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Shape derivatives for general objective functions and the incompressible Navier–Stokes equations*

by

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Abstract: The aim of this paper is to present the shape derivative for a wide array of objective functions using the incompressible Navier–Stokes equations as a state constraint. Most real world applications of computational fluid dynamics are shape optimization problems in nature, yet special shape optimization techniques are seldom used outside the field of elliptic partial differential equations and linear elasticity. This article tries to be self contained, also presenting many useful results from the literature. We conclude with a comparison of different objective functions for the shape optimization of an obstacle in a channel, which can be done quite conveniently when one knows the general form of the shape gradient.

Keywords: shape optimization, shape derivative, Navier–Stokes, adjoint calculus.

1. Introduction

Optimal control of fluids has seen much attention due to its importance for many technical, scientific, and engineering applications. A good overview on fluid control can, for example, be found in Gunzburger (2003). However, the problem is seldom treated from a pure shape optimization perspective. Notable exceptions are Pironneau (1973) and one section of Mohammadi and Pironneau (2001). When the problem is treated from a shape optimization approach, usually only one very specific type of objective function is considered: the volume dissipation of the kinetic energy of the fluid into heat. In the limit of the Stokes equations, this results in a self-adjoint problem, allowing for an elegant analysis. A more general volume objective function for the Navier–Stokes equations is considered in Ito et al. (2008), where the existence is shown using surprisingly weak regularity assumptions.

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Although many objective functions of practical relevance are defined on the surface of the flow obstacle alone, such objectives are seldom considered. On the one hand, the shape sensitivity analysis for surface functionals is much more complex in itself, but on the other hand, a surface functional often features a dependence on the geometry that adds to the difficulties in deriving the correct gradient expression in Hadamard form. The Hadamard form enables a very efficient computation of the gradient without the need to compute the so called "mesh sensitivity" Jacobian. This is especially true for aerodynamic quantities such as drag, lift, or matching a target surface pressure distribution. The shape derivative for such quantities can, for example, be found in Schmidt et al. (2008) for a compressible fluid model. Since many auxiliary results from a special shape analysis background are needed to derive the Hadamard expression, this paper seeks to be self-contained, listing them from multiple literature sources such as Amrouche, Nečasova and Sokolowski (2007), Boisgérault and Zolésio (1993), Delfour and Zolésio (2001) and Sokolowski and Zolésio (1992).

As such, the present work seeks to derive the expression for the shape derivative of a general objective function using an incompressible Navier–Stokes flow that is as general as possible, combining both a volume part and a surface objective function. A dependence on the geometry is also included.

This article is structured as follows: Section 2 presents the problem under consideration in more detail. Subsequently, Section 3 is used to give a detailed overview about shape sensitivity analysis from the literature, especially Delfour and Zolésio (2001), Sokolowski and Zolésio (1992). Finally, Section 4 presents the adjoint calculus, which in combination with the results from Section 3 leads to Theorem 4, the Hadamard representation of the shape derivative. Theorem 4 is the main purpose of this article and new to the best of our knowledge. Since the pressure in an incompressible fluid has an artificial character and usually no boundary condition on the fluid obstacle, there will be some restriction on the surface part of the objective function such that the adjoint state exists. For more detailed existence results we would like to refer to Plotnikov, Ruban and Sokolowski (2008) and Plotnikov and Sokolowski (2005, 2008). Section 5 concludes with the comparison of different objective functions for the shape optimization of an obstacle in a channel. When knowing the general form of the shape gradient for a Navier–Stokes fluid, such a comparison can be done quite conveniently.

2. The optimization problem

The aim of this paper is to show the structure of the shape derivative of a general objective function under a PDE constraint describing an incompressible Navier–Stokes fluid:

$$\min_{(u,p,\Omega)} J(u,p,\Omega) := \int_{\Omega} f(u, Du, p)\ dA + \int_{\Gamma_0} g(u, D_n u, p, n)\ dS \tag{1}$$

$$\begin{aligned} &\text{subject to} \\ -\mu\Delta u + \rho u \nabla u + \nabla p &= \rho G \quad \text{in} \quad \Omega \\ \operatorname{div} u &= 0 \\ u &= u_+ \quad \text{on} \quad \Gamma_+ \\ u &= 0 \quad\ \ \text{on} \quad \Gamma_0 \\ pn - \mu \frac{\partial u}{\partial n} &= 0 \quad\ \ \text{on} \quad \Gamma_-. \end{aligned} \tag{2}$$

Here, $f : \mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ are assumed to be continuously differentiable in each argument. Also, d is the dimension of the bounded domain $\Omega \subset \mathbb{R}^d$ and in the following $\Gamma := \partial\Omega$ is used to denote the whole boundary of Ω. Furthermore, $u : \Omega \to \mathbb{R}^d$ is the velocity of the fluid and $p : \Omega \to \mathbb{R}$ is the pressure. The viscosity is given by μ, and ρ denotes the density, which is constant in an incompressible fluid. The outflow boundary condition on Γ_- is the finite element "do nothing" outflow condition that naturally arises due to integration by parts during the finite element matrix assembly. Additionally, Γ_+ denotes the inflow boundary and Γ_0 is the fluid obstacle or the channel wall, using the no-slip boundary condition. The shape Γ_0 is the unknown to be found. Also, n is the normal vector with components n_i and ρG_i are the outside body forces, i.e. the forces per unit volume acting on the fluid. Due to the no-slip boundary condition on Γ_0 it is sufficient to consider the derivative in normal direction $D_n u := Du \cdot n$ on Γ_0 since the tangent derivative of the velocities is zero anyway. The domain is sketched in Fig. 1.

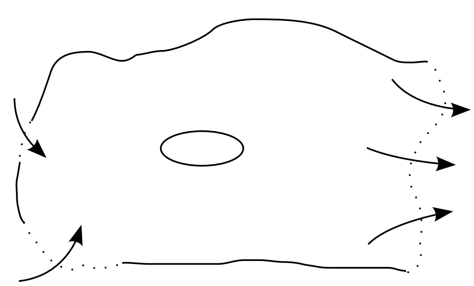

Figure 1. Exemplified domain under consideration. Solid lines denote the no-slip boundary Γ_0, dotted lines represent inflow Γ_+ and outflow Γ_-.

The control we are considering is the shape of the Dirichlet boundary Γ_0. As such, Γ_0 is the unknown and we seek the total derivative of the above with respect to Γ_0. The inflow direction is considered constant and independent of the shape of the boundary. Since the outflow boundary has an artificial character anyway, we also consider the shape of the outflow boundary to be fixed. In order to keep the notation readable we refer to the Jacobian components as follows:

$$\begin{aligned} Du &=: [a_{ij}]_{ij} \in \mathbb{R}^{d\times d} \\ D_n u = Du \cdot n &= \frac{\partial u}{\partial n} =: [b_i]_i \in \mathbb{R}^d. \end{aligned} \tag{3}$$

Since the pressure has no explicit boundary condition on Γ_0, but is implicitly linked with the velocity, we need to impose the following restriction on g, the boundary part of the objective, such that we can later arrive at a consistent adjoint boundary condition: we choose g such that there exists a functional $\lambda : \Omega \to \mathbb{R}^d$ satisfying the following conditions on Γ_0:

$$\begin{aligned} \lambda_i &= \frac{1}{\mu}\frac{\partial g}{\partial b_i}\ \forall i = 1, \dots, d \\ \langle \lambda, n\rangle &= -\frac{\partial g}{\partial p}. \end{aligned}$$

This is less restrictive than it might appear. A consequence is that for a force minimization, the forces should be chosen in line with the state equation, i.e. since the state equation describes a viscous fluid, the objective function should also include the viscous forces. For drag minimization at zero angle of attack, we have

$$g(u, D_n u, p, n) = \mu\frac{\partial u_1}{\partial n} - pn_1,$$

which leads to

$$\begin{aligned} \frac{\partial g}{\partial p} &= -n_1 \\ \frac{\partial g}{\partial b_i} &= \mu\delta_{1,i} \end{aligned}$$

and the above is satisfied with $\lambda_i = \delta_{1,i}$, where

$$\delta_{i,j} := \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

is the Kronecker symbol. The inclusion of higher derivatives on the velocities within the objective (1) is straightforward, but further limits the allowed surface functionals g and will not be considered here.

3. Review on shape calculus

Since we are interested in a gradient with respect to the shape of Γ_0, we first define a one parametric family of bijective mappings $T_t : (t, x) \mapsto T_t(x)$. A deformed domain Ω_t is then given by

$$\Omega_t := \{T_t(x_0) : x_0 \in \Omega\} .$$

Usually, the mapping T_t is either given by the perturbation of identity

$$T_t(x) = x + tV(x) \tag{4}$$

or implicitly by the speed method

$$\frac{dx}{dt} = V(t, x),\ x(0) = x_0,$$

where V is a vector field of appropriate smoothness. For first order calculus, it can be shown that both approaches are equivalent. Here, however, we will focus on the perturbation of identity (4). We seek to derive a formula for the shape derivative as defined in Sokolowski and Zolésio (1992) that can be computed very efficiently:

Definition 1 (Shape differentiability, shape derivative) *Let $D \subset \mathbb{R}^d$ be open and $\Omega \subset D$ measurable. Let V be a continuous vector field. A shape functional J is called shape differentiable at Ω, if the Eulerian derivative*

$$dJ(\Omega)[V] := \lim_{t\to 0^+} \frac{J(\Omega_t) - J(\Omega)}{t}, \quad \Omega_t := T_t(\Omega)$$

exists for all directions V and the mapping $V \mapsto dJ(\Omega)[V]$ is linear and continuous. The expression $dJ(\Omega)[V]$ is called the shape derivative of J at Ω in direction V.

Parameterization based approaches usually require knowledge of some "mesh sensitivity" for the gradient computation: suppose the Navier–Stokes state equation (2) is given in abstract form by $c(u, p, q) = 0$, where q is some design parameter defining the shape, e.g. b-splines or Bézier-curve parameters. Without taking into account the shape optimization nature of the problem, a formal Lagrangian approach results in:

$$\frac{dJ}{dq} = \frac{\partial J}{\partial q} - \lambda^T \frac{\partial c}{\partial q}$$
$$\left[\frac{\partial c}{\partial (u,p)}\right]^T \lambda = \frac{\partial J}{\partial (u,p)}.$$

Thus, computing this expression requires knowledge of the "mesh sensitivity" Jacobian $\frac{\partial c}{\partial q}$, i.e. the derivative of the solution procedure of the PDE with respect to perturbations in the mesh discretizing the domain. The key to avoid this expression is the so-called Hadamard theorem, a consequence of the Delfur–Zolésio structure theorem (Delfour and Zolésio, 2001; Sokolowski and Zolésio, 1992).

THEOREM 1 (HADAMARD THEOREM) *Let J be shape differentiable as in Definition 1. Then the relation*

$$dJ(\Omega)[V] = dJ(\Gamma)[\langle V, n\rangle n]$$

holds for all vector fields $V \in C^k(\bar{D}; \mathbb{R}^d)$.

Proof. See Proposition 2.26, pages 59–60, in Sokolowski and Zolésio (1992). ■

The consequence of the Hadamard formula is that under some mild smoothness assumptions, the shape derivative dJ has the structure of a scalar product with the normal component $\langle V, n\rangle$ of the prescribed perturbation V of the domain Ω. One can thus use the shape gradient directly as an update for the boundary, which results in the steepest descent direction and can be applied without knowledge of the costly mesh sensitivity Jacobian $\frac{\partial c}{\partial q}$.

REMARK 1 (SHAPE GRADIENT) *In Sokolowski and Zolésio (1992), the Hadamard theorem actually states the existence of a scalar distribution*

$$g(\Gamma) \in \mathcal{D}^{-k}(\Gamma),$$

such that the shape gradient $G(\Omega) \in \mathcal{D}^{-k}(\Omega, \mathbb{R}^d)$ is given by

$$G(\Omega) = \gamma_\Gamma^*(g \cdot n),$$

where γ_Γ^* is the adjoint of the trace operator on Γ. Here, however, it is always assumed that $G(\Omega)$ is an integrable function, i.e. Ω has piecewise smooth boundaries. Then the shape gradient g is much more conveniently expressed by

$$dJ(\Omega)[V] = \int_\Gamma \langle V, n\rangle\ g\ dS.$$

In order to find the shape gradient for the general Navier–Stokes problem we are considering, we need some additional results. Most of them are known from the literature (Amrouche, Nečasova and Sokolowski, 2007; Boisgérault and Zolésio, 1993; Delfour and Zolésio, 2001; Sokolowski and Zolésio, 1992), but we think that listing them here will create a much more self-contained derivation of the Navier–Stokes gradient.

3.1. Shape derivative for volume objectives

We start with recapitulating the Hadamard formula for objective functions, which are defined over the whole domain Ω, such as the first part of the mixed objective function (1):

LEMMA 1 (DERIVATIVE OF DEFORMATION DETERMINANT) *The derivative of the determinant of the perturbation of identity approach is given by:*

$$\left.\frac{d}{dt}\right|_{t=0} \det DT_t(x) = \operatorname{div} V(x). \tag{5}$$

Proof. For a matrix $A(t) \in \mathbb{R}^{m\times m}$ where each entry is a differentiable function such that $A(t)^{-1}$ exists for some interval $I \subset \mathbb{R}$, the derivative of the determinant with respect to t is given by

$$\frac{d}{dt}\det A(t) = \operatorname{tr}\left(\frac{dA(t)}{dt}A(t)^{-1}\right)\det A(t).$$

Since $DT_0(x) = I$, we have

$$\begin{aligned}\left.\frac{d}{dt}\right|_{t=0} \det DT_t(x) &= \operatorname{tr}\left(\left.\frac{dDT_t(x)}{dt}\right|_{t=0}\right)\\ &= \operatorname{tr}\left(DV(x)\right)\\ &= \operatorname{div} V(x).\end{aligned}$$

■

LEMMA 2 (HADAMARD FORMULA FOR VOLUME OBJECTIVE FUNCTIONS) *For a general volume objective function $f : \Omega \to \mathbb{R}$, not depending on a PDE constraint, i.e.*

$$J(\Omega) = \int_\Omega f \; dA,$$

the shape derivative is given by

$$dJ(\Omega)[V] = \int_\Gamma \langle V, n\rangle f \; dS.$$

Coincidentally, the shape gradient is already given by f in this case.

Proof. See Proposition 2.46 in Sokolowski and Zolésio (1992), or Theorem 4.1 in Delfour and Zolésio (2001). ■

3.2. Definitions and lemmas

Before we recapitulate the Hadamard formula for objective functions, which are defined on the boundary of the domain Ω, such as the second part of (1), some definitions and lemmas should be presented from the literature:

DEFINITION 2 (SUBMANIFOLD OF $\mathbb{R}^m$, PARAMETERIZATION, CHART, CO-DIMENSION) *A set $\Omega \subset \mathbb{R}^m$ is called d-dimensional submanifold of $\mathbb{R}^m$ if for each $x \in \Omega$ there exists an open neighborhood $U_1(x) \subset \mathbb{R}^m$ and a differentiable* *function $h : U_2 \to \mathbb{R}^m$ with $U_2 \subset \mathbb{R}^d$ open and with injective Jacobian and with continuous inverse mapping $h^{-1} : h(U_2) \to U_2$ such that*

$$h(U_2) \subset U_1 \cap \Omega.$$

Furthermore, h is called (local) parameterization, h^{-1} is called map, and the pair $(h^{-1}, h(U_2))$ is called chart. Thus, $x \in \Omega \subset \mathbb{R}^m$ is given by $x = h(\xi_1, ..., \xi_d)$ for $(\xi_1, ..., \xi_d) \in U_2 \subset \mathbb{R}^d$. The value $m - d$ is called co-dimension.

Definition 3 (Integral over submanifolds) *Let Ω be a d-dimensional compact submanifold in $\mathbb{R}^m$ with finite open atlas*

$$\Omega \subset \bigcup_{j=1}^{l} h_j(M_j)$$

such that $\Omega_j := h_j(M_j)$ and a corresponding partition of unity

$$\sum_{j=1}^{l} r_j(x) = 1$$

with r_j infinitely continuously differentiable with compact support for all j. Then, the integral over Ω is defined by

$$\begin{aligned}\int_\Omega g \; d\Omega := \sum_{j=1}^{l} \int_{\Omega_j} g r_j \; d\Omega &:= \sum_{j=1}^{l} \int_{M_j} g(h_j(s)) r_j(h_j(s)) \sqrt{\det({Dh_j}^T Dh_j)(s)} \; ds \\ &=: \int_M g(h(s)) \sqrt{\det(Dh^T Dh)(s)} \; ds, \qquad (6)\end{aligned}$$

where Dh_j is the Jacobian of h_j.

Lemma 3 (Integral over the surface of submanifolds) *Let Ω be as in Definition 3. The integral over the surface of Ω is then given by*

$$\int_{\partial\Omega} g \; dS = \int_{B_0} g(h(s)) |\det Dh| \| (Dh)^{-T} e_d \| \; ds, \qquad (7)$$

where $B_0 = \{\xi \in \mathbb{R}^d : \|\xi\| \leq 1, \; \xi_d = 0\}$ is the intersection of the open d-dimensional unit ball with the $\xi_d = 0$ hyperplane and e_d is the d-th unit vector.

Proof. Let $B := \{\xi \in \mathbb{R}^d : \|\xi\| \leq 1\} \subset \mathbb{R}^d$ be the open unit ball in $\mathbb{R}^d$. The unit ball is segmented by a cut with the $\xi_d = 0$ hyperplane in

$$\begin{aligned} B_+ &:= \{\xi \in B : \xi_d > 0\} \\ B_- &:= \{\xi \in B : \xi_d < 0\} \\ B_0 &:= \{\xi \in B : \xi_d = 0\}. \end{aligned}$$

Without loss of generality, one can assume that the interior of Ω_j is given by

$$\operatorname{int}\Omega_j = h_j(B_+)$$

and, consequently, the boundary is given by

$$\partial\Omega_j = h_j(B_0),$$

i.e. $\partial\Omega_j = \{h_j(\xi,0) : (\xi,0) := (\xi_1,...,\xi_{d-1},0) \in B_0\}$. Hence, for a proper computation of the surface integral it is necessary to project the integration density

$$\det({Dh_j}^T Dh_j)$$

of the volume case above to the $(\xi,0)$-hyperplane, i.e. dropping the last column and last row from the matrix, which is the dd-minor $[{Dh_j}^T Dh_j]_{dd}$ of ${Dh_j}^T Dh_j$. By the definition of the cofactor-matrix, the determinant of the dd-minor is exactly the m_{dd}-entry of the cofactor-matrix $M({Dh_j}^T Dh_j)$. Thus, the proper integration density for the surface integral is given by

$$\begin{aligned}
\sqrt{m_{dd}} &= \sqrt{e_d^T M({Dh_j}^T Dh_j) e_d} \\
&= \sqrt{e_d^T M({Dh_j}^T) M(Dh_j) e_d} \\
&= \sqrt{\|M(Dh_j)e_d\|_2^2} \\
&= \|M(Dh_j)e_d\|_2 \\
&= |\det(Dh_j)| \|Dh_j^{-T} e_d\|_2,
\end{aligned}$$

where in the last line the property $M(A) = \det(A)A^{-T}$ was used. Hence, the corresponding boundary integral is given by

$$\begin{aligned}
\int\limits_{\partial\Omega} g \; dS &:= \sum_{j=1}^{l} \int\limits_{\partial\Omega_j} g r_j \; dS \\
&= \sum_{j=1}^{l} \int\limits_{B_0} g r_j(h_j(s)) |\det Dh_j| \| \left(Dh_j\right)^{-T} e_d\| \; ds \\
&=: \int\limits_{B_0} g(h(s)) |\det Dh| \| \left(Dh\right)^{-T} e_d\| \; ds,
\end{aligned}$$

where $s = (\xi, 0) = (\xi_1, ..., \xi_{d-1}, 0)$. ∎

Lemma 4 (Unit normal field on $\partial\Omega$) *For a regular surface $\partial\Omega$, the unit normal field at $x = h(\xi,0)$ on $\partial\Omega$ is given by*

$$n(x) = \frac{Dh(\xi,0)^{-T} e_d}{\|Dh(\xi,0)^{-T} e_d\|}.$$

Proof. The tangent space is given by

$$T_x\Omega = \mathrm{span}(Dh(\xi,0)e_i, i = 1, ..., d-1),$$

i.e. one (non-unit) tangent direction is given by $\tau_i := Dh(\xi,0)e_i$. Hence,

$$\begin{aligned}\langle \tau_i, Dh(\xi,0)^{-T}e_d\rangle &= \langle Dh(\xi,0)e_i, Dh(\xi,0)^{-T}e_d\rangle \\ &= \langle Dh(\xi,0)^{-1}Dh(\xi,0)e_i, e_d\rangle \\ &= \langle e_i, e_d\rangle \\ &= 0 \ \forall i = 1, ..., d-1\end{aligned}$$

is normal to the tangent space. ■

REMARK 2 (ALTERNATIVE REPRESENTATIONS) *Since* $M(A) = \det(A)A^{-T}$, *the boundary integral can also be expressed as*

$$\int_{\partial\Omega} g \ dS = \int_{B_0} g(h(s))\|M(Dh(s))e_d\| \ ds.$$

Analogously, the outer normal is given by

$$n(x) = \frac{M(Dh(\xi,0))e_d}{\|M(Dh(\xi,0))e_d\|_2}. \tag{8}$$

The structure of the normal can now be used in the definition of the surface integral. Using the above, the integral over the perturbed surface Γ_t can now be expressed with respect to the unperturbed surface Γ:

LEMMA 5 (PERTURBED SURFACE INTEGRAL) *The surface integral over the perturbed surface* Γ_t *is given by*

$$\int_{\Gamma_t} g \ d\Gamma_t = \int_{\Gamma} g(T_t(x))\|M(DT_t(x))n(x)\|_2 \ d\Gamma(x),$$

where n *is the unit normal of the unperturbed boundary* Γ.

Proof. The perturbed submanifold Γ_t can be described by

$$h^t(\xi,0) := T_t(h(\xi,0)). \tag{9}$$

According to Remark 2, the surface integral is given by

$$\int_{\partial\Omega_t} g \ dS_t = \int_{B_0} g(h^t(s))\|M(Dh^t(s))e_d\|_2 \ ds.$$

The chain rule results in

$$Dh^t(\xi,0) = D[T_t(h(\xi,0))] = DT_t(h(\xi,0))Dh(\xi,0) \tag{10}$$

and

$$\begin{aligned} M(Dh^t(\xi,0)) &= M(DT_t(h(\xi,0)Dh(\xi,0))) \\ &= M(DT_t(h(\xi,0)))M(Dh(\xi,0)). \end{aligned}$$

Using the alternative representation of the normal, equation (8),

$$\begin{aligned} \|M(Dh^t(s))e_d\|_2 &= \|M(DT_t(h(\xi,0)))M(Dh(\xi,0))e_d\|_2 \\ &= \|M(DT_t(h(\xi,0)))\|M(Dh(\xi,0))e_d\|_2 n(h(\xi,0))\|_2 \\ &= \|M(Dh(\xi,0))e_d\|_2 \|M(DT_t(h(\xi,0)))n(h(\xi,0))\|_2. \end{aligned}$$

Thus,

$$\begin{aligned} \int_{\partial\Omega_t} g\ dS_t &= \int_{B_0} g(T_t(h(s))\|M(DT_t(h(s)))n(h(s))\|_2 \|M(Dh(s))e_d\|_2\ ds \\ &= \int_{\partial\Omega} g(T_t(x))\|M(DT_t(x))n(x)\|_2\ d\Gamma(x), \end{aligned}$$

where again $s = (\xi, 0)$ and $x = h(s)$. ∎

Remark 3 (Alternative representation) *Due to the definition of the cofactor matrix, the perturbed surface integral can also be written as*

$$\begin{aligned} \int_{\partial\Omega_t} g\ dS_t &= \int_{\partial\Omega} g(T_t(x))\|M(DT_t(x))n(x)\|_2\ d\Gamma(x) \\ &= \int_{\partial\Omega} g(T_t(x))|\det DT_t(x)|\|(DT_t(x))^{-T}n(x)\|_2\ d\Gamma(x). \end{aligned}$$

Since we assume that the deformation mapping T_t does not change the orientation of Ω_t relative to Ω, we can assume $\det DT_t > 0$ *in subsequent considerations.*

Remark 4 (Derivative through matrix inverse) *Let $A(t) \in \mathbb{R}^{m\times m}$ be a matrix where each entry is a differentiable function such that $A(t)^{-1}$ exists for some interval $I \subset \mathbb{R}$. The derivative of the matrix inverse with respect to t is then given by*

$$\frac{d}{dt}A(t)^{-1} = -A(t)^{-1}\frac{dA(t)}{dt}A(t)^{-1}.$$

Before the preliminary shape derivative for surface objectives is presented, some elements from tangential calculus are needed.

DEFINITION 4 (TANGENTIAL GRADIENT, TANGENTIAL DIVERGENCE, CURVATURE) *For a d-dimensional submanifold $\Omega \subset \mathbb{R}^m$ and a function $f \in C^2(\Omega, \mathbb{R})$, the tangential gradient of f is defined as the orthogonal projection of the classical gradient onto the tangent space:*

$$\nabla_\Gamma f := P_T(\nabla f) = \sum_{i=1}^{d-1} \frac{\partial f}{\partial \tau_i} \tau_i \ \in \mathbb{R}^{d-1},$$

where τ_i forms an orthonormal basis of the tangent space. For a differentiable vector field V, the tangential divergence is defined by

$$\operatorname{div}_\Gamma V := \sum_{i=1}^{d-1} \left\langle \frac{\partial V}{\partial \tau_i}, \tau_i \right\rangle \ \in \mathbb{R}.$$

This definition is independent of the choice of the orthonormal basis of the tangent space. Furthermore, the curvature is defined as the tangential divergence of the unit normal field:

$$\kappa := \operatorname{div}_\Gamma n.$$

REMARK 5 *In the following, we assume that all submanifolds Ω are of co-dimension 1, such that the normal is unique and $\{n, \tau_1, ..., \tau_{d-1}\}$ forms an orthonormal basis of $\mathbb{R}^d$. The gradient ∇f can then be expressed in this basis:*

$$\nabla f = \langle \nabla f, n \rangle n + \sum_{i=1}^{d-1} \langle \nabla f, \tau_i \rangle \tau_i.$$

Assuming f also exists in a neighborhood of Ω, such that $\frac{\partial f}{\partial n}$ exists, then the tangential gradient is equivalently given by

$$\nabla_\Gamma f = \nabla f - \frac{\partial f}{\partial n} n$$

and likewise

$$\operatorname{div}_\Gamma V = \operatorname{div} V - \langle DVn, n \rangle.$$

REMARK 6 *Similar to Remark 5, there also exists the equality*

$$D_\Gamma V = \left[\sum_{k=1}^{d-1} \frac{\partial V_i}{\partial \tau_k} \tau_k \right]_i^T = \left[\nabla V_i - \frac{\partial V_i}{\partial n} n \right]_i^T = DV - DVnn^T$$

should the required derivative in normal direction exist. This property is needed later in Lemma 9.

Definition 5 (Tangential Jacobian matrix) *Similar to Definition 4, the tangential Jacobian matrix for a differentiable vector valued function V is defined as*

$$D_\Gamma V = [\nabla_\Gamma V_i]_i^T ,$$

i.e. the rows of the tangential Jacobian are the tangential gradients of the respective component functions.

Lemma 6 (Preliminary shape derivative for surface objectives) *For $g : \Omega \to \mathbb{R}$, such that ∇g is defined on Γ, the preliminary shape derivative not yet in Hadamard form for the surface integral is given by*

$$\begin{aligned}\left.\frac{d}{dt}\right|_{t=0} \int\limits_{\Gamma_t} g\ dS_t &= \int\limits_{\Gamma} \langle \nabla g, V\rangle + g\cdot(\operatorname{div} V - \langle DVn, n\rangle)\ dS \\ &= \int\limits_{\Gamma} \langle \nabla g, V\rangle + g \operatorname{div}_\Gamma V\ dS.\end{aligned}$$

Proof. For simplicity reasons, perturbation of identity is assumed. The alternative representation from Remark 3 provides:

$$\begin{aligned}&\left.\frac{d}{dt}\right|_{t=0} \int\limits_{\partial\Omega_t} g\ dS_t \\ &= \int\limits_{\partial\Omega} \left.\frac{d}{dt}\right|_{t=0} (g(T_t(x)) \det DT_t(x) \|(DT_t(x))^{-T} n(x)\|_2)\ d\Gamma(x).\end{aligned}$$

Furthermore,

$$\gamma(t) := DT_t^{-T} n = ((I + tDV)^T)^{-1} n$$

gives

$$\left.\frac{d}{dt}\right|_{t=0} \|\gamma(t)\|_2 = \left.\frac{d}{dt}\right|_{t=0} \left(\sum_{i=1}^{d} \gamma_i(t)^2\right)^{\frac{1}{2}} = \frac{1}{\|\gamma(0)\|_2} \left(\gamma^T(0) \left.\frac{d}{dt}\right|_{t=0} \gamma(t)\right).$$

Due to Lemma 4 one has

$$\begin{aligned}\gamma(0) &= n \\ \left.\frac{d}{dt}\right|_{t=0} \gamma(t) &= -I^{-1} \left.\frac{d}{dt}\right|_{t=0} (I + tDV)^T I^{-1} n \\ &= -DV^T n.\end{aligned}$$

Thus,

$$\left.\frac{d}{dt}\right|_{t=0} \|\gamma(t)\|_2 = -n^T DV^T n = -\langle DVn, n\rangle.$$

Using $\det DT_0 = \det I = 1$ and the product rule, the above results in

$$\begin{aligned}\left.\frac{d}{dt}\right|_{t=0} \int_{\partial\Omega_t} g \; dS_t &= \int_{\partial\Omega} \left[\left.\frac{d}{dt}\right|_{t=0} (g(T_t) \det DT_t)\right] n - g \cdot \langle DVn, n\rangle \; dS \\ &= \int_{\partial\Omega} \langle \nabla g, V\rangle + g \cdot (\operatorname{div} V - \langle DVn, n\rangle) \; dS,\end{aligned}$$

where formula (5) for the determinant was used again. The final expression follows with Remark 5. ∎

3.3. Shape derivatives of geometric quantities

The derivative of the unit normal field with respect to shape perturbations is very often needed. Many objective functions stemming from physics, such as the fluid forces we are also considering, or any PDE constraint of the Neumann type require this knowledge.

LEMMA 7 (UNIT NORMAL ON PERTURBED DOMAIN) *The unit normal on the perturbed domain Ω_t is given by*

$$n_t(T_t(x)) = \frac{(DT_t(x))^{-T} n(x)}{\|(DT_t(x))^{-T} n(x)\|_2}.$$

Proof. According to Lemma 4, the unit normal on the perturbed domain is given by

$$n_t(x) = \frac{Dh^t(\xi, 0)^{-T} e_d}{\|Dh^t(\xi, 0)^{-T} e_d\|}.$$

Using equations (9) and (10) results in

$$\begin{aligned} n_t(T_t(x)) &= \frac{(DT_t(h(\xi, 0)))^{-T} (Dh(\xi, 0))^{-T} e_d}{\|(DT_t(h(\xi, 0)))^{-T} (Dh(\xi, 0))^{-T} e_d\|} \\ &= \frac{(DT_t(x))^{-T} n(x)}{\|(DT_t(x))^{-T} n(x)\|},\end{aligned}$$

where Lemma 4 was used again for the unperturbed domain. ∎

LEMMA 8 (PRELIMINARY SHAPE DERIVATIVE OF THE UNIT NORMAL) *The preliminary shape derivative of the unit normal is given by*

$$dn[V](x) := \left.\frac{d}{dt}\right|_{t=0} n_t(T_t(x)) = \langle n, (DV(x))^T n(x)\rangle n(x) - (DV(x))^T n(x).$$

Proof. Since $DT_0(x) = I$, the quotient rule simplifies to

$$dn[V](x) := \left(\frac{d}{dt}\bigg|_{t=0} \left[(DT_t(x))^{-T} n(x) \right] \right) - n(x) \left(\frac{d}{dt}\bigg|_{t=0} \|(DT_t(x))^{-T} n(x)\|_2 \right).$$

Using Lemma 4, the above transforms to

$$dn[V](x) = n(x) \left(\frac{d}{dt}\bigg|_{t=0} \|(DT_t(x))^{-T} n(x)\|_2 \right) - (DV(x))^T n(x).$$

For any vector $v(t)$, where the components are differentiable functions, the chain rule gives

$$\frac{d}{dt}\bigg|_{t=0} \|v(t)\|_2 = \frac{d}{dt}\bigg|_{t=0} \left(\sum_i v_i(t)^2 \right)^{\frac{1}{2}} = \frac{\langle v(0), v'(0) \rangle}{\|v(0)\|_2}.$$

Hence, for $v(t) = (DT_t(x))^{-T} n(x)$ one has $v(0) = n(x)$ and again due to Lemma 4 we have $v'(0) = (DV(x))^T n(x)$, resulting in

$$\frac{d}{dt}\bigg|_{t=0} \|DT_t(x) n(x)\|_2 = \langle n(x), (DV(x))^T n(x) \rangle,$$

which gives the desired expression. ∎

Unfortunately, Lemma 8 does not yet fulfill the Hadamard form, and additional transformations using tangential Jacobians from Definition 5 are required.

LEMMA 9 *The shape derivative of the normal is equivalently given by*

$$dn[V] = -\left(D_\Gamma V\right)^T n.$$

Proof. Assuming that the perturbation field V extends into a neighborhood, we have

$$D_\Gamma V = DV - DV n n^T$$

due to Remark 6. Likewise,

$$\left(D_\Gamma V\right)^T n = \left(DV\right)^T n - n \left(DV n\right)^T n = -dn[V]$$

due to Lemma 8. ∎

REMARK 7 *The tangential Jacobian of the unit normal field $n(x)$ at a point x lies in the tangent space $T_x\Omega$, i. e.*

$$0 = D_\Gamma 1 = D_\Gamma \left(n(x)^T n(x) \right) = 2 \left(D_\Gamma n(x) \right) n(x) = 2 \langle \nabla_\Gamma n, n \rangle,$$

meaning $D_\Gamma n \perp n$. This result is needed in the following lemma 10.

LEMMA 10 *For a perturbation normal to the boundary Γ, i.e. $\tilde{V} := \langle V, n\rangle n$ or equivalently $\langle \tilde{V}, \tau\rangle = 0$ for a vector $\tau \in T_x\Omega$ with $x \in \Gamma$, we have*

$$dn[\tilde{V}] = -\nabla_\Gamma \langle \tilde{V}, n\rangle.$$

Proof. For $x \in \Gamma$ let $\{\tau_i \in T_x\Omega : 1 \le i \le d-1\}$ be an orthonormal basis of the tangent space and let the unit normal be given by n with components n_k. By Definition 4 one has

$$\begin{aligned}\nabla_\Gamma \langle \tilde{V}, n\rangle &= \sum_{i=1}^{d-1} \frac{\partial \langle \tilde{V}, n\rangle}{\partial \tau_i} \tau_i \\ &= \sum_{i=1}^{d-1} \frac{\partial}{\partial \tau_i} \left[\sum_{k=1}^{d} \tilde{V}_k n_k \right] \tau_i \\ &= \sum_{i=1}^{d-1} \left[\sum_{k=1}^{d} \frac{\partial \tilde{V}_k}{\partial \tau_i} n_k + \tilde{V}_k \frac{\partial n_k}{\partial \tau_i} \right] \tau_i .\end{aligned}$$

According to Remark 7, the variation of the normal in tangent directions is perpendicular to the normal, and with the particular choice of $\tilde{V}$, the second part vanishes. This results in

$$\begin{aligned}\nabla_\Gamma \langle \tilde{V}, n\rangle &= \sum_{i=1}^{d-1} \sum_{k=1}^{d} \frac{\partial \tilde{V}_k}{\partial \tau_i} n_k \tau_i \\ &= (D_\Gamma \tilde{V})^T n = -dn[\tilde{V}]. \qquad \blacksquare\end{aligned}$$

The idea now is to apply the preliminary shape derivative of Lemma 6 to both sides of the divergence theorem, see below.

THEOREM 2 (DIVERGENCE THEOREM) *Let Ω be compact with piecewise smooth boundary Γ. If F is a continuously differentiable vector field on a neighborhood of Ω, then the following relation holds:*

$$\int_\Omega \operatorname{div} F \; dA = \int_\Gamma \langle F, n\rangle \; dS.$$

Proof. The expression follows immediately from integration by parts. See also Proposition 7.6.1 and Theorem 13.1.2 in Atkinson and Han (2007). ■

However, the preliminary gradient expression requires certain derivatives for which the functional under consideration must extend into a neighborhood of Γ. Unfortunately, this is not true for the outer normal n, so that an extension of the normal into a neighborhood is needed.

Remark 8 *When considering the shape functional*

$$J(g,\Gamma) = \int_\Gamma g(\varphi, n)\ dS,$$

where

$$g : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$
$$(\varphi, \psi) \mapsto g(\varphi, \psi)$$

is a sufficiently smooth function, the preliminary gradient for surface objectives, Lemma 6, requires the existence of the total derivative $\langle \nabla g(\varphi,\psi), V\rangle$. For the expression $g(\varphi, n)$ this existence is not given and a smooth unitary extension $\mathcal{N}$ of the unit normal n into a neighborhood of Γ is needed. Just as in Remark 7, this extension satisfies

$$0 = D\ 1 = D\ \left(\mathcal{N}(x)^T\mathcal{N}(x)\right) = 2\,(D\mathcal{N}(x))\,\mathcal{N}(x) = 2\langle \nabla\mathcal{N}, \mathcal{N}\rangle$$

in the domain Ω. For more details, see Sokolowski and Zolésio (1992). A popular choice for this extension $\mathcal{N}$ is the normalized gradient of the signed distance function $\nabla b/\|\nabla b\|$ due to the applicability in level-set methods, Hintermüller and Ring (2004).

The tangential Stokes formula can now be used to perform an integration by parts on surfaces, in order to arrive at more convenient expressions for surface shape functionals.

Lemma 11 (Tangential Stokes formula) *Let g be a real valued differentiable function on Γ and v be a differentiable vector valued function on Γ. Then the following relation holds:*

$$\int_\Gamma g \operatorname{div}_\Gamma v + \langle \nabla_\Gamma g, v\rangle\ dS = \int_\Gamma \kappa\ g\ \langle v, n\rangle\ dS.$$

Proof. Applying the Hadamard formula for volume objectives, Lemma 2, to the left side of the divergence theorem, Theorem 2 and the preliminary gradient expression of Lemma 6 to the right side, the expression

$$\int_\Gamma \langle V, n\rangle \operatorname{div} F\ dS = \int_\Gamma \langle \nabla\langle F, \mathcal{N}\rangle, V\rangle + \langle F, n\rangle\,(\operatorname{div}_\Gamma V) + \langle F, dn[V]\rangle\ dS$$

is created. The shape derivative of the normal $dn[V]$ enters due to the chain rule. Choosing $V = \mathcal{N}$ and applying Lemma 9 result in

$$\int_\Gamma \operatorname{div} F\ dS = \int_\Gamma \langle \nabla\langle F, \mathcal{N}\rangle, \mathcal{N}\rangle + \langle F, \mathcal{N}\rangle\,(\operatorname{div}_\Gamma \mathcal{N})\ dS,$$

because $D\mathcal{N}\mathcal{N} = 0$. The above now transforms into

$$\int_\Gamma \operatorname{div} F \; dS = \int_\Gamma \langle DFn, n\rangle + \langle F, n\rangle \kappa \; dS.$$

Because $\operatorname{div}_\Gamma F = \operatorname{div} F - \langle DFn, n\rangle$, the desired expression is created by choosing $F := g \cdot v$ for a scalar g and a vector v. ∎

3.4. Shape derivative for surface objectives

Using the tangential Stokes formula, the preliminary gradient expression from Lemma 6 for surface functionals such as the second part of (1) can now be brought into Hadamard form.

Lemma 12 (Hadamard formula for surface objectives) *For a general surface objective function $g : \Gamma \to \mathbb{R}$, which is independent of the shape and for which $\frac{\partial g}{\partial n}$ exists, the shape derivative for the surface objective*

$$J(\Omega) := \int_\Gamma g \; dS$$

is given by

$$dJ(\Omega)[V] = \int_\Gamma \langle V, n\rangle \left[\frac{\partial g}{\partial n} + \kappa g\right] \; dS,$$

where $\kappa = \operatorname{div}_\Gamma n$ is the tangential divergence of the normal, i.e. the additive mean curvature of Γ.

Proof. Starting from the preliminary gradient of Lemma 6, the derivative is given by

$$\begin{aligned} \left.\frac{d}{dt}\right|_{t=0} \int_{\partial\Omega_t} g \; dS_t &= \int_{\partial\Omega} \langle \nabla g, V\rangle + g\left(\operatorname{div} V - \langle DVn, n\rangle\right) \; dS \\ &= \int_{\partial\Omega} \langle \nabla g, V\rangle + g \operatorname{div}_\Gamma V \; dS. \end{aligned}$$

The desired expression is immediately obtained due to the tangential Stokes formula, Lemma 11 and the tangential quantities from Definition 4 and Remark 5. ∎

Lemma 13 (Hadamard formula of the shape derivative of the normal) *Let the objective function be given by*

$$J(g, \Gamma) := \int_\Gamma g(\varphi, D\varphi, n) \; dS,$$

where $g : \mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R}^d \to \mathbb{R}, (\varphi, \zeta, \psi) \mapsto g(\varphi, \zeta, \psi)$ *is a sufficiently smooth functional. The shape derivative of the above expression is then given by*

$$dJ(g,\Gamma)[V] = \int_\Gamma \langle V, n\rangle [D_\varphi g D\varphi\, n + D_\zeta g D^2\varphi\ n + \kappa\,(g - D_\psi g\ n) + \mathrm{div}_\Gamma\ (D_\psi g)^T]\, dS.$$

Proof. To ensure applicability of the Hadamard formula for boundary integrals, Lemma 12, the objective

$$J(g,\Gamma) := \int_\Gamma g(\varphi, D\varphi, \mathcal{N})\ dS$$

is considered. Here, $\mathcal{N}$ is a unitary extension of the normal into Ω just as in Remark 8. By construction, the extension fulfills $\mathcal{N} = n$ and $d\mathcal{N}[V] = dn[V]$ on Γ. The chain rule and Lemma 12 then yield

$$\begin{aligned} dJ(g,\Gamma)[V] = \int_\Gamma \langle V, n\rangle\, &[\langle \nabla g(\varphi, D\varphi, \mathcal{N}), n\rangle + \kappa g(\varphi, D\varphi, n)] \\ &+ D_\psi g(\varphi, D\varphi, n)\, dn[V]\ dS. \end{aligned}$$

The chain rule also leads to

$$\begin{aligned} \langle \nabla g(\varphi, D\varphi, \mathcal{N}), n\rangle &= Dg(\varphi, D\varphi, \mathcal{N})n \\ &= (D_\varphi g(\varphi, D\varphi, \mathcal{N})D\varphi + (D_\zeta g(\varphi, D\varphi, \mathcal{N})D^2\varphi \\ &\qquad + D_\psi g(\varphi, D\varphi, \mathcal{N})D\mathcal{N})n \\ &= D_\varphi g(\varphi, D\varphi, \mathcal{N})D\varphi\ n + D_\zeta g(\varphi, D\varphi, \mathcal{N})D^2\varphi\ n \\ &\qquad + D_\psi g(\varphi, \mathcal{N})D\mathcal{N}\mathcal{N} \\ &= D_\varphi g(\varphi, D\varphi, \mathcal{N})D\varphi\ n + D_\zeta g(\varphi, D\varphi, \mathcal{N})D^2\varphi\ n, \end{aligned}$$

where the second part vanishes due to Remark 8. Let $\tilde{V} := \langle V, n\rangle n$ be the perpendicular component of V. Applying Lemma 10 and inserting the above results in

$$dJ(g,\Gamma)[\tilde{V}] = \int_\Gamma \langle \tilde{V}, n\rangle \left[D_\varphi g D\varphi\ n + D_\zeta g D^2\varphi\, n + \kappa g\right] - D_\psi g\, \nabla_\Gamma \langle \tilde{V}, n\rangle\, dS.$$

The tangential Stokes formula, Lemma 11, gives

$$\int_\Gamma -D_\psi g \nabla_\Gamma \langle \tilde{V}, n\rangle = \int_\Gamma -\kappa \langle \tilde{V}, n\rangle D_\psi g\, n + \langle \tilde{V}, n\rangle \mathrm{div}_\Gamma\ (D_\psi g)^T\ dS,$$

which results in

$$\begin{aligned} dJ(g,\Gamma)[\tilde{V}] = \int_\Gamma \langle \tilde{V}, n\rangle [&D_\varphi g D\varphi\ n + D_\zeta g D^2\varphi\ n \\ &+ \kappa\,(g - D_\psi g\ n) + \mathrm{div}_\Gamma\ (D_\psi g)^T]\ dS. \end{aligned}$$

According to the Hadamard Theorem 1, the shape derivative depends only on the normal component of V. Hence, one has

$$dJ(g,\Gamma)[\tilde{V}] = dJ(g,\Gamma)[V],$$

and the above becomes the desired expression. ■

3.5. Shape derivatives under a state constraint

In the presence of a state constraint, i.e.

$$\begin{aligned}
\min_{(\varphi,\Omega)} J(\varphi,\Omega) \quad &:= \quad \int_{\Omega} f(\varphi)\ dA + \int_{\Gamma} g(\varphi)\ dS \\
\text{subject to} \quad & \\
L(\varphi) \quad &= \quad \varphi_f \text{ in } \Omega \\
L_b(\varphi) \quad &= \quad \varphi_b \text{ on } \Gamma,
\end{aligned}$$

where f and g do not depend on the geometry Ω (respective Γ), the chain rule immediately results in

$$\begin{aligned}
dJ(\varphi,\Omega) \quad &:= \quad \int_{\Gamma} \langle V,n\rangle \left[f(\varphi) + \frac{\partial g(\varphi)}{\partial n} + \kappa g(\varphi)\right]\ dS + \\
& \quad + \int_{\Omega} \frac{\partial f(\varphi)}{\partial \varphi}\varphi'[V]\ dA + \int_{\Gamma} \frac{\partial g(\varphi)}{\partial \varphi}\varphi'[V]\ dS \\
\text{subject to} \quad & \\
L(\varphi) \quad &= \quad \varphi_f \text{ in } \Omega \\
\frac{\partial L(\varphi)}{\partial \varphi}\varphi'[V] \quad &= \quad 0 \text{ in } \Omega,
\end{aligned}$$

which does not yet fulfill the Hadamard form. The Hadamard form for such a problem can now be found by the adjoint approach. Crucial for the adjoint approach is the knowledge of the boundary conditions of the linearized problem, which determines the local shape derivative $\varphi'[V]$ of the state.

A straightforward linearization of the PDE boundary conditions usually results in an expression for the so called "material derivative". However, the general strategy when deriving shape derivatives is to first transfer the problem back to the original boundary before computing the limit, resulting in the need to compute the "local shape derivative", i.e. the linearization of the state φ alone, without considering that the point where the state is being evaluated has moved:

Definition 6 (Material derivative, local Derivative) *Let φ_t solve the PDE constraint on the perturbed domain $\Omega_t = T_t(\Omega)$ and let $x_t := T_t(x)$ be a shifted boundary point. The material derivative is then defined as the total derivative*

$$d\varphi[V](x) := \left.\frac{d}{dt}\right|_{t=0} \varphi_t(x_t)$$

and the local shape derivative is defined as the partial derivative

$$\varphi'[V](x) := \left.\frac{d}{dt}\right|_{t=0} \varphi_t(x).$$

Remark 9 *The chain rule combines both by the relation*

$$d\varphi[V] = \varphi'[V] + \langle \nabla\varphi, V\rangle.$$

Thus, if the right hand side of the boundary condition does not depend on the geometry, one has

$$d\varphi_b[V] = \langle \nabla\varphi_b, V\rangle \quad on \quad \Gamma.$$

Lemma 14 (Shape derivative of the Dirichlet boundary condition) *Suppose the state φ is given as the solution of a PDE of the form*

$$\begin{aligned} L(\varphi) &= \varphi_f \ \ in\ \Omega \\ \varphi &= \varphi_b \ \ on\ \partial\Omega, \end{aligned}$$

such that φ_f and φ_b do not depend on the geometry of Ω, e.g. the unit normal n, etc. The local shape derivative under the perturbation V is then given as the solution of the problem

$$\begin{aligned} \frac{\partial L(\varphi)}{\partial \varphi}\varphi'[V] &= 0 \ \ in\ \Omega \\ \varphi'[V] &= \langle V, n\rangle \frac{\partial(\varphi_b - \varphi)}{\partial n} \ \ on\ \Gamma, \end{aligned}$$

where Γ is the variable part of the boundary of $\partial\Omega$.

Proof. The linearization in Ω is straightforward. Taking the total derivative of the boundary condition results in

$$d\varphi[V] = d\varphi_b[V] \text{ on } \Gamma.$$

Using Remark 9 the above can be transformed to

$$\begin{aligned} \varphi'[V] + \langle \nabla\varphi, V\rangle &= d\varphi[V] = d\varphi_b[V] = \langle \nabla\varphi_b, V\rangle \\ \Rightarrow \varphi'[V] &= \langle \nabla\left(\varphi_b - \varphi\right), V\rangle. \end{aligned}$$

The usual orthogonality argument gives the desired expression

$$\varphi'[V] = \langle V, n\rangle \left(\frac{\partial\left(\varphi_b - \varphi\right)}{\partial n}\right). \qquad \blacksquare$$

Lemma 15 (Shape derivative of the Neumann boundary condition) *Suppose the state φ is given as the solution of a PDE of the form*

$$\begin{aligned} L(\varphi) &= \varphi_f \text{ in } \Omega \\ \frac{\partial \varphi}{\partial n} &= \varphi_b \text{ on } \partial\Omega, \end{aligned}$$

such that φ_f and φ_b do not depend on the geometry of Ω, e.g. the unit normal n, etc. The local shape derivative under the perturbation V is then given as the solution of the problem

$$\begin{aligned} \frac{\partial L(\varphi)}{\partial \varphi}\varphi'[V] &= 0 \text{ in } \Omega \\ \frac{\partial \varphi'[V]}{\partial n} &= \langle \nabla \varphi_b, V\rangle - \langle D^2\varphi V, n\rangle - \langle \nabla_\Gamma \varphi, dn[V]\rangle \\ &= \langle V, n\rangle \left[\frac{\partial \varphi_b}{\partial n} - \frac{\partial^2 \varphi}{\partial n^2}\right] + \langle \nabla_\Gamma \varphi, \nabla_\Gamma \langle V, n\rangle\rangle, \end{aligned}$$

where the second identity holds for the orthogonal component of the perturbation field only.

Proof. The Neumann boundary condition at $x_t = T_t(x)$ on the deformed domain Ω_t reads

$$\begin{aligned} \varphi_b \circ x_t &= \langle \nabla \varphi_t, n_t\rangle \circ x_t \\ &= \langle \nabla \varphi_t, n_t\rangle \circ T_t(x) \\ &= \langle (\nabla \varphi_t) \circ T_t(x), n_t(x_t)\rangle. \end{aligned}$$

The chain rule results in

$$\begin{aligned} \nabla(\varphi_t \circ T_t(x)) &= ((\nabla \varphi_t) \circ T_t(x))^T \cdot DT_t(x) \\ &= (DT_t(x))^T \cdot [(\nabla \varphi_t) \circ T_t(x)] \end{aligned}$$

and the boundary condition becomes

$$\begin{aligned} \varphi_b(x_t) &= \langle (DT_t(x))^{-T} \nabla(\varphi_t \circ T_t(x)), n_t(x_t)\rangle \\ &= (\nabla(\varphi_t(x_t)))^T DT_t(x)^{-1} \cdot n_t(x_t). \end{aligned}$$

The total derivative with respect to t now yields the material derivative of $\varphi_t(x_t)$. Using Remark 4 we get:

$$d\varphi_b[V] = (\nabla d\varphi[V])^T n + (\nabla \varphi)^T (-DV)\, n + \langle \nabla \varphi, dn[V]\rangle,$$

which results in

$$\frac{\partial d\varphi[V]}{\partial n} = d\varphi_b[V] - \langle \nabla \varphi, (-DV)\, n\rangle - \langle \nabla \varphi, dn[V]\rangle. \tag{11}$$

Using the relationship from Remark 9,

$$d\varphi[V] = \varphi'[V] + \langle \nabla\varphi, V\rangle,$$

we have in addition to equation (11) also the relation

$$\frac{\partial d\varphi[V]}{\partial n} = \frac{\partial \varphi'[V]}{\partial n} + \langle D^2\varphi V, n\rangle + \langle \nabla\varphi, DVn\rangle. \tag{12}$$

Thus, taking (11) and (12) together, one obtains

$$\begin{aligned}\frac{\partial \varphi'[V]}{\partial n} &= \frac{\partial d\varphi[V]}{\partial n} - \langle D^2\varphi V, n\rangle - \langle \nabla\varphi, DVn\rangle \\ &= d\varphi_b[V] + \langle \nabla\varphi, DVn\rangle - \langle \nabla\varphi, dn[V]\rangle - \langle D^2\varphi V, n\rangle - \langle \nabla\varphi, DVn\rangle \\ &= d\varphi_b[V] - \langle \nabla\varphi, dn[V]\rangle - \langle D^2\varphi V, n\rangle,\end{aligned}$$

an equation for the local shape derivative. Since in addition one has

$$\begin{aligned} d\varphi_b[V] &= \langle \nabla\varphi_b, V\rangle \\ dn[V] &= -\nabla_\Gamma\langle V, n\rangle,\end{aligned}$$

the above can also be expressed as

$$\frac{\partial \varphi'[V]}{\partial n} = \langle \nabla\varphi_b, V\rangle - \langle D^2\varphi V, n\rangle - \langle \nabla\varphi, dn[V]\rangle.$$

Since $\langle \nabla\varphi, n\rangle = 0$, we have $\nabla\varphi = \nabla_\Gamma\varphi$, and with the usual orthogonality argument the boundary condition can be expressed as

$$\frac{\partial \varphi'[V]}{\partial n} = \langle V, n\rangle \left[\frac{\partial \varphi_b}{\partial n} - \frac{\partial^2\varphi}{\partial n^2}\right] + \langle \nabla_\Gamma\varphi, \nabla_\Gamma\langle V, n\rangle\rangle, \tag{13}$$

where the last part can be brought into Hadamard form using Lemma 11. ∎

Remark 10 *Note that a much simpler formula than* (13) *can be given in the special case of the standard Laplace problem*

$$\begin{aligned} -\Delta\varphi &= \varphi_f \ \text{ in } \Omega \\ \frac{\partial\varphi}{\partial n} &= \varphi_b \ \text{ on } \partial\Omega.\end{aligned}$$

The Laplace-Beltrami operator

$$\Delta_\Gamma\varphi := \operatorname{div}_\Gamma \nabla_\Gamma\varphi = \Delta\varphi - \kappa\frac{\partial\varphi}{\partial n} - \frac{\partial^2\varphi}{\partial n^2}$$

provides

$$\frac{\partial^2\varphi}{\partial n^2} = -\Delta_\Gamma\varphi - \varphi_f - \kappa\varphi_b,$$

which results in

$$\frac{\partial \varphi'[V]}{\partial n} = \mathrm{div}_\Gamma \left(\langle V, n\rangle \nabla_\Gamma \varphi\right) + \langle V, n\rangle \left(\frac{\partial \varphi_b}{\partial n} + \kappa\varphi_b + \varphi_f\right).$$

For more details see Sokolowski and Zolésio (1992).

Instead of conducting the adjoint calculus in a general setting, we now return to the Navier–Stokes problem.

4. Shape derivative and adjoint calculus for the general Navier–Stokes Problem

We begin with the shape derivative of (1) and (2) in sensitivity formulation:

THEOREM 3 (SHAPE DERIVATIVE IN SENSITIVITY FORMULATION) *The shape derivative of* (1) *and* (2) *in sensitivity formulation is given by:*

$$dJ(u,p,\Omega)[V] =$$

$$\int_{\Gamma_0} \langle V, n\rangle f(u, Du, p)\ dS \tag{14}$$

$$+ \int_{\Omega} \left(\sum_{i=1}^{d} \frac{\partial f}{\partial u_i} u_i'[V]\right) + \left(\sum_{i,j=1}^{d} \frac{\partial f}{\partial a_{ij}} \frac{\partial u_i'[V]}{\partial x_j}\right) + \frac{\partial f}{\partial p} p'[V]\ dA \tag{15}$$

$$+ \int_{\Gamma_0} \langle V, n\rangle \left[D_{(u,b,p)} g(u, D_n u, p, n)\cdot n + \kappa g(u, D_n u, p, n)\right]\ dS \tag{16}$$

$$+ \int_{\Gamma_0} \left(\sum_{i=1}^{d} \frac{\partial g}{\partial u_i} u_i'[V]\right) + \left(\sum_{i,j=1}^{d} \frac{\partial g}{\partial b_i} \frac{\partial u_i'[V]}{\partial x_j} n_j\right) + \frac{\partial g}{\partial p} p'[V]\ dS \tag{17}$$

$$+ \int_{\Gamma_0} \sum_{i=1}^{d} \frac{\partial g}{\partial n_i} dn_i[V]\ dS. \tag{18}$$

See also equation (3)*. The local shape derivatives $u'[V]$ and $p'[V]$ are given as the solution of the linearized Navier–Stokes equations*

$$\begin{aligned} -\mu\Delta u'[V] + \rho\left(u'[V]\nabla u + u\nabla u'[V]\right) + \nabla p'[V] = 0 \ \textit{in}\ \Omega \\ \mathrm{div}\, u'[V] = 0, \end{aligned}$$

with boundary conditions

$$\begin{aligned} u_i'[V] &= -\langle V, n\rangle \frac{\partial u_i}{\partial n} \quad \textit{on} \quad \Gamma_0 \\ u_i'[V] &= 0 \quad \textit{on} \quad \Gamma_+ \\ p'[V] n_i - \mu\langle \nabla u_i'[V], n\rangle &= 0 \quad \textit{on} \quad \Gamma_-. \end{aligned} \tag{19}$$

Proof. Formal shape differentiation of (1) and (2) is done according to Section 3. The boundary condition on Γ_0 is given by Lemma 14. Since the other boundaries are considered fixed, one does not have to consider differences between the material and the local shape derivative and a linearization is straightforward. ■

For the adjoint formulation of the shape derivative we need further discussions including adjoint functionals $\lambda : \Omega \to \mathbb{R}^d$ and $\lambda_p : \Omega \to \mathbb{R}$.

LEMMA 16 *For a sufficiently smooth arbitrary $\lambda : \Omega \to \mathbb{R}^d$ and $\lambda_p : \Omega \to \mathbb{R}$ the relation*

$$0 = \int_\Omega \sum_{i=1}^d \left[-\mu \Delta \lambda_i - \rho \left(\sum_{i,j=1}^d \frac{\partial \lambda_j}{\partial x_i} u_j + \frac{\partial \lambda_i}{\partial x_j} u_j \right) - \frac{\partial \lambda_p}{\partial x_i} \right] u_i'[V] \; dA \tag{20}$$

$$- \int_\Omega \sum_{i=1}^d \frac{\partial \lambda_i}{\partial x_i} p'[V] \; dA \tag{21}$$

$$+ \int_\Gamma \sum_{i=1}^d \left[\mu \frac{\partial \lambda_i}{\partial n} + \rho \sum_{j=1}^d (\lambda_j u_j n_i + \lambda_i u_j n_j) \right] u_i'[V] \; dS \tag{22}$$

$$+ \int_\Gamma \lambda_p \sum_{i=1}^d u_i'[V] n_i \; dS + \int_\Gamma \sum_{i=1}^d \lambda_i n_i p'[V] \; dS + \int_\Gamma \sum_{i=1}^d -\mu \lambda_i \frac{\partial u_i'[V]}{\partial n} \; dS \tag{23}$$

holds.

Proof. Multiplying the volume part of the linearized Navier–Stokes equations with arbitrary λ and λ_p results in

$$0 = \int_\Omega \sum_{i=1}^d \lambda_i \left[-\mu \Delta u_i'[V] + \rho \left(\sum_{j=1}^d u_j'[V] \frac{\partial u_i}{\partial x_j} + u_j \frac{\partial u_i'[V]}{\partial x_j} \right) + \frac{\partial p'[V]}{\partial x_i} \right] dA$$
$$+ \int_\Omega \lambda_p \mathrm{div}\, u'[V] \; dA.$$

Integration by parts gives

$$\int_\Omega \sum_{i=1}^d -\mu \lambda_i \Delta u_i'[V] \; dA = \int_\Gamma \sum_{i=1}^d -\mu \left(\lambda_i \frac{\partial u_i'[V]}{\partial n} - u_i'[V] \frac{\partial \lambda_i}{\partial n} \right) \; dS$$
$$+ \int_\Omega \sum_{i=1}^d -\mu u_i'[V] \Delta \lambda_i \; dA$$

and likewise, due to div $u'[V] = 0$:

$$\int_\Omega \sum_{i,j=1}^d \lambda_i u_j'[V] \frac{\partial u_i}{\partial x_j} \, dA = \int_\Gamma \sum_{i,j=1}^d \lambda_i u_j'[V] u_i n_j \, dS \quad - \int_\Omega \sum_{i,j=1}^d \frac{\partial \lambda_i}{\partial x_j} u_j'[V] u_i \, dA.$$

Note that in the above equation the index of the local shape derivative is j and not i. To derive the desired expression, the indices i and j must be switched. Integration by parts of the second part of the linearized convection results in

$$\int_\Omega \sum_{i,j=1}^d \lambda_i u_j \frac{\partial u_i'[V]}{\partial x_j} \, dA = \int_\Gamma \sum_{i,j=1}^d \lambda_i u_j u_i'[V] n_j \, dS - \int_\Omega \sum_{i,j=1}^d \frac{\partial \lambda_i}{\partial x_j} u_j u_i'[V] \, dA.$$

The pressure variation provides

$$\int_\Omega \sum_{i=1}^d \lambda_i \frac{\partial p'[V]}{\partial x_i} \, dA = \int_\Gamma \lambda_i n_i p'[V] \, dS - \int_\Omega \sum_{i=1}^d \frac{\partial \lambda_i}{\partial x_i} p'[V] \, dA$$

and the divergence constraint provides

$$\int_\Omega \lambda_p \sum_{i=1}^d \frac{\partial u_i'[V]}{\partial x_i} \, dA = \int_\Gamma \lambda_p \sum_{i=1}^d u_i'[V] n_i \, dS - \int_\Omega \sum_{i=1}^d \frac{\partial \lambda_p}{\partial x_i} u_i'[V] \, dA.$$

Summarizing the above yields the desired expression. ∎

Using Lemma 16, it is now possible to derive the adjoint right hand side in the volume:

LEMMA 17 (ADJOINT RIGHT HAND SIDE, VOLUME) *The adjoint equation must fulfill in the domain Ω:*

$$\begin{aligned} -\mu \Delta \lambda_i - \rho \sum_{j=1}^d \left(\frac{\partial \lambda_j}{\partial x_i} u_j + \frac{\partial \lambda_i}{\partial x_j} u_j \right) - \frac{\partial \lambda_p}{\partial x_i} &= \frac{\partial f}{\partial u_i} - \sum_{j=1}^d \frac{\partial}{\partial x_j} \frac{\partial f}{\partial a_{ij}} \\ \operatorname{div} \lambda &= \frac{\partial f}{\partial p}. \end{aligned}$$

Proof. Due to equations (20) - (23) summing to zero, they can be added to the preliminary gradient (14) - (18). Integration by parts of equation (15) yields

$$\begin{aligned} &\int_\Omega \left(\sum_{i=1}^d \frac{\partial f}{\partial u_i} u_i'[V] \right) + \left(\sum_{i,j=1}^d \frac{\partial f}{\partial a_{ij}} \frac{\partial u_i'[V]}{\partial x_j} \right) + \frac{\partial f}{\partial p} p'[V] \, dA \\ &= \int_\Gamma \sum_{i,j=1}^d \frac{\partial f}{\partial a_{ij}} u_i'[V] n_j \, dS \end{aligned} \tag{24}$$

$$+\int_\Omega \sum_{i=1}^d \left(\frac{\partial f}{\partial u_i} - \sum_{j=1}^d \frac{\partial}{\partial x_j}\frac{\partial f}{\partial a_{ij}}\right) u_i'[V]\; dA + \int_\Omega \frac{\partial f}{\partial p} p'[V]\; dA \tag{25}$$

and a direct comparison between the above and equations (20) and (21) reveals the required adjoint right hand side in Ω. Note that this has introduced a new boundary term. ∎

Lemma 18 (Adjoint boundary condition at inflow) *The adjoint boundary condition on the inflow boundary Γ_+ is given by*

$$\begin{aligned} \lambda &= 0 \\ \lambda_p &\quad \textit{free.} \end{aligned}$$

Proof. Since the inflow velocity is fixed and independent of the shape of the fluid obstacle, we have $u'[V] = 0$ on Γ_+. Hence, the only term appearing on Γ_+ is the normal variation of $u'[V]$ and the pressure variation $p'[V]$ from equation (23):

$$\int_{\Gamma_+} \sum_{i=1}^d \lambda_i n_i p'[V]\; dS + \int_{\Gamma_+} \sum_{i=1}^d -\mu\lambda_i \frac{\partial u_i'[V]}{\partial n}\; dS,$$

which is removed by $\lambda = 0$ on Γ_+. ∎

Lemma 19 (Adjoint Boundary Condition at No-Slip) *The adjoint boundary condition on the no-slip boundary Γ_0 is given by*

$$\begin{aligned} \lambda_i &= \frac{1}{\mu}\frac{\partial g}{\partial b_i}\ \forall i = 1,\ldots,d \\ \langle \lambda, n\rangle &= -\frac{\partial g}{\partial p} \\ \lambda_p &\quad \textit{free.} \end{aligned}$$

Proof. The sensitivities on Γ_0 are equations (24), (17), (22), and (23):

$$\begin{aligned} &\int_{\Gamma_0} \sum_{i,j=1}^d \frac{\partial f}{\partial a_{ij}} u_i'[V] n_j\; dS \\ &+ \int_{\Gamma_0} \left(\sum_{i=1}^d \frac{\partial g}{\partial u_i} u_i'[V]\right) + \left(\sum_{i,j=1}^d \frac{\partial g}{\partial a_{ij}} \frac{\partial u_i'[V]}{\partial x_j}\right) + \frac{\partial g}{\partial p} p'[V]\; dS \\ &+ \int_{\Gamma_0} \sum_{i=1}^d \left[\mu \frac{\partial \lambda_i}{\partial n} + \rho \sum_{j=1}^d (\lambda_j u_j n_i + \lambda_i u_j n_j)\right] u_i'[V]\; dS \end{aligned}$$

$$+\int_{\Gamma_0} \lambda_p \sum_{i=1}^{d} u_i'[V] n_i \; dS + \int_{\Gamma_0} \sum_{i=1}^{d} \lambda_i n_i p'[V] \; dS + \int_{\Gamma_0} \sum_{i=1}^{d} -\mu \lambda_i \frac{\partial u_i'[V]}{\partial n} \; dS.$$

Using the no-slip boundary condition and the boundary condition for the local shape derivative, the above transforms to

$$\begin{aligned} &\int_{\Gamma_0} \langle V, n\rangle \left[-\sum_{i=1}^{d} \left(\frac{\partial g}{\partial u_i} + \mu \frac{\partial \lambda_i}{\partial n} + \lambda_p n_i + \sum_{j=1}^{d} \frac{\partial f}{\partial a_{ij}} n_j \right) \frac{\partial u_i}{\partial n} \right] \; dS \\ &+ \int_{\Gamma_0} \left(\sum_{i=1}^{d} \frac{\partial g}{\partial b_i} \frac{\partial u_i'[V]}{\partial n} \right) + \left(\frac{\partial g}{\partial p} + \sum_{i=1}^{d} \lambda_i n_i \right) p'[V] \; dS \\ &+ \int_{\Gamma_0} \sum_{i=1}^{d} -\mu \lambda_i \frac{\partial u_i'[V]}{\partial n} \; dS, \end{aligned}$$

where the first part now also enters the gradient (14) - (18). Expressing ∇u_i in local coordinates on the boundary results in

$$\nabla u_i = \langle \nabla u_i, n\rangle n + \sum_{j=1}^{d} \langle \nabla u_i, \tau_j \rangle \tau_j,$$

hence

$$\frac{\partial u_i}{\partial x_j} = \frac{\partial u_i}{\partial n} n_j \Rightarrow 0 = \lambda_p \sum_{i=1}^{d} \frac{\partial u_i}{\partial n} n_i$$

due to the mass conservation on Γ_0. Hence, λ_p does not receive a boundary condition. The remaining sensitivities can be eliminated by

$$\begin{aligned} \lambda_i &= \frac{1}{\mu} \frac{\partial g}{\partial b_i} \; \forall i = 1, \ldots, d \\ \langle \lambda, n \rangle &= -\frac{\partial g}{\partial p}. \end{aligned}$$

In order to arrive at a complete adjoint system, we also need the boundary conditions for the adjoint variables at the outflow boundary:

LEMMA 20 (ADJOINT BOUNDARY CONDITION AT OUTFLOW) *The adjoint boundary condition on the outflow boundary Γ_- is given by*

$$\mu \frac{\partial \lambda_i}{\partial n} + \rho \left(\sum_{j=1}^{d} \lambda_j u_j n_i + \lambda_i u_j n_j \right) + \lambda_p n_i = 0.$$

Proof. After inserting equation (19) into equations (20) - (23), the remaining sensitivity is

$$\int_{\Gamma_-} \sum_{i=1}^{d} \left[\mu \frac{\partial \lambda_i}{\partial n} + \rho \sum_{j=1}^{d} (\lambda_j u_j n_i + \lambda_i u_j n_j) \right] u_i'[V]\, dS + \int_{\Gamma_-} \lambda_p \sum_{i=1}^{d} u_i'[V] n_i \, dS.$$

Hence, the required boundary condition is

$$\mu \frac{\partial \lambda_i}{\partial n} + \rho \left(\sum_{j=1}^{d} \lambda_j u_j n_i + \lambda_i u_j n_j \right) + \lambda_p n_i = 0.$$

THEOREM 4 (SHAPE DERIVATIVE FOR THE GENERAL NAVIER–STOKES PROBLEM) *The shape derivative in Hadamard form for the problem under consideration is given by*

$$\begin{aligned}
& dJ(u, p, \Omega)[V] = \\
& \int_{\Gamma_0} \langle V, n \rangle f(u, Du, p)\ dS \\
& + \int_{\Gamma_0} \langle V, n \rangle \left[D_{(u,b,p)} g(u, D_n u, p, n) \cdot n + \kappa g(u, D_n u, p, n) \right]\ dS \\
& + \int_{\Gamma_0} \langle V, n \rangle \left[- \sum_{i=1}^{d} \left(\frac{\partial g}{\partial u_i} + \mu \frac{\partial \lambda_i}{\partial n} + \sum_{j=1}^{d} \frac{\partial f}{\partial a_{ij}} n_j \right) \frac{\partial u_i}{\partial n} \right]\ dS \\
& + \int_{\Gamma_0} \langle V, n \rangle \left[(\operatorname{div}_\Gamma \nabla_n g) - \kappa \langle \nabla_n g, n \rangle \right]\ dS,
\end{aligned}$$

where $\nabla_n g$ *denotes the vector consisting of components* $\frac{\partial g}{\partial n_i}$. *Furthermore,* u *and* p *solve the incompressible Navier–Stokes equations*

$$\begin{aligned}
-\mu \Delta u + \rho u \nabla u + \nabla p = \rho G \quad & \text{in} \quad \Omega \\
\operatorname{div} u = 0 \quad & \\
u = u_+ \quad & \text{on} \quad \Gamma_+ \\
u = 0 \quad & \text{on} \quad \Gamma_0 \\
pn - \mu \frac{\partial u}{\partial n} = 0 \quad & \text{on} \quad \Gamma_-,
\end{aligned}$$

and λ *and* λ_p *solve the adjoint incompressible Navier–Stokes equations*

$$\begin{aligned}
-\mu \Delta \lambda_i - \rho \sum_{j=1}^{d} \left(\frac{\partial \lambda_j}{\partial x_i} u_j + \frac{\partial \lambda_i}{\partial x_j} u_j \right) - \frac{\partial \lambda_p}{\partial x_i} = \frac{\partial f}{\partial u_i} - \sum_{j=1}^{d} \frac{\partial}{\partial x_j} \frac{\partial f}{\partial a_{ij}} \quad & \text{in} \quad \Omega \\
\operatorname{div} \lambda = \frac{\partial f}{\partial p} \quad &
\end{aligned}$$

with boundary conditions

$$
\begin{aligned}
\lambda &= 0 && \textit{on} \quad \Gamma_+ \\
\lambda_i &= \frac{1}{\mu}\frac{\partial g}{\partial b_i} && \textit{on} \quad \Gamma_0 \\
\langle \lambda, n\rangle &= -\frac{\partial g}{\partial p} && \textit{on} \quad \Gamma_0 \\
\mu\frac{\partial \lambda_i}{\partial n} + \rho\left(\sum_{j=1}^{d} \lambda_j u_j n_i + \lambda_i u_j n_j\right) + \lambda_p n_i &= 0 && \textit{on} \quad \Gamma_- .
\end{aligned}
$$

Proof. The adjoint boundary conditions are derived in Lemma 18, 19, and 20. The adjoint right hand side is derived in Lemma 17, and removing the shape derivative of the normal is described in Lemma 13. ∎

5. Application

5.1. Volume and surface formulations

For theoretical considerations on optimal shapes in a Navier–Stokes fluid, the conversion of kinetic energy into heat is usually studied. This objective function is a volume integral, which is more accessible for analytic studies (Mohammadi and Pironneau, 2001; Pironneau, 1974). When we use the Stokes equation to model the flow, the expression is even self-adjoint and optimal shapes are known analytically (Pironneau, 1973). However, since the objective is integrated over the whole flow domain, the objective function value depends on the size of the simulation area. Also, the total dissipation of kinetic energy into heat cannot be split in the coordinate axis directions, meaning that lift and drag of the shape under consideration cannot easily be treated separately. Therefore, in actual aerodynamic design, the total force vector the fluid exerts on an obstacle is almost always computed as a boundary integral, which is then also non-dimensionalized to make the resulting lift and drag values applicable to a wider array of flow situations.

With the general formulation of the Navier–Stokes shape derivative at hand, it appears to be natural to compare both formulations with respect to their performance when actually computing optimal shapes discretely.

REMARK 11 (VOLUME FORMULATION: ENERGY DISSIPATION) *Using the same notation as in Theorem 4, the viscous dissipation of kinetic energy into heat in two dimensions is given by*

$$
\begin{aligned}
f(u, Du, p) &= \mu \sum_{i,j=1}^{2} \left(\frac{\partial u_i}{\partial x_j}\right)^2 \\
g(u, D_n u, p, n) &= 0,
\end{aligned}
$$

which results in

$$\frac{\partial f}{\partial a_{ij}} = 2\mu a_{ij} = 2\mu \frac{\partial u_i}{\partial x_j}$$
$$\frac{\partial f}{\partial u_i} = 0.$$

According to Theorem 4, the adjoint equation is given by

$$\begin{aligned} -\mu\Delta\lambda_i - \rho\sum_{j=1}^{d}\left(\frac{\partial \lambda_j}{\partial x_i}u_j + \frac{\partial \lambda_i}{\partial x_j}u_j\right) - \frac{\partial \lambda_p}{\partial x_i} &= \frac{\partial f}{\partial u_i} - \sum_{j=1}^{d}\frac{\partial}{\partial x_j}\frac{\partial f}{\partial a_{ij}} \\ &= -2\mu\Delta u_i \qquad \text{in} \quad \Omega \\ \operatorname{div}\lambda_p &= \frac{\partial f}{\partial p} = 0 \end{aligned}$$

with boundary conditions

$$\begin{aligned} \lambda &= 0 && \text{on} \quad \Gamma_+ \\ \lambda_i &= \frac{1}{\mu}\frac{\partial g}{\partial b_i} = 0 && \text{on} \quad \Gamma_0 \\ \langle \lambda, n\rangle &= -\frac{\partial g}{\partial p} = 0 && \text{on} \quad \Gamma_0 \\ \mu\frac{\partial \lambda_i}{\partial n} + \rho\left(\sum_{j=1}^{2}\lambda_j u_j n_i + \lambda_i u_j n_j\right) + \lambda_p n_i &= 0 && \text{on} \quad \Gamma_-. \end{aligned}$$

Both conditions on Γ_0 *are satisfied by* $\lambda = 0$ *and, consequently, the gradient is given by*

$$\begin{aligned} dJ(u,p,\Omega)[V] &= \int_{\Gamma_0}\langle V,n\rangle\left[\mu\sum_{i,j=1}^{2}\left(\frac{\partial u_i}{\partial x_j}\right)^2\right]\,dS \\ &+ \int_{\Gamma_0}\langle V,n\rangle\left[-\sum_{i=1}^{2}\left(\mu\frac{\partial \lambda_i}{\partial n} + \sum_{j=1}^{2}\frac{\partial f}{\partial a_{ij}}n_j\right)\frac{\partial u_i}{\partial n}\right]\,dS \\ &= \int_{\Gamma_0}\langle V,n\rangle\left[\mu\sum_{i=1}^{2}\left(\frac{\partial u_i}{\partial n}\right)^2\right]\,dS \\ &+ \int_{\Gamma_0}\langle V,n\rangle\left[-\sum_{i=1}^{2}\left(\mu\frac{\partial \lambda_i}{\partial n} + \sum_{j=1}^{2}2\mu\frac{\partial u_i}{\partial x_j}n_j\right)\frac{\partial u_i}{\partial n}\right]\,dS \\ &= \int_{\Gamma_0}\langle V,n\rangle\left[-\mu\sum_{i=1}^{2}\frac{\partial \lambda_i}{\partial n}\frac{\partial u_i}{\partial n} + \left(\frac{\partial u_i}{\partial n}\right)^2\right]\,dS. \end{aligned}$$

REMARK 12 (SURFACE FORMULATION: FLUID FORCES) *When considering flow around an airfoil or any other obstacle, one does not want to make a new mesh in case the airfoil has a different angle of attack. Instead, most flow solvers rotate the coordinate system internally. For drag at angle of attack* α*, the incident vector* a *is given by*

$$a := (\cos\alpha, \sin\alpha)^T .$$

The drag force an incompressible Navier–Stokes fluid exerts on Γ_0 *is given by*

$$F_D := \int_{\Gamma_0} -\mu \langle D_n u, a\rangle + p\langle n, a\rangle \; dS.$$

The gradient of F_D *is then given by*

$$\begin{aligned} dF_D(u,p,\Omega)[V] = & \int_{\Gamma_0} \langle V, n\rangle \left[-\mu (D_n)^2 ua + \frac{\partial p}{\partial n}\langle a, n\rangle - \sum_{i=1}^{2} \mu \frac{\partial \lambda_i}{\partial n}\frac{\partial u_i}{\partial n}\right] \; dS \\ & + \int_{\Gamma_0} \langle V, n\rangle \left[\mathrm{div}_\Gamma \; (-\mu Dua + pa)\right] \; dS \end{aligned}$$

with adjoint boundary condition $\lambda = -a$ *on* Γ_0*.*

Proof. Here, the function g is given by

$$g := -\mu\langle D_n u, a\rangle + p\langle n, a\rangle.$$

Furthermore,

$$\begin{aligned} \langle \nabla g, n\rangle &= -\mu (D_n)^2 ua + \frac{\partial p}{\partial n}\langle n, a\rangle \\ \frac{\partial g}{\partial u_i} &= 0 \\ \nabla_n g &= -\mu Dua + pa \\ \frac{\partial g}{\partial p} &= \langle a, n\rangle \\ \frac{\partial g}{\partial b} &= -\mu a, \end{aligned}$$

where $(D_n)^2 ua$ refers to the second normal derivative tensor of u, e.g.

$$(D_n)^2 ua = \sum_{i,j,k=1}^{2} n_i \frac{\partial^2 u_k}{\partial x_i \partial x_j} n_j a_k.$$

The structure of the gradient and the adjoint boundary conditions are a direct consequence of Theorem 4. Note that for this specific function, the terms $\kappa g(u, D_n u, p, n)$ and $\kappa\langle \nabla_n g, n\rangle$ cancel each other. ∎

5.2. Results

Here, the numerical performance of both formulations, i.e. the volume formulation from Remark 11 and the surface formulation from Remark 12, will be compared. The Navier–Stokes equations are discretized using mixed Taylor–Hood finite elements. The resulting non-linear system of equations is solved using Newton's method. The adjoint solver is constructed discretely out of the Newton iteration. Computation of the gradients requires knowledge of first and second order normal derivatives of the flow states, which are computed using finite differences. The tangential divergence is approximated discretely according to the definition

$$\operatorname{div}_\Gamma g = \sum_{i=1}^{d-1} \left\langle \frac{\partial g}{\partial \tau_i}, \tau_i \right\rangle,$$

where τ_i are the tangent vectors. The tangent derivative is computed using second order central finite differences.

The initial shape is a circle in a channel at Reynolds number $Re = 80$. The shape of the circle is subject to the no-slip boundary condition and is to be optimized using a constant volume constraint. The circle surface is discretized using 100 nodes, which are the design parameters. Due to the Taylor–Hood discretization, each edge mid-point also features a velocity value, such that there exist other 100 velocity-only nodes on the circle surface that are not shape design parameters. The channel walls are modeled as farfield. The initial shape is also shown in Fig. 2. For both versions, surface formulation and volume formulation, the optimization procedure is based on an approximative SQP method, where

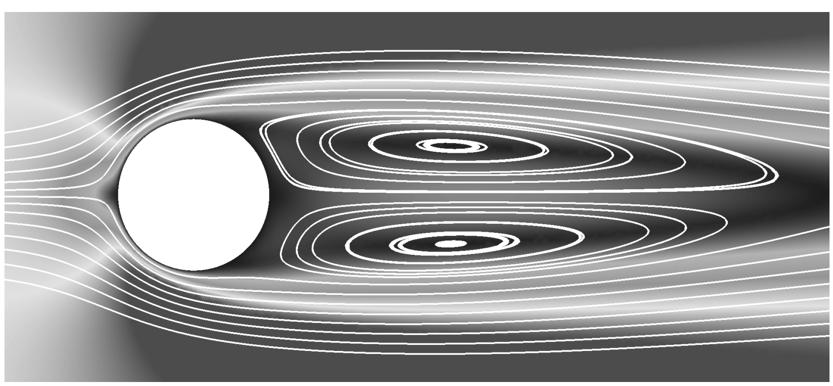

Figure 2. The initial shape. Flow around a circle with Reynolds number $Re = 80$. Speed and streamlines visualized. The apparent dissymmetry stems from the automatic generation of the seed points for the streamline integration.

the actual update J_S is computed from the shape gradient J according to

$$J = (k\Delta_\Gamma + I)J_S,$$

meaning the discrete shape Hessian is approximated by $k\Delta_\Gamma + I$, where Δ_Γ is the Laplace–Beltrami operator, I is the identity, and k is a smoothing parameter. For more details see Schmidt and Schulz (2009). Here, the parameter $k = 0.05$ was chosen as a constant in all following computations. Fig. 3 shows how both drag and energy dissipation evolve when optimizing according to the drag gradient. Likewise, Fig. 4 shows the same quantities when optimizing according to the energy dissipation shape gradient. Although optimization with respect to the volume objective function appears to be slightly faster, one has to

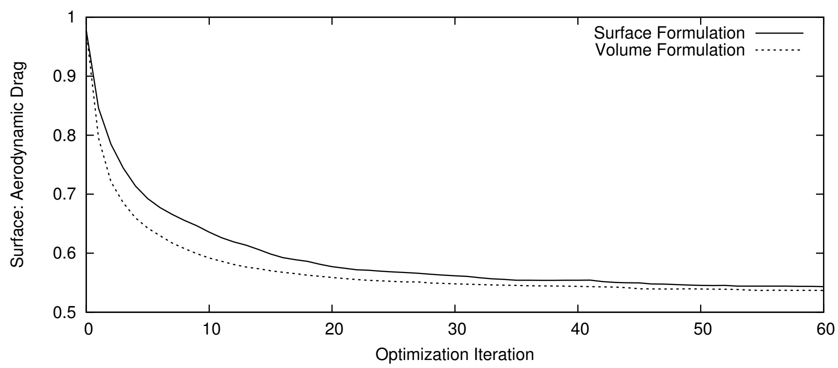

Figure 3. Optimization history for both energy dissipation and aerodynamic drag when using the gradient for the surface quantity “drag”.

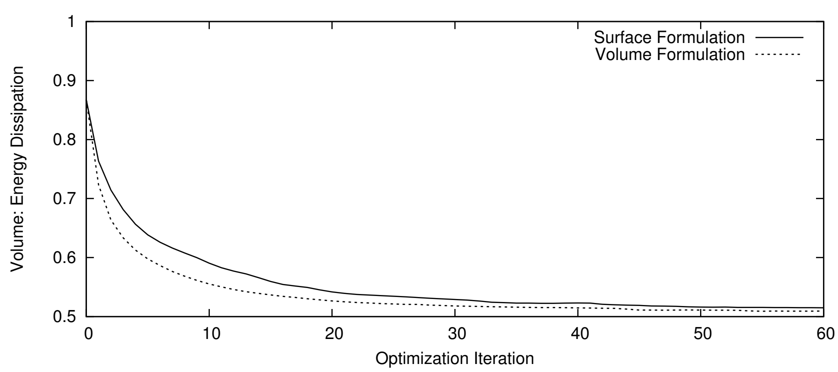

Figure 4. Optimization history for both energy dissipation and aerodynamic drag when using the gradient for the volume quantity “energy”.

take into account that both optimizations were conducted using a constant step length of 0.03 for the drag optimization and 0.08 for the energy optimization. Furthermore, the surface version requires knowledge of second order normal derivatives of the flow quantities. Since the solver is based on standard Taylor–Hood finite elements, the computation of second order finite differences can be problematic. The velocities are discretized using second order polynomials inside each of the six-noded Taylor–Hood elements, making the second order derivatives of the velocity constant within each element. Likewise, the same is true for first order pressure derivatives.

Fig. 5 shows the respective optimal shapes. Using the energy dissipation gradient, the rear end appears slightly rounder, which results in less separation and probably explains the slight difference in the objective functions. Since

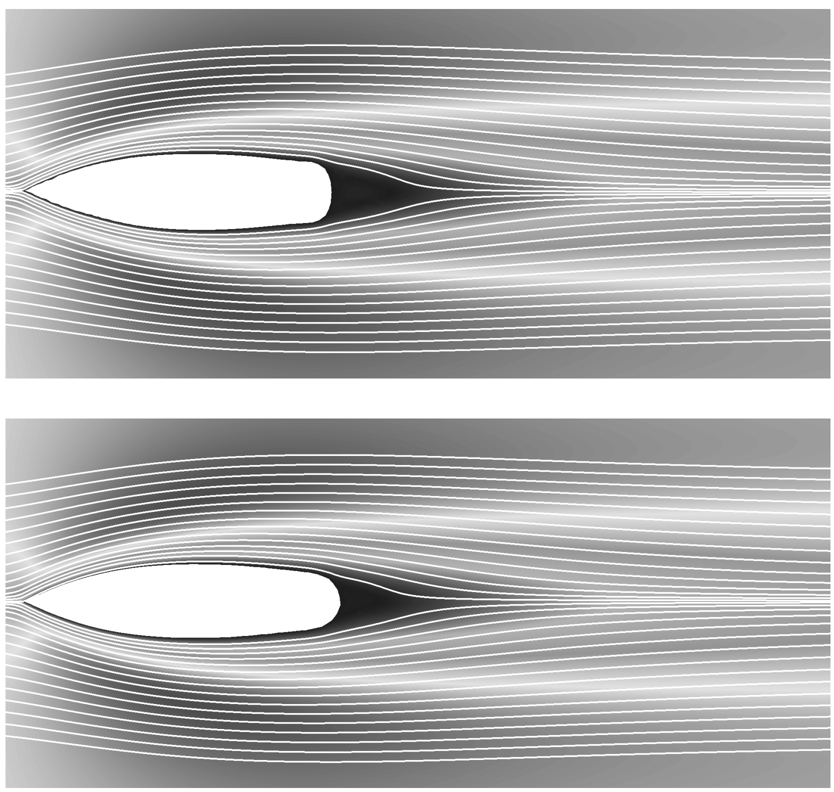

Figure 5. Speed and streamlines for the optimized shapes. Top figure shows the optimized shape when using the drag gradient, bottom shows the optimized shape when using the energy dissipation gradient.

the perimeter of the circle increases during the optimization, the number of variable boundary nodes is increased automatically during optimization. As such, the optimized shape with respect to the drag gradient has 135 variable nodes, while the optimized shape with respect to energy has 137 variable nodes. Since the number of surface nodes is allowed to be adapted during optimization, the volume mesh is re-created between each iteration.

6. Summary

The main purpose of this work has been the derivation of the Hadamard form of the shape derivative for a wide class of objective functions in a Navier–Stokes flow, especially also considering boundary integrals as the objective. The Hadamard form enables a very efficient computation of the gradient, since knowledge of the "mesh sensitivity" Jacobian is not required. Being an analytic expression, the Hadamard form must be re-derived for each problem unless a generic objective is considered as it is in this paper. Due to the artificial nature of the pressure in an incompressible flow, some restrictions appear on the surface part of the objective function. Otherwise one cannot formulate a consistent adjoint equation, since the pressure does not have a boundary condition but is implicitly given so that mass is conserved. We also list many important literature results from shape analysis and geometry, such that the paper is self contained and can easily be adapted to other kinds of shape problems. Having the general expression for the shape derivative at hand, we conclude with a comparison of two different approaches for the optimization of a fluid obstacle in a channel. One is based on the volume objective functional using the fluid energy, while the other is based on the surface objective functional of the aerodynamic drag. With the general form of the gradient at hand, such a comparison can be conducted quite conveniently.

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References

Amrouche, C., Nečasová, Š. and Sokolowski, J. (2007) Shape sensitivity analysis of the Neumann problem of the Laplace equation in the half-space. Technical Report preprint 2007-12-20, Institute of Mathematics, AS CR, Prague.

Atkinson, K. and Han, W. (2007) *Theoretical Numerical Analysis: A Functional Analysis Framework*. *Texts in Applied Mathematics*, **39**. Springer, 2nd edition.

Boisgérault, S. and Zolésio, J.P. (1993) Shape derivative of sharp functionals governed by Navier–Stokes flow. In: W. Jäger, J. Necas, O. John, K. Najzar and J. Stará, eds., *Partial Differential Equations: Theory and Numerical Solution. Research Notes in Mathematics.* Chapman & Hall/CRC, 49–63.

Delfour, M.C. and Zolésio, J.P. (2001) *Shapes and Geometries: Analysis, Differential Calculus, and Optimization. Advances in Design and Control.* SIAM, Philadelphia.

Gunzburger, M.D. (2003) *Perspectives in Flow Control and Optimization. Advances in Design and Control.* SIAM, Philadelphia.

Hintermüller, M. and Ring, W. (2004) An inexact Newton-CG-type active contour approach for the minimization of the Mumford-Shah functional. *Journal of Mathematical Imaging and Vision*, **20**, 19–42.

Ito, K., Kunisch, K., Gunther, G. and Peichl, H. (2008) Variational approach to shape derivatives. *Control, Optimisation and Calculus of Variations*, **14**, 517–539.

Mohammadi, B. and Pironneau, O. (2001) *Applied Shape Optimization for Fluids. Numerical Mathematics and Scientific Computation.* Clarendon Press, Oxford.

Pironneau, O. (1973) On optimum profiles in Stokes flow. *Journal of Fluid Mechanics*, **59** (1), 117–128.

Pironneau, O. (1974) On optimum design in fluid mechanics. *Journal of Fluid Mechanics*, **64** (1), 97–110.

Plotnikov, P.I., Ruban, E.V. and Sokolowski, J. (2008) Inhomogeneous boundary value problems for compressible Navier–Stokes equations: Well-posedness and sensitivity analysis. *Journal on Mathematical Analysis*, **40** (3), 1152–1200.

Plotnikov, P.I. and Sokolowski, J. (2005) On compactness, domain dependence and existence of steady state solutions to compressible isothermal Navier–Stokes equations. *Journal of Mathematical Fluid Mechanics*, **7** (4), 529–573.

Plotnikov, P.I. and Sokolowski, J. (2008) Stationary boundary value problems for compressible Navier–Stokes equations. *Handbook of Differential Equations*, **6**, 313–410.

Schmidt, S., Ilic, C., Gauger, N. and Schulz, V. (2008) Shape gradients and their smoothness for practical aerodynamic design optimization. Technical Report Preprint SPP1253-10-03, DFG-SPP 1253. Submitted to *OPTE*.

Schmidt, S. and Schulz, V. (2009) Impulse response approximations of discrete shape Hessians with application in CFD. *SIAM Journal on Control and Optimization*, **48** (4), 2562–2580.

Sokolowski, J. and Zolésio, J.P. (1992) *Introduction to Shape Optimization: Shape Sensitivity Analysis.* Springer.