mathrm{id}$

Let $(\boldsymbol{v}, p) \in Y_{\mathrm{ref}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\mathrm{ref}}}^*$ and $V, W \in S$. Then we have

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau\tau}((\boldsymbol{v}, p), \mathrm{id})(V)(W) \rangle_{{Z_{\mathrm{ref}}}^*, Z_{\mathrm{ref}}} \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda} (\text{ div } V \text{ div } W - \text{ tr } (W' V')) \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{v}_i^T \kappa_2 \nabla \boldsymbol{\lambda}_i \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T (- \text{ tr } (W' V') \, I + W'^T V'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda} \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T (- \text{ div } V W'^T + V'^T W'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda} \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T (\text{ div } V \text{ div } W \, I - \text{ div } W V'^T) \nabla \boldsymbol{v} \boldsymbol{\lambda} \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} p (\text{ tr } (V'^T \nabla \boldsymbol{\lambda}) \text{ div } W + \text{ tr } (W'^T \nabla \boldsymbol{\lambda}) \text{ div } V) \, dx \, dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} p (\text{ tr } (W'^T V'^T \nabla \boldsymbol{\lambda}) + \text{ tr } (V'^T W'^T \nabla \boldsymbol{\lambda})) \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} p \text{ div } \boldsymbol{\lambda} (\text{ tr } (W' V') - \text{ div } (V) \text{ div } (W)) \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} W^T \nabla \tilde{\boldsymbol{f}}(x,t) \boldsymbol{\lambda} \text{ div } V \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \tilde{\boldsymbol{f}}(x,t)^T \boldsymbol{\lambda} (\text{ div } V \text{ div } W - \text{ tr } (W' V')) \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} V^T (\sum_{i=1}^d \nabla^2 \tilde{\boldsymbol{f}}_i(x,t) W \boldsymbol{\lambda}_i + \nabla \tilde{\boldsymbol{f}}(x,t)) \boldsymbol{\lambda} \text{ div } W \, dx \, dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}(\cdot, 0)^T \boldsymbol{\lambda}_0 (\text{ div } V \text{ div } W - \text{ tr } (W' V')) \, dx \\
&+ \int_{\Omega_{\mathrm{ref}}} W^T \nabla \tilde{\boldsymbol{v}}_0 \boldsymbol{\lambda}_0 \text{ div } V \, dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \tilde{\boldsymbol{v}}_0^T \boldsymbol{\lambda}_0 (\text{ div } V \text{ div } W - \text{ tr } (W' V')) \, dx \\
&+ \int_{\Omega_{\mathrm{ref}}} V^T (\sum_{i=1}^d \nabla^2 (\tilde{\boldsymbol{v}}_0)_i W \lambda_0 + \nabla \tilde{\boldsymbol{v}}_0 \boldsymbol{\lambda}_0 \text{ div } W \, dx \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \mu (\text{ tr } (V'^T \nabla \boldsymbol{v}) \text{ div } W + \text{ tr } (W'^T \nabla \boldsymbol{v}) \text{ div } V) \, dx \, dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \mu (\text{ tr } (W'^T V'^T \nabla \boldsymbol{v}) + \text{ tr } (V'^T W'^T \nabla \boldsymbol{v})) \, dx \, dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \mu \text{ div } \boldsymbol{v} (\text{ tr } (W' V') - \text{ div } (V) \text{ div } (W)) \, dx \, dt.
\end{aligned}
$$

with

$$\begin{aligned}\kappa_2 :=& -W'\kappa + D\kappa + \kappa \text{ tr } (W') - \kappa W'^T \\ =& \text{ div } (V)(-W' - W'^T) + \text{div } (W)(-V' - V'^T) + (\text{div } (V)\text{div } (W) - \text{tr } (W'V'))I \\ &+ V'(W' + W'^T) + W'(V' + V'^T) + V'^T W'^T + W'^T V'^T.\end{aligned}$$

In the 2D case we obtain

$$\begin{aligned}&\langle(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau\tau}((\boldsymbol{v}, p), \text{id})(V)(W)\rangle_{Z_{\text{ref}}^*, Z_{\text{ref}}} \\ &= \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}_t^T \boldsymbol{\lambda} \text{ tr } (V'^{-1}W') \det V' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{v}_i^T \kappa_2 \nabla \boldsymbol{\lambda}_i \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} W^T \nabla \tilde{\boldsymbol{f}}(x,t) \boldsymbol{\lambda} \text{ div } V \; dx \; dt + \int_I \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{f}}(x,t)^T \boldsymbol{\lambda} \text{ tr } (V'^{-1}W') \det V' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} V^T (\sum_{i=1}^{d} \nabla^2 \tilde{\boldsymbol{f}}_i(x,t) W \boldsymbol{\lambda}_i + \nabla \tilde{\boldsymbol{f}}(x,t) \boldsymbol{\lambda} \text{ div } W) \; dx \; dt \\ &+ \int_{\Omega_{\text{ref}}} \boldsymbol{v}(\cdot, 0)^T \boldsymbol{\lambda}_0 \text{ tr } (V'^{-1}W') \det V' \; dx \\ &+ \int_{\Omega_{\text{ref}}} W^T \nabla \tilde{v}_0 \boldsymbol{\lambda}_0 \text{ div } V \; dx + \int_{\Omega_{\text{ref}}} \tilde{\boldsymbol{v}}_0^T \boldsymbol{\lambda}_0 \text{ tr } (V'^{-1}W') \det V' \; dx \\ &+ \int_{\Omega_{\text{ref}}} V^T (\sum_{i=1}^{d} \nabla^2 (\tilde{\boldsymbol{v}}_0)_i W (\boldsymbol{\lambda}_0)_i + \nabla \tilde{\boldsymbol{v}}_0 \boldsymbol{\lambda}_0 \text{ div } W) \; dx.\end{aligned}$$

B.1.3 Second derivative $E_{\tau,(v,p)}$

Let $((\boldsymbol{v}, p), \tau) \in Y_{\text{ref}} \times T_{\text{ad}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\text{ref}}}^*$, $V \in S$ and $(\boldsymbol{w}, q) \in Y_{\text{ref}}$. Then we have

$$\begin{aligned}&\langle(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau,(v,p)}((\boldsymbol{v}, p), \tau)(V)(w, q)\rangle_{Z_{\text{ref}}^*, Z_{\text{ref}}} \\ &= \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \text{ tr } (\tau'^{-1}V') \det \tau' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} \sum_{i=1}^{d} \nu \nabla \boldsymbol{w}_i^T \tau'^{-1} (\text{ tr } (\tau'^{-1}V')I - V'\tau'^{-1} - \tau'^{-T}V'^T) \tau'^{-T} \nabla \boldsymbol{\lambda}_i \det \tau' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{w}^T (\text{ tr } (\tau'^{-1}V')I - \tau'^{-T}V'^T) \tau'^{-T} \nabla \boldsymbol{v} \boldsymbol{\lambda} \det \tau' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} \boldsymbol{v}^T (\text{ tr } (\tau'^{-1}V')I - \tau'^{-T}V'^T) \tau'^{-T} \nabla \boldsymbol{w} \boldsymbol{\lambda} \det \tau' \; dx \; dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} q \left(\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{\lambda}) - \text{ tr } (\tau'^{-T}\nabla\boldsymbol{\lambda}) \text{ tr } (\tau'^{-1}V')\right) \det \tau' \; dx \; dt \\ &+ \int_{\Omega_{\text{ref}}} \boldsymbol{w}(\cdot, 0)^T \boldsymbol{\lambda}_0 \text{ tr } (\tau'^{-1}V') \det \tau' \; dx \\ &- \int_I \int_{\Omega_{\text{ref}}} \mu (\text{ tr } (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{w}) - \text{ tr } (\tau'^{-T}\nabla\boldsymbol{w}) \text{ tr } (\tau'^{-1}V')) \det \tau' \; dx \; dt.\end{aligned}$$

In the 2D case we have

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu),E_{\tau,(v,p)}((\boldsymbol{v},p),\tau)(V)(w,q)\rangle_{Z_{\mathrm{ref}}{}^*,Z_{\mathrm{ref}}}\\
&=\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}_t^T\boldsymbol{\lambda}\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx\ dt\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\sum_{i=1}^{d}\nu\nabla\boldsymbol{w}_i^T\tau'^{-1}(\ \mathrm{tr}\ (\tau'^{-1}V')I-V'\tau'^{-1}-\tau'^{-T}V'^T)\tau'^{-T}\nabla\boldsymbol{\lambda}_i\det\tau'\ dx\ dt\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}^TV'^{-T}\nabla\boldsymbol{v}\boldsymbol{\lambda}\det V'\ dx\ dt+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^TV'^{-T}\nabla\boldsymbol{w}\boldsymbol{\lambda}\det V'\ dx\ dt\\
&-\int_I\int_{\Omega_{\mathrm{ref}}}q\ \mathrm{tr}\ (V'^{-T}\nabla\boldsymbol{\lambda})\det V'\ dx\ dt\\
&+\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}(\cdot,0)^T\boldsymbol{\lambda}_0\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\mu\ \mathrm{tr}\ (V'^{-T}\nabla\boldsymbol{w})\det V'\ dx\ dt.
\end{aligned}
$$

B.1.4 Second derivative $E_{\tau,(v,p)}$ at $\tau=\mathrm{id}$

Let $(\boldsymbol{v},p)\in Y_{\mathrm{ref}}$, $(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu)\in Z_{\mathrm{ref}}{}^*$, $V\in S$ and $(\boldsymbol{w},q)\in Y_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle(\boldsymbol{\lambda},\boldsymbol{\lambda}_0,\mu),E_{\tau,(v,p)}((\boldsymbol{v},p),\mathrm{id})(V)(w,q)\rangle_{Z_{\mathrm{ref}}{}^*,Z_{\mathrm{ref}}}\\
&=\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}_t^T\boldsymbol{\lambda}\ \mathrm{div}\ V\ dx\ dt+\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}(\cdot,0)^T\boldsymbol{\lambda}_0\ \mathrm{div}\ V\ dx\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\sum_{i=1}^{d}\nu\nabla\boldsymbol{w}_i^T(\ \mathrm{div}\ (V)I-V'-V'^T)\nabla\boldsymbol{\lambda}_i\ dx\ dt\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{w}^T(\ \mathrm{div}\ V)I-V'^T)\nabla\boldsymbol{v}\boldsymbol{\lambda}\ dx\ dt\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}\boldsymbol{v}^T(\ \mathrm{div}\ V)I-V'^T)\nabla\boldsymbol{w}\boldsymbol{\lambda}\ dx\ dt\\
&+\int_I\int_{\Omega_{\mathrm{ref}}}q\left(\ \mathrm{tr}\ (V'^T\nabla\boldsymbol{\lambda})-\ \mathrm{div}\ \boldsymbol{\lambda}\ \mathrm{div}\ V)\right)\ dx\ dt\\
&-\int_I\int_{\Omega_{\mathrm{ref}}}\mu(\ \mathrm{tr}\ (V'^T\nabla\boldsymbol{w})-\ \mathrm{div}\ \boldsymbol{w}\ \mathrm{div}\ V)\ dx\ dt.
\end{aligned}
$$

In the 2D case we have

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{\tau,(v,p)}((\boldsymbol{v}, p), \mathrm{id})(V)(w, q)\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \operatorname{div} V \; dx \; dt + \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}(\cdot, 0)^T \boldsymbol{\lambda}_0 \operatorname{div} V \; dx \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{w}_i^T (\operatorname{div} (V) I - V' - V'^T) \nabla \boldsymbol{\lambda}_i \; dx \; dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}^T V'^T \nabla \boldsymbol{v} \boldsymbol{\lambda} \det V' \; dx \; dt + \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{v}^T V'^{-T} \nabla \boldsymbol{w} \boldsymbol{\lambda} \det V' \; dx \; dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} q \operatorname{tr} (V'^{-T} \nabla \boldsymbol{\lambda}) \det V' \; dx \; dt + \int_I \int_{\Omega_{\mathrm{ref}}} \mu \operatorname{tr} (V'^{-T} \nabla \boldsymbol{w}) \det V' \; dx \; dt.
\end{aligned}
$$

B.1.5 Second derivative $E_{(v,p),\tau}$

Let $((\boldsymbol{v}, p), \tau) \in Y_{\mathrm{ref}} \times T_{\mathrm{ad}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in Z_{\mathrm{ref}}{}^*$, $V \in S$ and $(\boldsymbol{w}, q) \in Y_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{(v,p),\tau}((\boldsymbol{v}, p), \tau)(w, q)(V))\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}_t^T \boldsymbol{\lambda} \operatorname{tr} (\tau'^{-1} V') \det \tau' \; dx \; dt \\
&\quad + \int_{\Omega_{\mathrm{ref}}} \boldsymbol{w}(\cdot, 0)^T \boldsymbol{\lambda}_0 \operatorname{tr} (\tau'^{-1} V') \det \tau' \; dx \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \sum_{i=1}^d \nu \nabla \boldsymbol{w}_i^T \tau'^{-1} (\operatorname{tr} (\tau'^{-1} V') I - V' \tau'^{-1} - \tau'^{-T} V'^T) \tau'^{-T} \nabla \boldsymbol{\lambda}_i \det \tau' \; dx \; dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} (\boldsymbol{w}^T \tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v} + \boldsymbol{v}^T \tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{w}) \boldsymbol{\lambda} \det \tau' \; dx \; dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} (\boldsymbol{w}^T \tau'^{-T} \nabla \boldsymbol{v} + \boldsymbol{v}^T \tau'^{-T} \nabla \boldsymbol{w}) \boldsymbol{\lambda} \operatorname{tr} (\tau'^{-1} V') \det \tau' \; dx \; dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} q(\operatorname{tr} (-\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{\lambda}) + \operatorname{tr} (\tau'^{-T} \nabla \boldsymbol{\lambda}) \operatorname{tr} (\tau'^{-1} V')) \det \tau' \; dx \; dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \mu(\operatorname{tr} (-\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{w}) + \operatorname{tr} (\tau'^{-T} \nabla \boldsymbol{w}) \operatorname{tr} (\tau'^{-1} V')) \det \tau' \; dx \; dt
\end{aligned}
$$

A short calculation shows

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \mu), E_{(v,p),\tau}((\boldsymbol{v}, p), \tau)(w, q)(V))\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}} = \\
&\langle (\boldsymbol{\lambda}, \mu), E_{\tau,(v,p)}((\boldsymbol{v}, p), \tau)(V)(w, q))\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}}.
\end{aligned}
$$

B.1.6 Second derivative $E_{(v,p),(v,p)}$

Let $((\boldsymbol{v}, p), \tau) \in Y_{\mathrm{ref}} \times T_{\mathrm{ad}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in Z_{\mathrm{ref}}{}^*$ and $(\boldsymbol{w}, q), (\boldsymbol{u}, s) \in Y_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{(\boldsymbol{v},p),(\boldsymbol{v},p)}((\boldsymbol{v}, p), \tau)(\boldsymbol{w}, q)(\boldsymbol{u}, s)\rangle_{Z_{\mathrm{ref}}{}^*, Z_{\mathrm{ref}}} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \left(\boldsymbol{w}^T \tau'^{-T} \nabla \boldsymbol{u} + \boldsymbol{u}^T \tau'^{-T} \nabla \boldsymbol{w} \right) \boldsymbol{\lambda} \det \tau' \; dx \; dt.
\end{aligned}
\tag{B.1}
$$

B.1.7 Second derivative $E_{(v,p),(v,p)}$ at $\tau = \mathrm{id}$

Let $(\boldsymbol{v}, p) \in Y_{\mathrm{ref}}$, $(\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu) \in {Z_{\mathrm{ref}}}^*$ and $(\boldsymbol{w}, q), (\boldsymbol{u}, s) \in Y_{\mathrm{ref}}$. Then we have

$$\begin{aligned} &\langle (\boldsymbol{\lambda}, \boldsymbol{\lambda}_0, \mu), E_{(\boldsymbol{v},p),(\boldsymbol{v},p)}((\boldsymbol{v}, p), \mathrm{id})(\boldsymbol{w}, q)(\boldsymbol{u}, s) \rangle_{{Z_{\mathrm{ref}}}^*, Z_{\mathrm{ref}}} \\ &\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \left(\boldsymbol{w}^T \nabla \boldsymbol{u} + \boldsymbol{u}^T \nabla \boldsymbol{w} \right) \boldsymbol{\lambda} \; dx \; dt. \end{aligned} \tag{B.2}$$

B.2 Second Derivatives of J

We will use the following definitions in formula (3.56) of J_τ to document the derivation of the second derivatives $J_{\tau\tau}$ and $J_{\tau,(\boldsymbol{v},p)}$:
Let $(\boldsymbol{v},\tau) \in \hat{Y}_{\text{ref}} \times T_{\text{ad}}$ and $V \in S$. Then we have

$$\begin{aligned}
&\langle J_\tau(\boldsymbol{v},\tau), V\rangle_{S^*,S} \\
&= \underbrace{\int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t)) \text{ tr } (\tau'^{-1}V') \det\tau' \; dx \; dt}_{=:A'} \\
&\underbrace{- \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial(\nabla\tilde{\boldsymbol{v}})} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\, \tau'^{-T} V'^T \tau'^{-T}\nabla\boldsymbol{v} \det\tau' \; dx \; dt}_{=:B'} \\
&+ \underbrace{\int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{x}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t)) V \; \det\tau' \; dx \; dt}_{=:C'} \\
&+ \underbrace{\int_{\Omega_{\text{ref}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \text{ tr } (\tau'^{-1}V') \det\tau' \; dx}_{=:D'} \\
&+ \underbrace{\int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{x}} f_2(\tau(x), \boldsymbol{v}(x,T)) V \det\tau' \; dx.}_{=:E'}
\end{aligned}$$

We will use the following definitions in the formula (3.59) of $J_{\boldsymbol{v}}$ to document the derivation of the second derivatives $J_{\boldsymbol{v}\tau}$ and $J_{\boldsymbol{v}\boldsymbol{v}}$:
Let $(\boldsymbol{v},\tau) \in \hat{Y}_{\text{ref}} \times T_{\text{ad}}$ and $\boldsymbol{w} \in \hat{Y}_{\text{ref}}$. Then we have

$$\begin{aligned}
&\langle J_{\boldsymbol{v}}(\boldsymbol{v},\tau), \boldsymbol{w}\rangle_{\hat{Y}^*_{\text{ref}}),\hat{Y}_{\text{ref}}} \\
&= \underbrace{\int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\boldsymbol{w} \det\tau' \; dx \; dt}_{=:A''} \\
&+ \underbrace{\int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\tau'^{-T}\nabla\boldsymbol{w} \det\tau' \; dx \; dt}_{=:B''} \\
&+ \underbrace{\int_{\Omega_{\text{ref}}} \frac{\partial}{\partial\tilde{\boldsymbol{v}}} f_2(\tau(x), \boldsymbol{v}(x,T))\boldsymbol{w}(x,T) \det\tau' \; dx\,.}_{=:C''}
\end{aligned}$$

B.2.1 Second derivative $J_{\tau\tau}$

Let $(\boldsymbol{v},\tau) \in \hat{Y}_{\text{ref}} \times T_{\text{ad}}$ and $V, W \in S$. Then we have

$$
\begin{aligned}
&\langle J_{\tau\tau}(\boldsymbol{v},\tau)V,W\rangle_{S^*,S} \\
&= \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{x}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))W \ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx\ dt \\
&- \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v}\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ \mathrm{tr}\ (-\tau'^{-1}W'\tau'^{-1}V')\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ \mathrm{tr}\ (\tau'^{-1}V')\ \mathrm{tr}\ (\tau'^{-1}W')\det\tau'\ dx\ dt \\
&- \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{x}}\frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (W)\ (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v})\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v})\ (\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v})\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\tau'^{-T}W'^T\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v}\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\tau'^{-T}V'^T\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v}\det\tau'\ dx\ dt \\
&- \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\tau'^{-T}V'^T\tau'^{-T}\nabla\boldsymbol{v}\ \mathrm{tr}\ (\tau'^{-1}W')\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\tilde{x}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (W)\ (V)\det\tau'\ dx\ dt \\
&- \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}}\frac{\partial}{\partial\tilde{x}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\tau'^{-T}W'^T\tau'^{-T}\nabla\boldsymbol{v})\ (V)\det\tau'\ dx\ dt \\
&+ \int_I\int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{x}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))V\ \mathrm{tr}\ (\tau'^{-1}W')\det\tau'\ dx\ dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{x}} f_2(\tau(x),\boldsymbol{v}(x,T))W\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} f_2(\tau(x),\boldsymbol{v}(x,T))\ \mathrm{tr}\ (-\tau'^{-1}W'\tau'^{-1}V')\det\tau'\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} f_2(\tau(x),\boldsymbol{v}(x,T))\ \mathrm{tr}\ (\tau'^{-1}W')\ \mathrm{tr}\ (\tau'^{-1}V')\det\tau'\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\tilde{x}} f_2(\tau(x),\boldsymbol{v}(x,T))(W)(V)\det\tau'\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{x}} f_2(\tau(x),\boldsymbol{v}(x,T))V\ \mathrm{tr}\ (\tau'^{-1}W')\det\tau'\ dx.
\end{aligned}
$$

The first four integrals stem from term A', integral 5-9 from term B', integral 10-12 from term C', integral 13-15 from term D' and integral 16-17 from term E'.

B.2.2 Second derivative $J_{\tau\tau}$ at $\tau = \mathrm{id}$

Let $\boldsymbol{v} \in \hat{Y}_{\mathrm{ref}}$ and $V, W \in S$. Then we have

$$
\begin{aligned}
&\langle J_{\tau\tau}(\boldsymbol{v}, \mathrm{id})V, W\rangle_{S^*,S} \\
&= -\int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) W'^T \nabla \boldsymbol{v} \ \mathrm{div}\ V \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) W \ \mathrm{div}\ V \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ \mathrm{tr}\ (-W'V') \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ \mathrm{div}\ V \ \mathrm{div}\ W \ dx \ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (W) \ (V'^T \nabla \boldsymbol{v}) \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (W'^T \nabla \boldsymbol{v}) \ (V'^T \nabla \boldsymbol{v}) \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) W'^T V'^T \nabla \boldsymbol{v} \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) V'^T W'^T \nabla \boldsymbol{v} \ dx \ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) V'^T \nabla \boldsymbol{v} \ \mathrm{div}\ W \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (W) \ (V) \ dx \ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (W'^T \nabla \boldsymbol{v}) \ (V) \ dx \ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) V \ \mathrm{div}\ W \ dx \ dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} f_2(x, \boldsymbol{v}(x,T)) W \ \mathrm{div}\ V \ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} f_2(x, \boldsymbol{v}(x,T)) \ \mathrm{tr}\ (-W'V') \ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} f_2(x, \boldsymbol{v}(x,T)) \ \mathrm{div}\ W \ \mathrm{div}\ V \det \tau' \ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \tilde{x}} f_2(x, \boldsymbol{v}(x,T))(W)(V) \ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} f_2(x, \boldsymbol{v}(x,T)) V \ \mathrm{div}\ W \ dx.
\end{aligned}
$$

Grouping some terms we obtain

$$
\begin{aligned}
&\langle J_{\tau\tau}(\boldsymbol{v}, \mathrm{id})V, W\rangle_{S^*,S} \\
&= \int_{\Omega_{\mathrm{ref}}} (\int_I f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ dt + f_2(x, \boldsymbol{v}(x,T)))(\ \mathrm{div}\ V\ \mathrm{div}\ W -\ \mathrm{tr}\ (W'V'))\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} (\int_I \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ dt + \frac{\partial}{\partial \tilde{x}} f_2(x, \boldsymbol{v}(x,T)))(W\ \mathrm{div}\ V + V\ \mathrm{div}\ W)\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} (\int_I \frac{\partial^2}{\partial^2 \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ dt + \frac{\partial^2}{\partial^2 \tilde{x}} f_2(x, \boldsymbol{v}(x,T)))\ (W)\ (V)\ dx \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})(W'^T V'^T + V'^T W'^T -\ \mathrm{div}\ V W'^T -\ \mathrm{div}\ W V'^T)\nabla \boldsymbol{v}\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ (W'^T \nabla \boldsymbol{v})\ (V'^T \nabla \boldsymbol{v})\ dx\ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ (W)\ (V'^T \nabla \boldsymbol{v})\ dx\ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})\ (W'^T \nabla \boldsymbol{v})\ (V)\ dx\ dt.
\end{aligned}
$$

B.2.3 Second derivative $J_{\tau \boldsymbol{v}}$

Let $(\boldsymbol{v}, \tau) \in \hat{Y}_{\mathrm{ref}} \times T_{\mathrm{ad}}$, $V \in S$ and $\boldsymbol{w} \in \hat{Y}_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle J_{\tau \boldsymbol{v}}(\boldsymbol{v}, \tau)V, \boldsymbol{w}\rangle_{\hat{Y}^*_{\mathrm{ref}}, \hat{Y}_{\mathrm{ref}}} \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \boldsymbol{w}\ \mathrm{tr}\ (\tau'^{-1} V') \det \tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \tau'^{-T} \nabla \boldsymbol{w}\ \mathrm{tr}\ (\tau'^{-1} V') \det \tau'\ dx\ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t))\ (\boldsymbol{w})\ (\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v}) \det \tau'\ dx\ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t))\ (\tau'^{-T} \nabla \boldsymbol{w})\ (\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v}) \det \tau'\ dx\ dt \\
&- \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t))(\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{w}) \det \tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t))\ (\boldsymbol{w})\ (V) \det \tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t))\ (\tau'^{-T} \nabla \boldsymbol{w})\ (V) \det \tau'\ dx\ dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \boldsymbol{w}(x,T)\ \mathrm{tr}\ (\tau'^{-1} V') \det \tau'\ dx \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_2(\tau(x), \boldsymbol{v}(x,T))(\boldsymbol{w}(x,T))(V) \det \tau'\ dx.
\end{aligned}
$$

The first three integrals stem from term A', integrals 4-7 from term B', integrals 8-10 from term C', integral 11 from term D' and integral 12 from term E'.

B.2.4 Second derivative $J_{\tau\boldsymbol{v}}$ at $\tau = \mathrm{id}$

Let $\boldsymbol{v} \in \hat{Y}_{\mathrm{ref}}$, $V \in S$ and $\boldsymbol{w} \in \hat{Y}_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle J_{\tau\boldsymbol{v}}(\boldsymbol{v}, \mathrm{id})V, \boldsymbol{w}\rangle_{\hat{Y}^*_{\mathrm{ref}}, \hat{Y}_{\mathrm{ref}}} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \boldsymbol{w} \ \mathrm{div}\ V \ dx \ dt + \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(x, \boldsymbol{v}(x,T)) \boldsymbol{w}(x,T) \ \mathrm{div}\ V \ dx \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (\boldsymbol{w}) \ (V) \ dx \ dt \\
&\quad + \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_2(x, \boldsymbol{v}(x,T))(\boldsymbol{w}(x,T))(V) \ dx \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v})(\nabla \boldsymbol{w} \ \mathrm{div}\ V - V'^T \nabla \boldsymbol{w}) \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (\boldsymbol{w}) \ (V'^T \nabla \boldsymbol{v}) \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \nabla \tilde{\boldsymbol{v}}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (\nabla \boldsymbol{w}) \ (V'^T \nabla \boldsymbol{v}) \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \boldsymbol{v}, \nabla \boldsymbol{v}) \ (\nabla \boldsymbol{w}) \ (V) \ dx \ dt.
\end{aligned}
$$

B.2.5 Second derivative $J_{\boldsymbol{v}\tau}$

Let $(\boldsymbol{v}, \tau) \in \hat{Y}_{\mathrm{ref}} \times T_{\mathrm{ad}}$, $V \in S$ and $\boldsymbol{w} \in \hat{Y}_{\mathrm{ref}}$. Then we have

$$
\begin{aligned}
&\langle J_{\boldsymbol{v}\tau}(\boldsymbol{v}, \tau)\boldsymbol{w}, V\rangle_{S^*, S} \\
&\quad = \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \ (V) \ (\boldsymbol{w}) \det \tau' \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \ (\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v}) \ (\boldsymbol{w}) \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \boldsymbol{w} \ \mathrm{tr}\ (\tau'^{-1} V') \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \ (V) \ (\tau'^{-1} \nabla \boldsymbol{w}) \det \tau' \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \ (\tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{v}) \ (\tau'^{-1} \nabla \boldsymbol{w}) \det \tau' \ dx \ dt \\
&\quad - \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \tau'^{-T} V'^T \tau'^{-T} \nabla \boldsymbol{w} \det \tau' \ dx \ dt \\
&\quad + \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \nabla \tilde{\boldsymbol{v}}} f_1(\tau(x), \boldsymbol{v}, \tau'(x)^{-T} \nabla \boldsymbol{v}(x,t)) \tau'^{-T} \nabla \boldsymbol{w} \ \mathrm{tr}\ (\tau'^{-1} V') \det \tau' \ dx \ dt \\
&\quad + \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{x}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tau(x), \boldsymbol{v}(x,T)) \ (V) \ (\boldsymbol{w}(x,T)) \det \tau' \ dx \\
&\quad + \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial \tilde{\boldsymbol{v}}} f_2(\tau(x), \boldsymbol{v}(x,T))(\boldsymbol{w}(x,T)) \ \mathrm{tr}\ (\tau'^{-1} V') \det \tau' \ dx.
\end{aligned}
$$

The first three integrals stem from term A", integrals 4-7 from term B" and integrals 8-9 from term C".
Comparing terms shows

$$\langle J_{\tau,\boldsymbol{v}}(\boldsymbol{v},\tau)V,\boldsymbol{w}\rangle_{\hat{Y}^*_{\mathrm{ref}},\hat{Y}_{\mathrm{ref}}} = \langle J_{\boldsymbol{v},\tau}(\boldsymbol{v},\tau)\boldsymbol{w},V\rangle_{S^*,S}.$$

B.2.6 Second derivative $J_{\boldsymbol{vv}}$

Let $(\boldsymbol{v},\tau) \in \hat{Y}_{\mathrm{ref}} \times T_{\mathrm{ad}}$ and $\boldsymbol{w},\boldsymbol{u} \in \hat{Y}_{\mathrm{ref}}$. Then we have

$$\begin{aligned}
&\langle J_{\boldsymbol{vv}}(\boldsymbol{v},\tau)\boldsymbol{w},\boldsymbol{u}\rangle_{\hat{Y}^*_{\mathrm{ref}},\hat{Y}_{\mathrm{ref}}} \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2 \tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\boldsymbol{u})\ (\boldsymbol{w}) \det\tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}}\frac{\partial}{\partial\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\tau'^{-T}\nabla\boldsymbol{u})\ (\boldsymbol{w}) \det\tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{\boldsymbol{v}}}\frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\boldsymbol{u})\ (\tau'^{-T}\nabla\boldsymbol{w}) \det\tau'\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\nabla\tilde{\boldsymbol{v}}} f_1(\tau(x),\boldsymbol{v},\tau'(x)^{-T}\nabla\boldsymbol{v}(x,t))\ (\tau'^{-T}\nabla\boldsymbol{u})\ (\tau'^{-T}\nabla\boldsymbol{w}) \det\tau'\ dx\ dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\tilde{\boldsymbol{v}}} f_2(\tau(x),\boldsymbol{v}(x,T))\ (\boldsymbol{u}(x,T))\ (\boldsymbol{w}(x,T)) \det\tau'\ dx.
\end{aligned}$$

The first 2 integrals stem from term A", integrals 3-4 from term B", and integral 5 from term C".

B.2.7 Second derivative $J_{\boldsymbol{vv}}$ at $\tau = \mathrm{id}$

Let $\boldsymbol{v} \in \hat{Y}_{\mathrm{ref}}$ and $\boldsymbol{w},\boldsymbol{u} \in \hat{Y}_{\mathrm{ref}}$. Then we have

$$\begin{aligned}
&\langle J_{\boldsymbol{vv}}(\boldsymbol{v},\mathrm{id})\boldsymbol{w},\boldsymbol{u}\rangle_{\hat{Y}^*_{\mathrm{ref}},\hat{Y}_{\mathrm{ref}}} \\
&= \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\tilde{\boldsymbol{v}}} f_1(x,\boldsymbol{v},\nabla\boldsymbol{v})\ (\boldsymbol{u})\ (\boldsymbol{w})\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}}\frac{\partial}{\partial\tilde{\boldsymbol{v}}} f_1(x,\boldsymbol{v},\nabla\boldsymbol{v})\ (\nabla\boldsymbol{u})\ (\boldsymbol{w})\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial}{\partial\tilde{\boldsymbol{v}}}\frac{\partial}{\partial\nabla\tilde{\boldsymbol{v}}} f_1(x,\boldsymbol{v},\nabla\boldsymbol{v})\ (\boldsymbol{u})\ (\nabla\boldsymbol{w})\ dx\ dt \\
&+ \int_I \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\nabla\tilde{\boldsymbol{v}}} f_1(x,\boldsymbol{v},\nabla\boldsymbol{v})\ (\nabla\boldsymbol{u})\ (\nabla\boldsymbol{w})\ dx\ dt \\
&+ \int_{\Omega_{\mathrm{ref}}} \frac{\partial^2}{\partial^2\tilde{\boldsymbol{v}}} f_2(x,\boldsymbol{v}(x,T))\ (\boldsymbol{u}(x,T))\ (\boldsymbol{w}(x,T))\ dx.
\end{aligned}$$

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