Journal of Computational and Applied Mathematics 296 (2016) 334–351

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Shape derivatives for the compressible Navier–Stokes equations in variational form

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ARTICLE INFO

Article history:
Received 6 February 2015
Received in revised form 30 July 2015

MSC:
49Q10
49Q12
65K10
76Nxx
76M30

Keywords:
Shape derivative
Variational form
Compressible Navier–Stokes equations

ABSTRACT

Shape optimization based on surface gradients and the Hadamard-form is considered for a compressible viscous fluid. Special attention is given to the difference between the "function composition" approach involving local shape derivatives and an alternate methodology based on the weak form of the state equation. The resulting gradient expressions are found to be equal only if the existence of a strong form solution is assumed. Surface shape derivatives based on both formulations are implemented within a Discontinuous Galerkin flow solver of variable order. The gradient expression stemming from the variational approach is found to give superior accuracy when compared to finite differences.

0. Introduction

Shape optimization is a research field that has received much attention in the past. In general, any problem where the boundary of the domain is part of the unknown can be considered a shape optimization problem. In most applications, the physics are modeled by partial differential equations, making shape optimization a special sub-class within the field of PDE-constrained optimization. Usually, the derivation of the sensitivities and adjoint equations follows a function composition approach, i.e. some set of design variables defines the geometry and within this geometry the PDE is solved, thereby generating the state variables that enter the objective function [1–3]. Therefore, the necessity to consider sensitivities or derivative information with respect to the geometry adds additional complexity to the shape optimization problem when compared to general PDE-constrained optimization. Because it is often not immediately clear how to compute these "mesh sensitivities", that is the variation of the PDE with respect to a change in the geometry, there is often a strong desire for a very smooth parameterization of the domain with as few design parameters as possible. Although there have been successful attempts to incorporate problem structure exploitations in order to efficiently compute these partial derivatives for very large problems, such as differentiating the entire design chain at once or by considering the adjoint process of the mesh deformation [4,5], very often one is still forced into finite differencing, which means the PDE residual at steady state has to be evaluated on meshes that have been perturbed by a variation in each design parameter of the shape, a process that makes large scale optimization usually prohibitive. This negates some of the advantages of the adjoint approach, such as

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http://dx.doi.org/10.1016/j.cam.2015.09.010
0377-0427/

the independence of the number of design parameters. More severely, it also makes fast optimization strategies such as the one-shot approach [6–8] somewhat unattractive in terms of wall-clock-time.

A more recent trend to overcome the cumbersome computation of these geometric sensitivities is the use of shape calculus. Shape calculus summarizes the mathematical framework used when considering problems where the shape is the unknown in the continuous setting. Manipulations in the tangent space of the unknown object can be used to circumvent any necessity of knowing discrete geometric sensitivities, because these can be directly included in a surface gradient expression on the continuous level. More details on this theoretical framework can be found in [9,10]. Traditionally, this methodology was primarily used to address the very difficult question of existence and uniqueness of optimal shapes [11], but more recently this methodology has also been used in very large scale aerodynamic design and computational optimization [12–14]. In [15], for example, the complete optimization of a blended wing–body aircraft in a compressible inviscid fluid is considered. Because this approach solely relies on the problem formulation in the continuous setting and only afterwards discretizes the continuous boundary integral expressions for the shape derivative, great care must be taken when making the initial assumptions and when implementing the respective continuous expressions, especially at singular points in the geometry, such as the trailing edge of an airfoil [16]. Because this approach is indeed truly independent of the number of design parameters, it enables the most detailed possible parameterization, that is using all surface mesh nodes as design unknowns. This is sometimes called "free node parameterization". However, these highly detailed shape parameterizations usually lack any kind of inherent regularity preservation and as such, one usually finds this approach paired with some sort of smoothing procedure that projects or embeds the respective optimization iterations into a desired regularity class, which can nicely be paired with an SQP or Newton-type optimization scheme, which is sometimes also called a "Sobolev Method" [17,18].

As part of this work, we study how to further increase the accuracy of shape derivatives when used within viscous compressible aerodynamic design optimization. Within applied aerodynamic shape optimization, it is customary to exploit the above mentioned function composition approach in order to derive and implement the adjoint equation and gradient expression. This has been used with great success, both within the context of continuous and discrete adjoint based aerodynamic shape optimization [19,20,13,21] and general shape optimization [22]. However, common to these approaches is the assumption that the state equation has a strong form solution and each of the steps within the shape differentiation process of the function composition exists, which usually means the existence of so-called local shape derivatives. For elliptic problems, this existence can usually be shown, making the above mentioned approach somewhat of an established procedure, see for example Chapter 3.3 in [10]. However, for the hyperbolic equations governing some compressible fluids, the existence of a strong form solution is not clear. Rather, in the presence of shock waves and discontinuities in the flow, one can usually only expect the variational form of the equation to hold, a property which is very often not taken into account when studying the derivative. Shape differentiation of problems governed by PDEs in weak or variational forms are not very often considered in the literature, except in [23] and especially in [24], where the incompressible Navier–Stokes equations are considered for this purpose from a rigorous theoretical standpoint. Thus, we revisit the shape optimization problem previously considered in [25], but the gradient is derived using elements of the variational approach as shown in [24]. Furthermore, we simultaneously follow the function composition approach, outlining the exact differences comparing these two approaches. One can nicely see how both methodologies reduce to the same gradient expression when assuming the existence of a strong from solution of the state equation. We conclude with a numerical error analysis based on comparing finite differencing with either implementation, demonstrating the higher accuracy of the gradient formulation based on the variational form of the compressible Navier–Stokes equations.

The structure of the paper is as follows. In Section 1, we begin by recapitulating the compressible Navier–Stokes equations in both strong and variational form. Next, Section 2 serves as an introduction and quick overview of shape calculus, including shape derivatives and the Hadamard or Hadamard–Zolésio Structure Theorem, which leads to a preliminary form of the shape derivative of the aerodynamic cost functions. The next section, Section 3, is used to work out the differences between the shape derivative of the compressible Navier–Stokes equations stemming from either the function composition or the variational approach. In Section 4, we then summarize the idea of adjoint calculus. This is used to differentiate the Navier–Stokes equations, thereby discussing the Hadamard form of the respective objective functions both for the strong as well as the variational form of the state constraint. Finally, in the last section, numerical results achieved with both methods are compared to shape derivatives computed by finite differences, showing a considerable gain in accuracy when using shape derivatives based on the variational form.

1. Fluid mechanics

1.1. Flow domain and boundary conditions

In the following ρ, $v = (v_1, v_2)^\top$, p, E and T denote the density, velocity, pressure, total energy and temperature. The domain of the fluid is denoted by Ω, with wall and far-field boundaries Γ_W and Γ_∞. At the wall Γ_W, the no-slip boundary condition $v = 0$ is imposed for the velocity. With respect to temperature, either the isothermal boundary condition $T = T_W$ or the adiabatic boundary condition $\nabla T \cdot n = 0$ holds. The isothermal and adiabatic parts of the wall are named Γ_{iso} and Γ_{adia} and we assume $\Gamma_W = \Gamma_{iso} \cup \Gamma_{adia}$ disjoint.

Furthermore κ, e, H, μ and γ denote the thermal conductivity, the internal energy, the enthalpy, the viscosity and the adiabatic exponent. The relation $T\kappa = \frac{\mu\gamma}{Pr}\left(E - \frac{1}{2}\|v\|^2\right)$ is fulfilled for the temperature, where Pr is the Prandtl number.

1.2. Navier–Stokes equations and aerodynamic objective functions

In this subsection, we state the Navier–Stokes equations in both strong and weak form. As discussed later, the shape derivative of the aerodynamic cost functions differs depending on which form of the Navier–Stokes equations is used. Using the viscous stress tensor τ, defined by

$$\tau = \mu\left(\nabla v + (\nabla v)^\top - \frac{2}{3}(\nabla\cdot v)I\right), \tag{1}$$

the compressible Navier–Stokes equations in strong form are given by

$$\nabla\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u},\nabla\mathbf{u})\right) \equiv \sum_k\left(\frac{\partial}{\partial x_k}f_k^c(\mathbf{u}) - \frac{\partial}{\partial x_k}f_k^v(\mathbf{u},\nabla\mathbf{u})\right) = 0 \quad \text{in } \Omega, \tag{2}$$

where $\mathbf{u}$ denotes the vector of conserved variables, $\mathcal{F}^c = (f_1^c, f_2^c)$ the convective fluxes

$$\mathbf{u} = \begin{pmatrix}\rho\\ \rho v_1\\ \rho v_2\\ \rho E\end{pmatrix} \qquad f_1^c(\mathbf{u}) = \begin{pmatrix}\rho v_1\\ \rho v_1^2 + p\\ \rho v_1 v_2\\ \rho H v_1\end{pmatrix}, \qquad f_2^c(\mathbf{u}) = \begin{pmatrix}\rho v_2\\ \rho v_1 v_2\\ \rho v_2^2 + p\\ \rho H v_2\end{pmatrix}$$

and $\mathcal{F}^v = (f_1^v, f_2^v)$ denotes the viscous fluxes

$$f_1^v(\mathbf{u},\nabla\mathbf{u}) = \begin{pmatrix}0\\ \tau_{11}\\ \tau_{21}\\ \sum_j \tau_{1j}v_j + \kappa\dfrac{\partial T}{\partial x_1}\end{pmatrix}, \qquad f_2^v(\mathbf{u},\nabla\mathbf{u}) = \begin{pmatrix}0\\ \tau_{12}\\ \tau_{22}\\ \sum_j \tau_{2j}v_j + \kappa\dfrac{\partial T}{\partial x_2}\end{pmatrix}.$$

Furthermore, temperature T and pressure p are linked to the state variables using the perfect gas assumption, that is

$$p = \rho R T = \rho R\frac{E - \frac{1}{2}\|v\|^2}{c_v} = \frac{R}{c_v}\rho\left(E - \frac{1}{2}\|v\|^2\right),$$

where $e = c_v T$, $E = e + \frac{1}{2}\|v\|^2$ and c_v denotes the heat capacity of the gas at constant volume.

Furthermore, the compressible Navier–Stokes equations in variational form are given by the following:

Definition 1.1 (*Variational Form of the Navier–Stokes Equations*)**.** We assume that $\mathcal{H} := H^1 \times H^2 \times H^3 \times H^4$, where H^i is a suitable Hilbert-Space. Multiplication of the pointwise Navier–Stokes (2) with an arbitrary test function $\mathbf{v} \in \mathcal{H}$ and integration by parts results in the problem to find $\mathbf{u} \in \mathcal{H}$, such that

$$\langle F(\mathbf{u},\Omega),\mathbf{v}\rangle_{\mathcal{H}^*\times\mathcal{H}} := -\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u},\nabla\mathbf{u}), \nabla\mathbf{v}\right)_\Omega + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u},\nabla\mathbf{u})\right), \mathbf{v}\right)_\Gamma = 0 \quad \forall\mathbf{v}\in\mathcal{H} \tag{3}$$

with the boundary conditions

$$\begin{aligned}\begin{pmatrix}v_1\\ v_2\end{pmatrix} &= 0 && \text{on } \Gamma_W,\\ \nabla T\cdot n &= 0 && \text{on } \Gamma_{adia},\\ T &= T_{wall} && \text{on } \Gamma_{iso}.\end{aligned} \tag{4}$$

Definition 1.2 (*Cost Function*)**.** The cost functions under consideration are the lift and drag coefficients, given by

$$J(\mathbf{u}) = \frac{1}{C_\infty}\int_{\Gamma_W}(pn - \tau n)\cdot\psi\,\mathrm{d}s, \tag{5}$$

where C_∞ is a constant and ψ is either $\psi_l = (-\sin(\alpha), \cos(\alpha))^\top$ for the lift or $\psi_d = (\cos(\alpha), \sin(\alpha))^\top$ for the drag coefficient.

2. Shape calculus

2.1. Definition of the shape derivative and the Hadamard theorem

In this section the concept of shape derivatives and especially the Hadamard Theorem, as stated in [9,10], are summarized. Let therefore D, the so-called hold-all, be an open set in $\mathbb{R}^d$ and the domain Ω be a measurable subset of D. For vector fields

$V \in C_0^k(D;\mathbb{R}^d)$ the perturbation of identity

$$T_t[V] : D \times [0,\delta) \to \mathbb{R}^d, \quad (x,t) \mapsto x + tV(x)$$

is a common approach to describe a deformation $\Omega_t = T_t[V](\Omega)$ of the domain Ω. With such a deformation, the shape derivative of a domain functional $J(\Omega)$ at Ω in the direction of a vector field $V \in C_0^k(D;\mathbb{R}^d)$ is defined as the Eulerian derivative

$$dJ(\Omega;V) := \lim_{t\searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}.$$

The functional $J(\Omega)$ is called shape differentiable at Ω if this Eulerian derivative exists for all directions V and the mapping $G(\Omega) : C_0^k(D;\mathbb{R}^d) \to \mathbb{R},\ V \mapsto dJ(\Omega;V)$ is linear and continuous.

If the functional $J(\Omega)$ is shape differentiable on measurable sets $\Omega \subset D$, then there exists the shape gradient $G(\Omega) \in \left(C_0^k(D;\mathbb{R}^d)\right)^*$ such that

$$dJ(\Omega;V) = \langle G(\Omega), V\rangle_{\left(C_0^k(D;\mathbb{R}^d)\right)^* \times C_0^k(D;\mathbb{R}^d)} \quad \forall\, V \in C_0^k(D;\mathbb{R}^d). \tag{6}$$

This means that the shape derivative, as a directional derivative in direction V, can be computed by the dual pair, which is a generalized scalar product, of the shape gradient $G(\Omega)$ and the vector field V. Furthermore in [10] it is shown, that if a vector field V fulfills $V \cdot n = 0$, meaning it is tangential to the boundary $\Gamma = \partial\Omega \in C^k$, then the shape derivative in this direction vanishes, which is intuitively clear, since a deformation of the domain Ω in a tangential direction, being a form of reparameterization, does not change the domain and therefore the shape derivative vanishes, because the flow solution and the cost functional stay the same.

Consequently, there exists a continuous linear mapping $dJ(\Gamma;\cdot) : C^k(\Gamma) \to \mathbb{R}$ such that for all vector fields $V \in C^k(\bar{D};\mathbb{R}^d)$ the relation

$$dJ(\Omega;V) = dJ(\Gamma; V\cdot n)$$

holds, which implies that the shape derivative only depends on the normal component of the vector field V at the boundary of the domain. The following theorem states the existence of a scalar distribution $g(\Gamma)$, which takes the role of the shape gradient $G(\Omega)$ in Eq. (6) for the mapping $dJ(\Gamma;\cdot)$ on the boundary of the domain.

Theorem 2.1 (*Hadamard Theorem, Hadamard Formula*)**.** *For every domain $\Omega \subset D$ of class C^k, let $J(\Omega)$ be a shape differentiable function. Furthermore let the boundary Γ be of class C^{k-1}. There exists the following scalar distribution $g(\Gamma) \in C_0^k(\Gamma)^*$, such that the shape gradient $G(\Omega) \in C_0^k(\Omega,\mathbb{R}^d)^*$ of $J(\Omega)$ is given by*

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

where $\gamma_\Gamma \in L\left(C_0^k(\Omega,\mathbb{R}^d), C_0^k(\Gamma,\mathbb{R}^d)\right)$ and γ_Γ^* denote the trace operator and its adjoint operator. In this situation, one can show that [10]

$$dJ(\Omega;V) = dJ(\Gamma;V\cdot n) = \langle g, V\cdot n\rangle_{\left(C_0^k(\Gamma,\mathbb{R}^d)\right)^* \times C_0^k(\Gamma,\mathbb{R}^d)}.$$

If $g(\Gamma)$ is integrable over Γ, then the Hadamard Formula

$$dJ(\Omega;V) = \int_\Gamma (V\cdot n) g\, ds$$

is fulfilled. In the following we will call terms that are of the structure "$(V\cdot n)\ldots$" to be in Hadamard form.

Proof. A proof can for example be found in [9] or in [10]. □

Remark 2.2. Assuming the boundary Γ_W is of sufficient regularity such that the tangential component only describes a reparameterization but no actual change of the shape, then the shape derivative $dJ(\Omega;V)$ only depends on the normal component $(V\cdot n)n$ of the vector field V, which will later eliminate certain normal components within the derivation of the surface gradient expression of the cost functions. Further studies of the ramifications of this assumption can be found in [16].

Definition 2.3 (*Material Derivative/Local Shape Derivative*)**.** The total derivative

$$d_V[f](x) := \left.\frac{d}{dt}\right|_{t=0} f(t, T_t(x))$$

of f is called the material derivative. Furthermore, the partial derivative

$$f'(x) := f'[V](x) := \frac{\partial}{\partial t} f(t,x)$$

is called the local shape derivative of f.

Remark 2.4. The material and the local shape derivative are related to each other by the chain rule if both exist, i.e.

$$d_V[f](x) = f'[V](x) + \nabla f(0,x) \cdot V(x) = f' + \nabla f \cdot V,$$

where we used $\frac{d}{dt}\big|_{t=0} T_t(x) = \frac{d}{dt}\big|_{t=0}(x + tV(x)) = V(x)$ for the perturbation of identity. If the geometry is as such that the local shape derivative does not exist, a sharp convex corner for example, one usually accepts the above formula as a definition of the local shape derivative instead.

2.2. Tangential calculus

Before we state the shape derivative of volume and boundary integrals, we give a minimal summary of tangential calculus, which will later be used to derive a preliminary shape derivative of the lift and drag coefficients. This is also required to find the local shape derivative of quantities fulfilling Neumann boundary conditions. A more detailed discussion on tangential calculus can be found in [9, Chapter 8, Section 5].

Let $f \in C^1(\Gamma)$ be a function with a C^1-extension F into a tubular neighborhood of Γ. The tangential gradient is the ordinary gradient minus its normal component, i.e.

$$\nabla_\Gamma f := \nabla F|_\Gamma - \frac{\partial F}{\partial n} n. \tag{7}$$

Analogously, the tangential divergence of a smooth vector field $W \in (C^1(\Gamma))^d \cap (C^1(\Omega))^d$ is defined by

$$\operatorname{div}_\Gamma W := \operatorname{div} W - DWn \cdot n. \tag{8}$$

For f and W as defined above, the tangential Green's formula is given by

$$\int_\Gamma W \cdot \nabla_\Gamma f \, ds = \int_\Gamma fK(W \cdot n) - f \operatorname{div}_\Gamma W \, ds, \tag{9}$$

where $K := \operatorname{div}_\Gamma n$ denotes the sum of the principal curvatures, the so called additive curvature, or $(d-1)$ times the mean curvature. A proof can be found in [9, Chapter 8].

2.3. Shape derivative for volume and boundary integrals

In this subsection, we recapitulate shape derivatives of general volume and boundary integrals, as they can be found in [9] for example. Furthermore, we show a preliminary shape derivative of the drag and lift coefficients, which is later transformed into Hadamard form using adjoint calculus. The shape derivative of a general volume cost function $J(\Omega) = \int_\Omega f(x)\, dx$ is given by

$$dJ(\Omega; V) = \int_\Omega f' \, dx + \int_\Gamma (V \cdot n) f \, ds \tag{10}$$

and for a general boundary cost function $J(\Omega) = \int_\Gamma f \, ds$ the shape derivative fulfills

$$dJ(\Omega; V) = \int_\Gamma f' + (V \cdot n)\left(\frac{\partial f}{\partial n} + Kf\right) ds. \tag{11}$$

Furthermore, if the vector field V is orthogonal to the boundary Γ, the material derivative of the normal vector fulfills

$$d_V[n] = -\nabla_\Gamma (V \cdot n), \tag{12}$$

which can be found in [26].

Theorem 2.5 (*Preliminary Shape Derivative of the Cost Functional*)**.** *If the vector field of the perturbation of identity fulfills $V = 0$ in the neighborhood of the farfield boundary Γ_∞, then the shape derivative of the lift and drag coefficients, Eq. (5), is given by*

$$dJ(\Omega; V) = \frac{1}{C_\infty} \int_{\Gamma_W} (p'n - \tau' n) \cdot \psi + (V \cdot n) \operatorname{div}(p\psi - \tau\psi) \, ds. \tag{13}$$

Proof. The proof of the above expression is not fully straight forward, because the objective function (5) depends on the local normal, which first needs to be extended into a tubular neighborhood as discussed within the subsection on tangential calculus. Following the same argumentation as in [26], let $\mathcal{N}$ be an extension of the normal n into a tubular neighborhood. It is easy to see that as a result of the normalization of this extension, the property

$$\begin{aligned} 0 &= \nabla \mathcal{N} \cdot \mathcal{N} \\ &= \nabla \mathcal{N} \cdot n \quad \text{on } \Gamma_W \end{aligned} \tag{14}$$

holds. Because $p\mathcal{N}\cdot\psi$ and $\tau\mathcal{N}\cdot\psi$ have the same structure, we restrict ourselves to $p\mathcal{N}\cdot\psi$, that is we consider the functional $j=\int_{\Gamma_W} p\mathcal{N}\cdot\psi\,\mathrm{d}s$, for which the shape derivative of a general boundary integral as stated in Eq. (11) is applicable. Paired with the properties of the normal extension (14), this leads to

$$\begin{aligned} dj(\Omega;V) &= \int_{\Gamma_W} p'\mathcal{N}\cdot\psi + p\mathcal{N}'\cdot\psi + (V\cdot\mathcal{N})\left(\frac{\partial(p\mathcal{N}\cdot\psi)}{\partial n} + K(p\mathcal{N}\cdot\psi)\right)\mathrm{d}s \\ &= \int_{\Gamma_W} p'n\cdot\psi + pn'\cdot\psi + (V\cdot n)\left(\frac{\partial(p\cdot\psi)}{\partial n}n + K(pn\cdot\psi)\right)\mathrm{d}s. \end{aligned} \tag{15}$$

From Remark 2.4 we have $\mathcal{N}'=d_V[\mathcal{N}]-\nabla\mathcal{N}\cdot V$ for the local shape derivative of the extended normal vector. Combining Remark 2.2, i.e. assuming $V=(V\cdot n)n$, with Eq. (14), one arrives at $n'=d_V[n]$. Also using $d_V[n]=-\nabla_\Gamma(V\cdot n)$ from (12) gives us the relation

$$\int_{\Gamma_W} pn'\cdot\psi\,\mathrm{d}s = -\int_{\Gamma_W} p\nabla_\Gamma(V\cdot n)\cdot\psi\,\mathrm{d}s.$$

Application of the tangential Green's formula to the right hand side of the above equation yields

$$\int_{\Gamma_W} pn'\cdot\psi\,\mathrm{d}s = -\int_{\Gamma_W} (V\cdot n)K(p\psi\cdot n) - (V\cdot n)\,\mathrm{div}_\Gamma(p\psi)\,\mathrm{d}s,$$

where the assumption $V=0$ in the neighborhood of the farfield boundary Γ_∞ was used to employ the tangential Green's formula at the wall boundary only. We will now insert the above equation into (15). As one can see, the terms containing the additive curvature K cancel out and the following expression remains

$$dj(\Omega;V) = \int_{\Gamma_W} p'n\cdot\psi + (V\cdot n)\left[\mathrm{div}_\Gamma(p\psi) + \frac{\partial(p\cdot\psi)}{\partial n}n\right]\mathrm{d}s.$$

The terms within the bracket now exactly align with the definition of the tangential divergence, Eq. (8), such that

$$\mathrm{div}_\Gamma(p\psi) + \frac{\partial(p\cdot\psi)}{\partial n}n = \mathrm{div}_\Gamma(p\psi) + D(p\psi)n\cdot n = \mathrm{div}(p\psi).$$

The same argumentation can now be also applied to $\tau n\cdot\psi$ instead of $pn\cdot\psi$. □

The above theorem already supplies one possible representation of the shape derivative of the objective functional. However, this preliminary shape derivative is not yet in Hadamard form because it still contains the local shape derivatives p' and τ'. Computation of these would require one forward flow solution for each design parameter of the parameterization of the shape, which is prohibitively costly. In Section 4, adjoint calculus is used to remove these local shape derivatives p' and τ', thereby transforming the above gradient expression into the Hadamard form.

2.4. Shape derivatives of boundary conditions

Transformation of the gradient expression from Theorem 2.5 requires explicit knowledge of the boundary conditions defining the local shape derivatives p' and τ'. These are governed by the respective boundary conditions imposed within the forward problem. As such, we now consider how the Dirichlet condition, the Neumann condition and the slip condition of the forward problem determine these local shape derivatives. The general argumentation again follows [10].

2.4.1. Dirichlet boundaries

First, we consider a general Dirichlet boundary condition $w = w_D$ on the wall Γ_W, where w_D does not depend on the geometry, meaning w_D is independent of the parameter t of the deformation T_t. This is especially true for the no-slip condition $v=0$, which should also be fulfilled on the perturbed boundary. Application of the material derivative paired with Remark 2.4 applied to both sides of the Dirichlet boundary condition $w=w_D$ yields

$$d_V[w] = w' + \nabla w\cdot V = d_V[w_D] = \nabla w_D\cdot V,$$

where the local shape derivative of w_D equals zero, since w_D does not depend on t. From this equation, we can extract a condition defining the local shape derivative $w'=\nabla(w_D-w)\cdot V$. According to Remark 2.2, it is sufficient to consider only the normal direction $(V\cdot n)n$ of the vector field V, which leads to

$$w' = \nabla(w_D-w)\cdot n(V\cdot n) = \frac{\partial w_D - w}{\partial n}(V\cdot n).$$

2.4.2. Neumann boundaries

Similar to the Dirichlet boundary condition, we again would like to consider the material derivative of the boundary condition of the forward problem and then apply the chain rule argument given by Remark 2.4 to find a corresponding expression for the local shape derivatives. This will again require the quantities under consideration to exist at least within a tubular neighborhood for which we again assume an extension of the normal $\mathcal{N}$ just as in Theorem 2.5. If we apply the material derivative to both sides of the Neumann boundary condition $\frac{\partial w}{\partial \mathcal{N}} = \nabla w \cdot \mathcal{N} = w_N$, where w_N does not depend on the shape, meaning on the parameter t, we get with Remark 2.4

$$d_V[\nabla w \cdot \mathcal{N}] = (\nabla w \cdot \mathcal{N})' + \nabla(\nabla w \cdot \mathcal{N}) \cdot V = d_V[w_N] = \nabla w_N \cdot V.$$

Since $\nabla w' \cdot \mathcal{N} = (\nabla w \cdot \mathcal{N})' - \nabla w \cdot \mathcal{N}'$ holds, we get from this equation

$$\nabla w' \cdot \mathcal{N} = \nabla w_N \cdot V - \nabla w \cdot \mathcal{N}' - \nabla(\nabla w \cdot \mathcal{N}) \cdot V.$$

Using the usual orthogonality argumentation again, Remark 2.2 and again employing Remark 2.4, we can insert the relation $n' = \mathcal{N}' = d_V[\mathcal{N}] - \nabla \mathcal{N} \cdot V = d_V[n]$ and furthermore use $\nabla(\nabla w \cdot \mathcal{N}) \cdot V = D^2 w \mathcal{N} \cdot V + \nabla w \cdot (\nabla \mathcal{N} \cdot V) = D^2 wn \cdot V$ to obtain

$$\begin{aligned}\nabla w' \cdot n &= \nabla w_N \cdot V - \nabla w \cdot d_V[n] - D^2 wn \cdot V \\ &= (V \cdot n)\left[\nabla w_N \cdot n - D^2 wn \cdot n\right] - \nabla w \cdot d_V[n].\end{aligned}$$

From Eq. (12) we get the equality $d_V[n] = -\nabla_\Gamma (V \cdot n)$, which results in

$$\begin{aligned}\frac{\partial w'}{\partial n} &= (V \cdot n)\left[\frac{\partial w_N}{\partial n} - \frac{\partial^2 w}{\partial n^2}\right] + \nabla w \cdot \nabla_\Gamma (V \cdot n) \\ &= (V \cdot n)\left[\frac{\partial w_N}{\partial n} - \frac{\partial^2 w}{\partial n^2}\right] + \nabla_\Gamma w \cdot \nabla_\Gamma (V \cdot n),\end{aligned}$$

where the last transformation directly results from $\nabla w \cdot n = 0$ being inserted into the definition of the tangential gradient. This expression is still not entirely in Hadamard form, but we will later use the tangential Green's formula to conclude this transformation.

3. Shape derivative of the Navier–Stokes equations in strong and variational form

Before adjoint calculus can be used in Section 4 to finalize the Hadamard form, one first needs to establish the corresponding forward problem. Therefore, we now consider the linearization of the compressible Navier–Stokes equations with respect to a variation of the domain. As mentioned above, we distinguish between the Navier–Stokes equations in pointwise and in variational form. Unsurprisingly, both versions of the forward problem lead to distinct linearizations and this section will be used to discuss the respective differences.

Theorem 3.1 (*Shape Derivative of the Pointwise Navier–Stokes Equations*)**.** *The local shape derivative* $\mathbf{u}'$ *of the Navier–Stokes equations in strong form (2) is given as the solution of*

$$0 = \nabla \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right) \quad \text{in } \Omega, \tag{16}$$

where $\mathcal{F}^c_{\mathbf{u}} := \frac{\partial \mathcal{F}^c}{\partial \mathbf{u}}$, $\mathcal{F}^v_{\mathbf{u}} := \frac{\partial \mathcal{F}^v}{\partial \mathbf{u}}$ *and* $\mathcal{F}^v_{\nabla \mathbf{u}} := \frac{\partial \mathcal{F}^v}{\partial \nabla \mathbf{u}}$.

Proof. Applying the local shape derivative to both sides of Eq. (2) results in

$$\begin{aligned}0 &= \left(\nabla \cdot \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right)\right)' \\ &= \nabla \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right). \quad \square\end{aligned}$$

Theorem 3.2 (*Shape Derivative of the Variational Navier–Stokes Equations*)**.** *The shape derivative of the variational form of the Navier–Stokes equations (3) is given by the problem: Find* $\mathbf{u}' \in \mathcal{H}$*, such that*

$$\begin{aligned}0 = &- \left(\mathbf{u}', \left[\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right]^\top \nabla \mathbf{v}\right)_\Omega - \left(\langle V, n\rangle \left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right], \nabla \mathbf{v}\right)_{\Gamma_W} \\ &- \left(\mathbf{u}', \nabla \cdot \left[\left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{v}\right]\right)_\Omega + \left(\mathbf{u}', n \cdot \left[\left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{v}\right]\right)_\Gamma \\ &+ \left(\mathbf{u}', \left[n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)\right]^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} \\ &- \left(\nabla \mathbf{u}', \left(n \cdot \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} + \left(n \cdot \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right)', \mathbf{v}\right)_{\Gamma_W} \\ &+ \int_{\Gamma_W} \langle V, n\rangle \nabla \cdot \left(\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right] \cdot \mathbf{v}\right) ds \quad \forall \mathbf{v} \in \mathcal{H}.\end{aligned} \tag{17}$$

Proof. A shape differentiation of the variational form (3) results in

$$
\begin{aligned}
0 &= -\frac{d}{dt}\bigg|_{t=0} \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u}), \nabla\mathbf{v}\right)_\Omega + \frac{d}{dt}\bigg|_{t=0} \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right), \mathbf{v}\right)_\Gamma \\
&= -\left(\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)', \nabla\mathbf{v}\right)_\Omega - \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u}), \nabla\mathbf{v}'\right)_\Omega - \left(\langle V, n\rangle\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right], \nabla\mathbf{v}\right)_\Gamma \\
&\quad + \left(\left[n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)\right]', \mathbf{v}\right)_{\Gamma\setminus\Gamma_W} \\
&\quad + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right), \mathbf{v}'\right)_{\Gamma\setminus\Gamma_W} + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)', \mathbf{v}\right)_{\Gamma_W} \\
&\quad + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right), \mathbf{v}'\right)_{\Gamma_W} + \int_{\Gamma_W} \langle V, n\rangle \nabla\cdot\left(\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right]\cdot\mathbf{v}\right) \,\mathrm{d}s \quad \forall\mathbf{v}\in\mathcal{H},
\end{aligned}
\tag{18}
$$

where we used Eqs. (10) and (11) for the volume and the farfield integrals and Theorem 2.5 for the wall boundary integral. The terms containing $\mathbf{v}'$ vanish due to the forward equation (3) being satisfied. Using the product rule on $[n\cdot(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u}))]'$ and the chain rule on $(\mathcal{F}^c(\mathbf{u}))'$ and $(\mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u}))'$ at the farfield boundary and in the volume leads to

$$
\begin{aligned}
0 &= -\left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\nabla\mathbf{u}', \nabla\mathbf{v}\right)_\Omega - \left(\langle V, n\rangle\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right], \nabla\mathbf{v}\right)_\Gamma \\
&\quad + \left(n\cdot\left[\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\nabla\mathbf{u}'\right], \mathbf{v}\right)_{\Gamma\setminus\Gamma_W} \\
&\quad + \left(n'\cdot\left[\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)\right], \mathbf{v}\right)_{\Gamma\setminus\Gamma_W} + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)', \mathbf{v}\right)_{\Gamma_W} \\
&\quad + \int_{\Gamma_W} \langle V, n\rangle \nabla\cdot\left(\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right]\cdot\mathbf{v}\right) \,\mathrm{d}s \quad \forall\mathbf{v}\in\mathcal{H}.
\end{aligned}
$$

Since $V = 0$ is fulfilled in the neighborhood of the farfield boundary $\Gamma\setminus\Gamma_W$ the local shape derivative of normal vector n' vanishes and it remains

$$
\begin{aligned}
0 &= -\left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\nabla\mathbf{u}', \nabla\mathbf{v}\right)_\Omega - \left(\langle V, n\rangle\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right], \nabla\mathbf{v}\right)_{\Gamma_W} \\
&\quad + \left(n\cdot\left[\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\nabla\mathbf{u}'\right], \mathbf{v}\right)_{\Gamma\setminus\Gamma_W} + \left(n\cdot\left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right)', \mathbf{v}\right)_{\Gamma_W} \\
&\quad + \int_{\Gamma_W} \langle V, n\rangle \nabla\cdot\left(\left[\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})\right]\cdot\mathbf{v}\right) \,\mathrm{d}s \quad \forall\mathbf{v}\in\mathcal{H}.
\end{aligned}
$$

We shift n, $\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})$, $\mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})$ and $\mathcal{F}^v_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})$ to the other side of the products and integrate the volume term containing $\nabla\mathbf{u}'$ by parts to obtain the stated expression. □

4. Adjoint calculus

We now recall adjoint calculus to reformulate a shape optimization problem as documented in [1,27] or [28]. In our case the cost function J to be shape optimized is the drag or lift coefficient

$$J = J(\mathbf{u}, S),$$

which depends on a function S describing the shape and the flow solution $\mathbf{u}$ of the governing equation

$$N(\mathbf{u}, S) = 0. \tag{19}$$

Since $\mathbf{u}$ depends, through the governing equation, on the shape function S, a variation of the shape δS leads to the following variation of the cost function

$$\delta J = \frac{\partial J}{\partial \mathbf{u}}\delta\mathbf{u} + \frac{\partial J}{\partial S}\delta S. \tag{20}$$

Therefore, to compute the variation δJ, one needs to know the sensitivity of the flow solution $\delta\mathbf{u}$ for each degree of freedom within the shape deformation. To calculate this variation for each such parameter, a flow solution has to be computed. This prohibitive numerical effort of multiple flow computations can be omitted if it is possible to eliminate the variation $\delta\mathbf{u}$. For this purpose, we look at the variation of the governing equation

$$\delta N = \frac{\partial N}{\partial \mathbf{u}}\delta\mathbf{u} + \frac{\partial N}{\partial S}\delta S = 0, \tag{21}$$

which provides another equation determining the variation $\delta \mathbf{u}$. Because the variation δN equals zero, it can be multiplied by a Lagrange multiplier $\mathbf{z}$ and then be subtracted from the variation of the cost function:

$$\delta J = \delta J - \mathbf{z}^\top \delta N.$$

Inserting Eqs. (20) and (21) for the variations δJ and δN into this equation yields

$$\begin{aligned}\delta J &= \frac{\partial J}{\partial \mathbf{u}}\delta \mathbf{u} + \frac{\partial J}{\partial S}\delta S - \mathbf{z}^\top \left(\frac{\partial N}{\partial \mathbf{u}}\delta \mathbf{u} + \frac{\partial N}{\partial S}\delta S\right)\\ &= \left(\frac{\partial J}{\partial \mathbf{u}} - \mathbf{z}^\top \frac{\partial N}{\partial \mathbf{u}}\right)\delta \mathbf{u} + \left(\frac{\partial J}{\partial S} - \mathbf{z}^\top \frac{\partial N}{\partial S}\right)\delta S.\end{aligned}$$

The first term, containing $\delta \mathbf{u}$, is then eliminated if $\mathbf{z}$ satisfies the adjoint equation

$$\frac{\partial J}{\partial \mathbf{u}} - \mathbf{z}^\top \frac{\partial N}{\partial \mathbf{u}} = 0. \tag{22}$$

Therewith the variation of the cost function becomes

$$\delta J = \left(\frac{\partial J}{\partial S} - \mathbf{z}^\top \frac{\partial N}{\partial S}\right)\delta S, \tag{23}$$

which can be computed without multiple primal flow solutions.

Although the nature of Eq. (19) makes the above motivation more reminiscent of the strong form approach, it is nevertheless presented here to illustrate the methodology. Furthermore, as stated before, we are also considering the strong form for our shape optimization problem so we have a procedure to gauge against. Thus, we are going to consider the shape derivative of the objective function as given by Theorem 2.5, but under the assumption of a state equation in weak form, Eq. (3).

4.1. Variational formulation of the continuous adjoint problem

We will use this section to derive the variational formulation of the adjoint problem. For more details on the variational approach also see [24] and the respective integral transforms are covered in more depth in [29].

Theorem 4.1 (*Variational Form of the Adjoint Navier–Stokes Equations*)**.** *The variational formulation of the adjoint Navier–Stokes equations is given by finding* $\mathbf{z} \in \mathcal{H}$ *such that*

$$\begin{aligned}&-\left(\mathbf{w}, (\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})^\top \nabla \mathbf{z}\right)_\Omega - \left(\mathbf{w}, \nabla \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_\Omega + \left(\mathbf{w}, n \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_\Gamma\\ &\quad + \left(\mathbf{w}, \left(n \cdot \left(\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}}\right)\right)^\top \mathbf{z}\right)_\Gamma - \left(\nabla \mathbf{w}, \left(n \cdot \mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \mathbf{z}\right)_\Gamma = J'[\mathbf{u}](\mathbf{w}) \quad \forall \mathbf{w} \in \mathcal{H},\end{aligned} \tag{24}$$

where the linearization of the cost function in case of drag or lift coefficient is given by

$$J'[\mathbf{u}](\mathbf{w}) = \left(\tfrac{1}{C_\infty}\left(p_{\mathbf{u}} n - \tau_{\mathbf{u}} n\right) \cdot \psi, \mathbf{w}\right)_{\Gamma_W} - \left(\tfrac{1}{C_\infty}\left(\tau_{\nabla \mathbf{u}} n\right) \cdot \psi, \nabla \mathbf{w}\right)_{\Gamma_W}.$$

Proof. Following the outline given by [24], the linearization in direction $\mathbf{w} \in \mathcal{H}$ of the Navier–Stokes equations in variational form (3) is given by

$$\begin{aligned}\langle F'(\mathbf{u}, \Omega)\mathbf{w}, \mathbf{z}\rangle_{\mathcal{H}^* \times \mathcal{H}} = &-\left(\frac{\partial \mathcal{F}^c}{\partial \mathbf{u}}\mathbf{w} - \frac{\partial \mathcal{F}^v}{\partial \mathbf{u}}\mathbf{w} - \frac{\partial \mathcal{F}^v}{\partial \nabla \mathbf{u}}\nabla \mathbf{w}, \nabla \mathbf{z}\right)_\Omega + \left(n \cdot \left(\frac{\partial \mathcal{F}^c}{\partial \mathbf{u}}\mathbf{w} - \frac{\partial \mathcal{F}^v}{\partial \mathbf{u}}\mathbf{w} - \frac{\partial \mathcal{F}^v}{\partial \nabla \mathbf{u}}\nabla \mathbf{w}\right), \mathbf{z}\right)_\Gamma\\ &\forall \mathbf{z} \in \mathcal{H}.\end{aligned}$$

The adjoint equation in variational form is then given by the problem of finding $\mathbf{z} \in \mathcal{H}$ such that

$$\langle F'(\mathbf{u}, \Omega)\mathbf{w}, \mathbf{z}\rangle_{\mathcal{H}^* \times \mathcal{H}} = J'[\mathbf{u}](\mathbf{w}) \quad \forall \mathbf{w} \in \mathcal{H}. \tag{25}$$

Thus, we have

$$\begin{aligned}&-\left((\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})\mathbf{w} - \mathcal{F}^v_{\nabla \mathbf{u}}\nabla \mathbf{w}, \nabla \mathbf{z}\right)_\Omega + \left(n \cdot ((\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})\mathbf{w} - \mathcal{F}^v_{\nabla \mathbf{u}}\nabla \mathbf{w}), \mathbf{z}\right)_\Gamma\\ &\quad = -\left(\mathbf{w}, (\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})^\top \nabla \mathbf{z}\right)_\Omega + \left(\nabla \mathbf{w}, \left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)_\Omega + \left(\mathbf{w}, \left(n \cdot \left(\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}}\right)\right)^\top \mathbf{z}\right)_\Gamma - \left(\nabla \mathbf{w}, \left(n \cdot \mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \mathbf{z}\right)_\Gamma\\ &\quad = J'[\mathbf{u}](\mathbf{w}) \quad \forall \mathbf{w} \in \mathcal{H}.\end{aligned}$$

Integration by parts resolves the remaining gradient $\nabla \mathbf{w}$ in the second volume integral and the variational formulation of the adjoint Navier–Stokes equations becomes the desired expression. □

Corollary 4.2. *Choosing* $\mathbf{w}$ *in Eq. (24) with appropriate compact support in either* Ω *or on* Γ_W *and* $\Gamma \setminus \Gamma_W$*, one can see that*

$$-\left(\mathbf{w}, (\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})^\top \nabla \mathbf{z}\right)_\Omega - \left(\mathbf{w}, \nabla \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_\Omega = 0 \quad \forall \mathbf{w} \in \mathcal{H}_0(\Omega) \tag{26}$$

for the volume. For a test function with compact support on Γ_W *we see that*

$$\begin{aligned}&\left(\mathbf{w}, n \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_{\Gamma_W} + \left(\mathbf{w}, \left(n \cdot (\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})\right)^\top \mathbf{z}\right)_{\Gamma_W} - \left(\nabla \mathbf{w}, \left(n \cdot \mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \mathbf{z}\right)_{\Gamma_W} \\ &\quad = \left(\tfrac{1}{C_\infty} (p_{\mathbf{u}} n - \tau_{\mathbf{u}} n) \cdot \psi, \mathbf{w}\right)_{\Gamma_W} - \left(\tfrac{1}{C_\infty} (\tau_{\nabla \mathbf{u}} n) \cdot \psi, \nabla \mathbf{w}\right)_{\Gamma_W} \quad \forall \mathbf{w} \in \mathcal{H} \cap \mathcal{H}_0(\Gamma_W)\end{aligned} \tag{27}$$

and finally using the same argumentation on all remaining boundaries $\Gamma \setminus \Gamma_W$

$$\begin{aligned}&\left(\mathbf{w}, n \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_{\Gamma \setminus \Gamma_W} + \left(\mathbf{w}, \left(n \cdot (\mathcal{F}^c_{\mathbf{u}} - \mathcal{F}^v_{\mathbf{u}})\right)^\top \mathbf{z}\right)_{\Gamma \setminus \Gamma_W} \\ &\quad - \left(\nabla \mathbf{w}, \left(n \cdot \mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \mathbf{z}\right)_{\Gamma \setminus \Gamma_W} = 0 \quad \forall \mathbf{w} \in \mathcal{H} \cap \mathcal{H}_0(\Gamma \setminus \Gamma_W).\end{aligned} \tag{28}$$

4.2. Application of adjoint equation to the shape derivative of the Navier–Stokes equations

Recalling our goal of eliminating the local shape derivatives p' and τ' in Eq. (13), we will now derive two intermediate relationships between the adjoint equation and the respective linearizations of the Navier–Stokes equations. One stems from a consideration of a pointwise linearization while the other stems from the same procedure applied to the linearization of the weak form. The resulting two different intermediate expressions (29) and (30) will then be transformed further in Section 4.3. There, the corresponding variations in terms of the pressure-based variables will be made explicit. The variation of the boundary conditions will be taken into consideration in Section 4.4.

We begin by considering the pointwise problem. Multiplying the shape derivative of the pointwise Navier–Stokes equations from Theorem 3.1 by a test function $\mathbf{v}$ and integrating over the domain Ω gives us

$$0 = \left(\nabla \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right), \mathbf{v}\right)_\Omega \quad \forall \mathbf{v} \in \mathcal{H}.$$

Integration by parts yields

$$\begin{aligned}0 = &-\left(\left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right), \nabla \mathbf{v}\right)_\Omega \\ &+ \left(n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right), \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} \\ &+ \left(n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right), \mathbf{v}\right)_{\Gamma_W} \quad \forall \mathbf{v} \in \mathcal{H}.\end{aligned}$$

Shifting n, $\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})$, $\mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})$ and $\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})$ to the other side of the products results in

$$\begin{aligned}0 = &-\left(\mathbf{u}', \left[\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right]^\top \nabla \mathbf{v}\right)_\Omega + \left(\nabla \mathbf{u}', \left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{v}\right)_\Omega \\ &+ \left(\mathbf{u}', \left[n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)\right]^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} - \left(\nabla \mathbf{u}', \left[n \cdot \left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)\right]^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} \\ &+ \left(n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\mathbf{u}' - \mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\nabla \mathbf{u}'\right), \mathbf{v}\right)_{\Gamma_W} \quad \forall \mathbf{v} \in \mathcal{H}.\end{aligned}$$

Integration by parts in the 2nd volume integral and applying the chain rule backwards to the wall integral leads to

$$\begin{aligned}0 = &-\left(\mathbf{u}', \left[\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right]^\top \nabla \mathbf{v}\right)_\Omega - \left(\mathbf{u}', \nabla \cdot \left[\left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{v}\right]\right)_\Omega + \left(\mathbf{u}', n \cdot \left[\left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{v}\right]\right)_\Gamma \\ &+ \left(\mathbf{u}', \left[n \cdot \left(\mathcal{F}^c_{\mathbf{u}}(\mathbf{u}) - \mathcal{F}^v_{\mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)\right]^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} \\ &- \left(\nabla \mathbf{u}', \left[n \cdot \left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)\right]^\top \mathbf{v}\right)_{\Gamma \setminus \Gamma_W} + \left(n \cdot \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right)', \mathbf{v}\right)_{\Gamma_W} \quad \forall \mathbf{v} \in \mathcal{H}.\end{aligned}$$

Using adjoint conditions (26) and (28) and changing the name of the dependent variable from $\mathbf{v}$ to $\mathbf{z}$, one obtains

$$0 = \left(\mathbf{u}', n \cdot \left[\left(\mathcal{F}^v_{\nabla \mathbf{u}}(\mathbf{u}, \nabla \mathbf{u})\right)^\top \nabla \mathbf{z}\right]\right)_{\Gamma_W} + \left(n \cdot \left(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla \mathbf{u})\right)', \mathbf{z}\right)_{\Gamma_W} \quad \forall \mathbf{z} \in \mathcal{H}. \tag{29}$$

Using Eqs. (26) and (28), which stem from a weak form adjoint equation, within the strong form linearization here might appear counter intuitive at first glance. However, it should be noted that a pointwise interpretation of those does not effect the above equation.

Contrary to the above preliminary result stemming from the strong form of the Navier–Stokes equations, we next follow the same process, now considering the interaction with the adjoint equation and the variational Navier–Stokes equations from Theorem 3.2, which results in

$$0 = \left(\mathbf{u}', n \cdot \left[\left(\mathcal{F}^{v}_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\right)^{\top} \nabla\mathbf{z}\right]\right)_{\Gamma_W} + \left(n \cdot \left(\mathcal{F}^{c}(\mathbf{u}) - \mathcal{F}^{v}(\mathbf{u}, \nabla\mathbf{u})\right)', \mathbf{z}\right)_{\Gamma_W}$$
$$+ \int_{\Gamma_W} \langle V, n\rangle \nabla \cdot \left(\left[\mathcal{F}^{c}(\mathbf{u}) - \mathcal{F}^{v}(\mathbf{u}, \nabla\mathbf{u})\right] \cdot \mathbf{z}\right) \mathrm{d}s - \left(\langle V, n\rangle \left[\mathcal{F}^{c}(\mathbf{u}) - \mathcal{F}^{v}(\mathbf{u}, \nabla\mathbf{u})\right], \nabla\mathbf{z}\right)_{\Gamma_W} \quad \forall \mathbf{z} \in \mathcal{H}.$$

We apply the product rule to the divergence and get

$$0 = \left(\mathbf{u}', n \cdot \left[\left(\mathcal{F}^{v}_{\nabla\mathbf{u}}(\mathbf{u}, \nabla\mathbf{u})\right)^{\top} \nabla\mathbf{z}\right]\right)_{\Gamma_W} + \left(n \cdot \left(\mathcal{F}^{c}(\mathbf{u}) - \mathcal{F}^{v}(\mathbf{u}, \nabla\mathbf{u})\right)', \mathbf{z}\right)_{\Gamma_W}$$
$$+ \boxed{\left(\langle V, n\rangle \nabla \cdot [\mathcal{F}^{c}(\mathbf{u}) - \mathcal{F}^{v}(\mathbf{u}, \nabla\mathbf{u})], \mathbf{z}\right)_{\Gamma_W}} \quad \forall \mathbf{z} \in \mathcal{H}. \tag{30}$$

Comparing Eqs. (29) and (30) we see that for the variational form of the Navier–Stokes equations, there is one extra term (framed), which vanishes if the Navier–Stokes equations are fulfilled pointwise. In the following, we can therefore avoid a fork and always use Eq. (30), keeping in mind that all framed terms only occur in the variational approach. Also, expressing the variation $\mathbf{u}'$ in terms of the non-conserved variables works likewise, irrespective of the underlying form of the state equation.

4.3. Transformation to non-conserved variables

In this subsection we insert in particular the no-slip condition into the shape derivative of the Navier–Stokes equations (30). Therefore we first state the so called homogeneity tensor $G = \mathcal{F}^{v}_{\nabla\mathbf{u}}$ at the no-slip wall. We also use $v = 0$ to get the representations of $\mathbf{u}'$, $(\mathcal{F}^{c})'$ and $(\mathcal{F}^{v})'$ at the wall boundary. With these terms the local shape derivative $\mathbf{u}'$ is then reformulated, such that we form the respective local shape derivative of the pressure p' and the viscous stress tensor τ', which will later eliminate their counterparts in the preliminary shape derivative of the cost function, given by Eq. (13).

As in [29], the homogeneity tensor is given by

$$G = \left[G^{ij}_{kl}\right]^{ij}_{kl} = \frac{\partial\left(f^{v}_{k}\right)_{i}}{\partial \frac{\partial \mathbf{u}_j}{\partial x_l}},$$

where $(f^{v}_{k})_i$ denotes the ith component of the kth viscous flux vector and $\frac{\partial \mathbf{u}_j}{\partial x_l}$ denotes the derivative of the jth component of the vector of conserved variables with respect to x_l. Therefore in two dimensions the indices fulfill $i, j \in \{1, \dots, 4\}$ and $k, l \in \{1, 2\}$. The homogeneity tensor G at the no-slip wall is given by

$$G_{11} = \frac{\mu}{\rho}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{4}{3} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\frac{\gamma}{Pr}E & 0 & 0 & \frac{\gamma}{Pr} \end{pmatrix}, \qquad G_{12} = \frac{\mu}{\rho}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{3} & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$
$$G_{21} = \frac{\mu}{\rho}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -\frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad G_{22} = \frac{\mu}{\rho}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{4}{3} & 0 \\ -\frac{\gamma}{Pr}E & 0 & 0 & \frac{\gamma}{Pr} \end{pmatrix}.$$

See [29] for a more detailed discourse on the general homogeneity tensor. The shape derivative of the vector of conserved variables $\mathbf{u}'$ reduces with $(\rho v_i)' = \rho v_i' + \rho' v_i = \rho v_i'$ at the no-slip wall to

$$\mathbf{u}' = \begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho E \end{pmatrix}' = \begin{pmatrix} \rho' \\ \rho v_1' \\ \rho v_2' \\ (\rho E)' \end{pmatrix} \quad \text{on } \Gamma_W.$$

Because $(\rho v_i v_j)' = (\rho v_i)' v_j + \rho v_i v_j' = 0$ holds due the no-slip condition, the shape derivative of the convective flux $(\mathcal{F}^{c})'$ reduces to

$$(\mathcal{F}^{c})' = \begin{pmatrix} \rho v_1 & \rho v_2 \\ \rho v_1^2 + p & \rho v_1 v_2 \\ \rho v_1 v_2 & \rho v_2^2 + p \\ \rho H v_1 & \rho H v_2 \end{pmatrix}' = \begin{pmatrix} \rho v_1' & \rho v_2' \\ p' & 0 \\ 0 & p' \\ \rho H v_1' & \rho H v_2' \end{pmatrix} \quad \text{on } \Gamma_W. \tag{31}$$

For the shape derivative of the viscous flux $(\mathcal{F}^v)'$ we can use $(\tau_{ij}v_j)' = \tau_{ij}v_j'$ at the no-slip boundary to obtain

$$(\mathcal{F}^v)' = \begin{pmatrix} 0 & 0 \\ \tau_{11}' & \tau_{12}' \\ \tau_{21}' & \tau_{22}' \\ \sum_j \tau_{1j}v_j' + \kappa \frac{\partial T'}{\partial x_1} & \sum_j \tau_{2j}v_j' + \kappa \frac{\partial T'}{\partial x_2} \end{pmatrix} \quad \text{on } \Gamma_W. \tag{32}$$

These terms are now inserted into the shape derivative of the Navier–Stokes equations for each scalar product of Eq. (30) separately. First we consider the second scalar product of Eq. (30) and insert the representations (31) and (32) of $(\mathcal{F}^c)'$ and $(\mathcal{F}^v)'$ into this integral:

$$\left(n \cdot \left(\left(\mathcal{F}^c\right)' - (\mathcal{F}^v)'\right), \mathbf{z}\right)_{\Gamma_W} = \left(\left[\begin{pmatrix} \rho v_1' & \rho v_2' \\ p' & 0 \\ 0 & p' \\ \rho H v_1' & \rho H v_2' \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ \tau_{11}' & \tau_{12}' \\ \tau_{21}' & \tau_{22}' \\ \sum_j \tau_{1j}v_j' + \kappa \frac{\partial T'}{\partial x_1} & \sum_j \tau_{2j}v_j' + \kappa \frac{\partial T'}{\partial x_2} \end{pmatrix}\right] n, \mathbf{z}\right)_{\Gamma_W}.$$

From the first line we read $\rho(v' \cdot n)\mathbf{z}_1$, from the second and third lines $(p'n - \tau'n) \cdot \mathbf{z}_{2,3}$ and the last line gives $\big(\rho H v' - (\tau v' + \kappa \nabla T')\big) \cdot n\mathbf{z}_4$. Altogether this yields

$$\left(n \cdot \left(\left(\mathcal{F}^c\right)' - (\mathcal{F}^v)'\right), \mathbf{z}\right)_{\Gamma_W} = \int_{\Gamma_W} (p'n - \tau'n) \cdot \mathbf{z}_{2,3} + v' \cdot (\rho n \mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4) - \nabla T' \cdot n\kappa \mathbf{z}_4 \, ds. \tag{33}$$

Next we use the homogeneity tensor to rewrite the first scalar product of Eq. (30):

$$\left(\mathbf{u}', n \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_{\Gamma_W} = \left(\mathbf{u}', n \cdot \left(G^\top \nabla \mathbf{z}\right)\right)_{\Gamma_W} = \int_{\Gamma_W} \sum_{k,l,i,j} \mathbf{u}_j' n_l G_{kl}^{ij} \frac{\partial \mathbf{z}_i}{\partial x_k} \, ds.$$

As we can see, the first component of $\mathbf{z}$ is multiplied with the first lines of the matrices G_{kl}, which are all zero. Therefore there is no contribution for $\mathbf{z}_1$. The non-zero entries in the second and third lines of G at the no-slip wall look familiar to the coefficients of $\frac{\partial v_i}{\partial x_j}$ in the viscous stress tensor. If we define the adjoint stress tensor as

$$\Sigma := \mu \left(\nabla \mathbf{z}_{2,3} + (\nabla \mathbf{z}_{2,3})^\top - \frac{2}{3}\left(\nabla \cdot \mathbf{z}_{2,3}\right) I\right)$$

one can actually see that the second and third lines yield

$$\int_{\Gamma_W} \sum_{\substack{i,j=2,3 \\ k,l}} \mathbf{u}_j' n_l G_{kl}^{ij} \frac{\partial \mathbf{z}_i}{\partial x_k} \, ds = \int_{\Gamma_W} v' \cdot (n \cdot \Sigma) \, ds.$$

For the fourth component of $\mathbf{z}$, meaning the fourth lines of G, we only get contributions for $k = l$ and $j = 1$ or 4, meaning the first and last entries in the fourth line of the matrices G_{11} and G_{22}. Since the jth columns of the matrices G_{kl} are multiplied by the jth component of $\mathbf{u}$, the remaining expression is

$$\int_{\Gamma_W} \sum_{\substack{i=4 \\ j=1,4 \\ k=l}} \mathbf{u}_j' n_l G_{kl}^{ij} \frac{\partial \mathbf{z}_i}{\partial x_k} \, ds = \int_{\Gamma_W} \frac{\mu}{\rho} \frac{\gamma}{Pr} \left(-E\mathbf{u}_1' + \mathbf{u}_4'\right) n \cdot \nabla \mathbf{z}_4 \, ds.$$

With $\mathbf{u}_1' = \rho'$ and $\mathbf{u}_4' = (\rho E)' = \rho' E + \rho E'$ this integral is simplified to

$$\int_{\Gamma_W} \frac{\mu}{\rho} \frac{\gamma}{Pr} \rho E' n \cdot \nabla \mathbf{z}_4 \, ds = \int_{\Gamma_W} T' \kappa n \cdot \nabla \mathbf{z}_4 \, ds,$$

where we use $T\kappa = \frac{\mu\gamma}{Pr}\left(E - \frac{1}{2}v^2\right)$ and the no-slip condition to substitute

$$T'\kappa = \frac{\mu\gamma}{Pr}\left(E' - \left(\frac{1}{2}v^2\right)'\right) = \frac{\mu\gamma}{Pr} E'.$$

In total we obtain for the first scalar product of Eq. (30)

$$\left(\mathbf{u}', n \cdot \left(\left(\mathcal{F}^v_{\nabla \mathbf{u}}\right)^\top \nabla \mathbf{z}\right)\right)_{\Gamma_W} = \int_{\Gamma_W} v' \cdot (n \cdot \Sigma) \, ds + \int_{\Gamma_W} T' \kappa n \cdot \nabla \mathbf{z}_4 \, ds. \tag{34}$$

Combining the results of (33) and (34) the preliminary shape derivative equation (30), now containing the variation of the boundary condition and the explicit variations of the primal variables, becomes

$$
\begin{aligned}
0 &= \int_{\Gamma_W} v' \cdot (n \cdot \Sigma)\,\mathrm{d}s + \int_{\Gamma_W} T'\kappa n \cdot \nabla \mathbf{z}_4\,\mathrm{d}s \\
&\quad + \int_{\Gamma_W} (p'n - \tau' n)\cdot \mathbf{z}_{2,3} + v' \cdot (\rho n \mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4) - \nabla T' \cdot n \kappa \mathbf{z}_4\,\mathrm{d}s + \boxed{((V\cdot n)(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v)), \mathbf{z})_{\Gamma_W}}.
\end{aligned}
$$

4.4. Subtraction of the shape derivative of the Navier–Stokes equations from the preliminary shape derivative of the cost function

The above equality is now, in accordance with the adjoint approach, subtracted from the preliminary shape derivative of the cost function (13), thereby obtaining a representation that does not contain any local shape derivatives.

$$
\begin{aligned}
dJ(\Omega; V) &= \frac{1}{C_\infty}\int_{\Gamma_W} (p'n - \tau' n)\cdot \psi^{\boxed{1}} + (V\cdot n) \div (p\psi - \tau\psi)^{\boxed{2}}\,\mathrm{d}s \\
&\quad - \int_{\Gamma_W} v' \cdot (n\cdot\Sigma)\,\mathrm{d}s - \int_{\Gamma_W} T'\kappa n \cdot \nabla\mathbf{z}_4\,\mathrm{d}s \\
&\quad - \int_{\Gamma_W} (p'n - \tau' n)\cdot \mathbf{z}_{2,3}{}^{\boxed{3}} + v'\cdot(\rho n \mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4) - \nabla T' \cdot n\kappa \mathbf{z}_4\,\mathrm{d}s \\
&\quad - \boxed{((V\cdot n)(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v)), \mathbf{z})_{\Gamma_W}}^{\boxed{4}}.
\end{aligned}
\tag{35}
$$

To ease the following discussions we use framed numbers $\boxed{1}, \boxed{2}, \boxed{3}, \ldots$ to refer to certain terms. Term $\boxed{3}$ and term $\boxed{1}$ cancel each other if the adjoint boundary condition $\mathbf{z}_{2,3} = \frac{1}{C_\infty}\psi$ on Γ_W is fulfilled. Furthermore, this boundary condition also implies that the $\mathbf{z}_{2,3}$-component of expression $\boxed{4}$ cancels out term $\boxed{2}$, because due to $\frac{\partial \rho v_i v_j}{\partial x_k} = \frac{\partial \rho v_i}{\partial x_k} v_j + \rho v_i \frac{\partial v_j}{\partial x_k} = 0$ at the no-slip boundary, the equation

$$
\left(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v)\right)_{2,3} = \nabla\cdot\left[(\rho v_i v_j)_{ij} + pI - \tau\right] = \operatorname{div}(pI - \tau)
\tag{36}
$$

and therewith $(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v))_{2,3}\cdot \mathbf{z}_{2,3} = \frac{1}{C_\infty}\operatorname{div}(p\psi - \tau\psi)$ holds.

When considering the pointwise equations the scalar product $\boxed{4}$ is not present and one would expect $\boxed{2}$ to remain untouched. In this situation, however, Eq. (36), being the pointwise conservation of momentum, equals zero and therefore term $\boxed{2}$ vanishes anyway. Summarizing the above, the first and last components of $\boxed{4}$ are the only differences between the shape derivatives of the two approaches. We mark them by $\boxed{4_{1,4}}$.

$$
\begin{aligned}
dJ(\Omega; V) &= -\int_{\Gamma_W} v'\cdot(n\cdot\Sigma)\,\mathrm{d}s - \int_{\Gamma_W} T'\kappa n\cdot\nabla\mathbf{z}_4\,\mathrm{d}s - \int_{\Gamma_W} v'\cdot(\rho n\mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4) - \nabla T'\cdot n\kappa\mathbf{z}_4\,\mathrm{d}s \\
&\quad - \boxed{\left((V\cdot n)(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v))_{1,4}, \mathbf{z}_{1,4}\right)_{\Gamma_W}}^{\boxed{4_{1,4}}}.
\end{aligned}
\tag{37}
$$

To achieve independence of the remaining local shape derivatives v' and T', we use the variation of the boundary conditions, as described in Section 2.4, for the no-slip, adiabatic and isothermal boundary condition:

$$
\begin{aligned}
v' &= -(V\cdot n)\frac{\partial v}{\partial n} && \text{on } \Gamma_W, \\
T' &= (V\cdot n)\frac{\partial T_W - T}{\partial n} && \text{on } \Gamma_{iso}, \\
\nabla T'\cdot n &= -(V\cdot n)\frac{\partial^2 T}{\partial n^2} + \nabla T\cdot\nabla_\Gamma(V\cdot n) && \text{on } \Gamma_{adia}.
\end{aligned}
$$

Inserting these conditions on the respective parts of the wall, Eq. (37) becomes

$$
\begin{aligned}
dJ(\Omega; V) &= \int_{\Gamma_W} (V\cdot n)\frac{\partial v}{\partial n}\cdot(n\cdot\Sigma)\,\mathrm{d}s - \int_{\Gamma_{iso}} (V\cdot n)\frac{\partial T_W - T}{\partial n}\kappa n\cdot\nabla\mathbf{z}_4\,\mathrm{d}s - \int_{\Gamma_{adia}} T'\kappa n\cdot\nabla\mathbf{z}_4\,\mathrm{d}s^{\boxed{5}} \\
&\quad + \int_{\Gamma_W} (V\cdot n)\frac{\partial v}{\partial n}\cdot(\rho n\mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4)\,\mathrm{d}s + \int_{\Gamma_{iso}} \nabla T'\cdot n\kappa\mathbf{z}_4\,\mathrm{d}s^{\boxed{6}} - \int_{\Gamma_{adia}} (V\cdot n)\frac{\partial^2 T}{\partial n^2}\kappa\mathbf{z}_4\,\mathrm{d}s \\
&\quad + \int_{\Gamma_{adia}} \nabla T\cdot\nabla_\Gamma(V\cdot n)\kappa\mathbf{z}_4\,\mathrm{d}s^{\boxed{7}} - \boxed{\left((V\cdot n)(\nabla\cdot(\mathcal{F}^c - \mathcal{F}^v)_{1,4}), \mathbf{z}_{1,4}\right)_{\Gamma_W}}^{\boxed{4_{1,4}}}.
\end{aligned}
\tag{38}
$$

Application of the tangential Green's formula (9) to integral $\boxed{7}$ leads to

$$\begin{aligned}\int_{\Gamma_{adia}} \nabla T \cdot \nabla_\Gamma (V \cdot n)\kappa \mathbf{z}_4 \, ds &= \int_{\Gamma_{adia}} (V \cdot n)K(\nabla T \cdot n)\kappa \mathbf{z}_4 - (V \cdot n)\,\mathrm{div}_\Gamma(\nabla T \kappa \mathbf{z}_4)\, ds \\ &= -\int_{\Gamma_{adia}} (V \cdot n)\,\mathrm{div}_\Gamma(\nabla T \kappa \mathbf{z}_4)\, ds,\end{aligned}$$

where the adiabatic wall condition $\nabla T \cdot n = 0$ was used in the second line.

Integrals of Eq. (37) containing the remaining local shape derivatives T' at the adiabatic wall $\boxed{5}$ and $\nabla T'$ at the isothermal wall $\boxed{6}$ vanish if the following adjoint boundary conditions are fulfilled

$$\mathbf{z}_4 = 0, \quad \text{on } \Gamma_{iso} \quad \text{and} \quad \nabla \mathbf{z}_4 \cdot n = 0, \quad \text{on } \Gamma_{adia}.$$

The last step is to give an expression for the term $\boxed{4_{1,4}}$. We therefore consider this expression separately for the first and fourth components, denoted by $\nabla \cdot (\mathcal{F}^c - \mathcal{F}^v)_{1,4}$. Because the first line of the viscous flux $\mathcal{F}^v$ equals zero anyway and furthermore the no-slip condition holds, the first component simplifies to

$$\nabla \cdot (\mathcal{F}^c - \mathcal{F}^v)_1 = \nabla \cdot (\rho v_1, \rho v_2) = \rho(\nabla \cdot v).$$

For the fourth component we get, again with the no-slip condition,

$$\begin{aligned}\nabla \cdot (\mathcal{F}^c - \mathcal{F}^v)_4 &= \nabla \cdot (\rho H v_1, \rho H v_2) - \nabla \cdot \left(\sum_j \tau_{1j} v_j + \kappa \frac{\partial T}{\partial x_1}, \sum_j \tau_{2j} v_j + \kappa \frac{\partial T}{\partial x_2} \right) \\ &= \rho H(\nabla \cdot v) - \sum_{i,j} \tau_{ij} \frac{\partial v_j}{\partial x_i} - \kappa \Delta T.\end{aligned}$$

Altogether the shape derivative of the drag or lift coefficient in Hadamard form becomes

$$\begin{aligned}dJ(\Omega; V) = &\int_{\Gamma_W} (V \cdot n)\frac{\partial v}{\partial n} \cdot (n \cdot \Sigma)\, ds - \int_{\Gamma_{iso}} (V \cdot n)\frac{\partial T_W - T}{\partial n} \kappa n \cdot \nabla \mathbf{z}_4 \, ds \\ &+ \int_{\Gamma_W} (V \cdot n)\frac{\partial v}{\partial n} \cdot (\rho n \mathbf{z}_1 + (\rho H n - \tau n)\mathbf{z}_4)\, ds \\ &- \int_{\Gamma_{adia}} (V \cdot n)\left(\frac{\partial^2 T}{\partial n^2} \kappa \mathbf{z}_4 + \div_\Gamma (\nabla T \kappa \mathbf{z}_4) \right) ds - \boxed{\int_{\Gamma_W} (V \cdot n)\rho(\nabla \cdot v)\mathbf{z}_1 \, ds} \\ &- \boxed{\int_{\Gamma_{adia}} (V \cdot n)\left(\rho H(\nabla \cdot v) - \sum_{i,j} \tau_{ij} \frac{\partial v_j}{\partial x_i} - \kappa \Delta T \right) \mathbf{z}_4 \, ds},\end{aligned} \tag{39}$$

where the difference between the variational and the pointwise approach is based on the two framed integrals in the last line, which only appear upon consideration of the variational form of the Navier–Stokes equations.

5. Numerical results

We now present numerical results to show the difference between the pointwise and the variational approach in application. The shape derivative of both drag and lift coefficient is implemented in the discontinuous Galerkin solver PADGE developed primarily at the German Aerospace Center (DLR), Braunschweig. This flow solver is already capable to also compute the necessary adjoint solutions, originally implemented for error estimation and p-/h-refinement. This adjoint solution, together with the primal solution, is directly used to calculate the Hadamard form (39) of the drag and lift coefficient. This formula only consists of boundary integrals on the airfoil and contains multiple terms depending on geometrical quantities like the normal vector. Hence, an accurate approximation of the shape of the airfoil is necessary to gain maximum accuracy of our high order method, especially with regard to those geometric quantities:

The initial geometry is given by a fine structured hexahedral mesh consisting of straight elements. Before the initial flow calculation, the fine resolution hexahedral elements are merged into spatially coarser elements, but with curved boundaries. Thus, information about the geometry is preserved by transforming many straight sided elements to fewer curved ones. Internally, these curved elements are defined by a 4th order polynomial, mapping the reference element to the physical element. Thus, the actual geometrical information stemming from the fine straight sided mesh is preserved and transformed into spatially coarse elements and a 4th order polynomial map linking them to the reference element. Consequently, the boundary curve is given by a piecewise per element polynomial of 4th order. In order to calculate the integrals of the weak form, a Gaussian quadrature rule of 8th order is used, resulting in considerably more quadrature points per element than degrees of freedom for the Test- and Ansatz functions of the DG discretization.

Our finite difference validations are then conducted by modifying the mapping of the reference element to the physical element, meaning the spatial position of the vertices of the coarse mesh elements are never actually moved, but rather

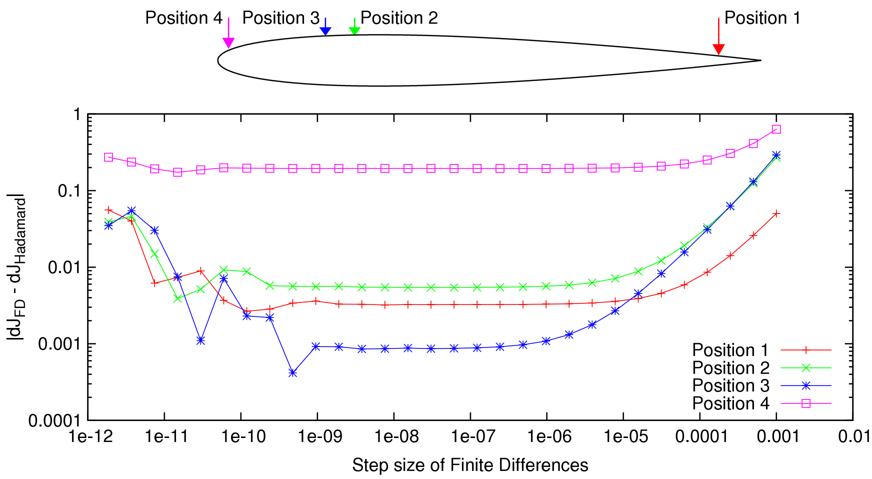

Fig. 1. Error of FD-shape gradient versus shape gradient in variational Hadamard form over different FD step sizes at four different positions.

included in the curvature information. To conduct our finite difference studies, we thus add a polynomial f to the reference-to-physical element map satisfying

$$\begin{aligned} f(0) &= 0, & f'(0) &= 0, \\ f(1) &= 0, & f'(1) &= 0, \\ & & f(0.5) &= \epsilon, \end{aligned}$$

where ϵ is the finite difference step-length and the line segment in physical dimensions is normalized to the interval [0, 1] with midpoint 0.5.

For evaluating the Hadamard-Form, we have 5 quadrature points on the boundary stemming from our 8th order Gaussian quadrature as mentioned above. As a first step, we evaluate the shape Gradient without the $\langle V, n\rangle$ expression on these 5 quadrature points using the polynomial representation of Ansatz functions of the state and adjoint solution. In order to achieve comparability with the finite difference perturbation and the Hadamard approach, we transform the above polynomial f operating on the element mappings into an effective physical boundary movement, represented by a corresponding vector field V, which is then used as the $\langle V, n\rangle$ term and multiplied with the preliminary Hadamard form. The resulting expression is then integrated over the respective element, creating a discretized gradient vector in $\mathbb{R}^n$ where each component corresponds to one element and consequently one ϵ in the definition of f.

Part of the PADGE environment is the ADIGMA MTC3 test case, which is defined as the calculation of flow around a NACA0012 airfoil at Mach $M = 0.5$, angle of attack $\alpha = 2.0°$ and a Reynolds number of $Re = 5000$. Because this test case is thoroughly verified, it is a good basis gauge our shape derivatives. Our grid consists of 1640 cells and the profile as the boundary of the mesh is represented by 40 curved edges of polynomial order four. To obtain a very accurate solution and study the error and behavior for varying polynomial degree p of the Galerkin ansatz, we use a p-refinement from degree three to five. The polynomial degree of the adjoint solution was always chosen to be one degree higher, i.e. four to six. We verify our two respective shape derivative implementations against finite differences, considering lift and drag separately. The finite difference reference solution is created as follows. Each edge is disturbed by a fourth order polynomial individually as described above, such that the profile stays smooth. A flow solution is then computed for each such perturbation. Because the shape gradient can be evaluated in every boundary quadrature point of these degree-4-polynomials representing the edges of the profile, we initially calculate five times as many gradient components as edges. Using this information from all boundary quadrature nodes, we integrate over each edge individually to find the respective value to be used in our figures and comparisons, which corresponds to the center "bump" created by our finite difference approach given by f above. Since the step size of the perturbation for finite differences is unknown in general, we compute the absolute difference of the shape derivative in variational Hadamard form and the finite differences for step sizes ranging from 10^{-12} to 10^{-3}, that is we interpret the finite difference error as a function of the perturbation parameter ϵ at four given spacial positions on the airfoil. In Fig. 1 these errors are shown and despite a quite substantial difference at the nose of the airfoil, all curves show a step size between about 10^{-9} and 10^{-5} to be acceptable. Another possible way to find the optimal step size for the finite differences is to consider the finite difference error as a function of spacial position with respect to fixed perturbation size ϵ, which is studied in Fig. 2 and leads to similar conclusions as those above. The spacial finite difference error for all step sizes 10^{-5}, 10^{-7} and 10^{-9} coincides perfectly, both for drag and lift. Consequently, we chose a step size of $\epsilon = 10^{-7}$ to be used as a reference for validating the Hadamard representation, because selecting $\epsilon = 10^{-7}$ is between the upper and lower bound of the suitable range and is very robust with respect to cancellation errors.

In Fig. 3 finite differences of the drag and lift coefficient are plotted against the shape derivatives in Hadamard form for the variational and the pointwise approach. Both the finite differences and the two Hadamard forms were calculated for a

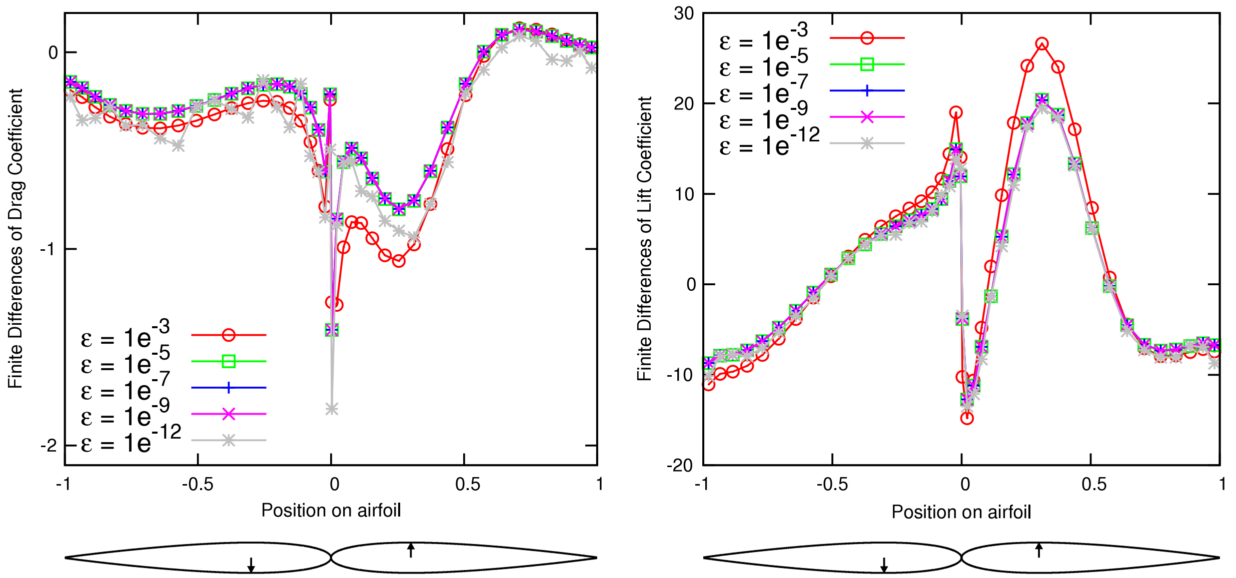

Fig. 2. Finite differences of shape gradient for drag and lift coefficient at five different step sizes.

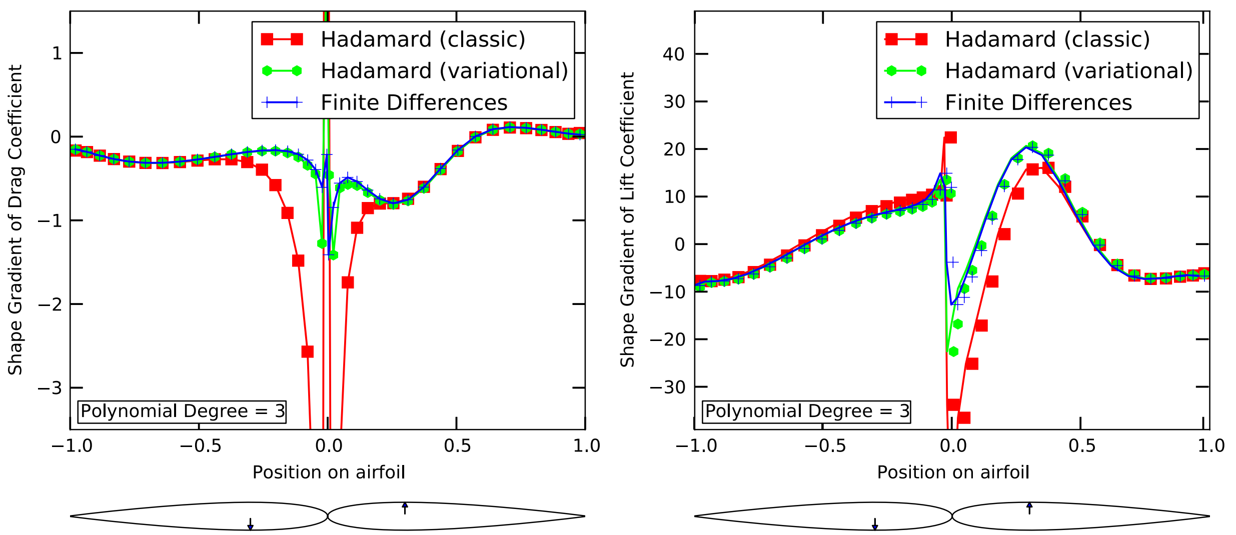

Fig. 3. Shape Gradient of Drag/Lift Coefficient to polynomial degree $p = 3$.

solution made of third order polynomials. One can observe that the shape derivative of the variational approach matches very nicely with the finite differences, whereas the shape derivative of the pointwise approach deviates noticeably.

As we increase the polynomial degree of the flow solution, see Fig. 4, both Hadamard forms fit the finite differences better overall. However, around the nose of the profile and the forward pressure stagnation point, the offset of the Hadamard form of the pointwise approach is still unmissable, most likely due to the magnitude of the gradients of the flow solution. Remarkably, the shape derivative stemming from the variational approach aligns nearly perfectly with the finite difference reference.

Further p-refinement and therewith enhancement of the accuracy of the solution follows this trend: In Fig. 5 we see an excellent match between the variational approach and finite differences, whereas the pointwise approach still exhibits a fairly substantial gap in the region around the nose, although somewhat diminished when compared to the lower degree case.

The natural next step after deriving the gradients is conducting the actual design optimization. A very popular choice for an optimization strategy is the so called one-shot methodology, where the design update is made simultaneously to the iteration of the primal and adjoint solver [6,15,7]. Consequently, gradients created from an inexact and not fully converged flow and adjoint solution are used initially, before all three residuals are driven to convergence simultaneously. Thus, the precision of the shape derivative for inaccurate flow solutions is of crucial importance.

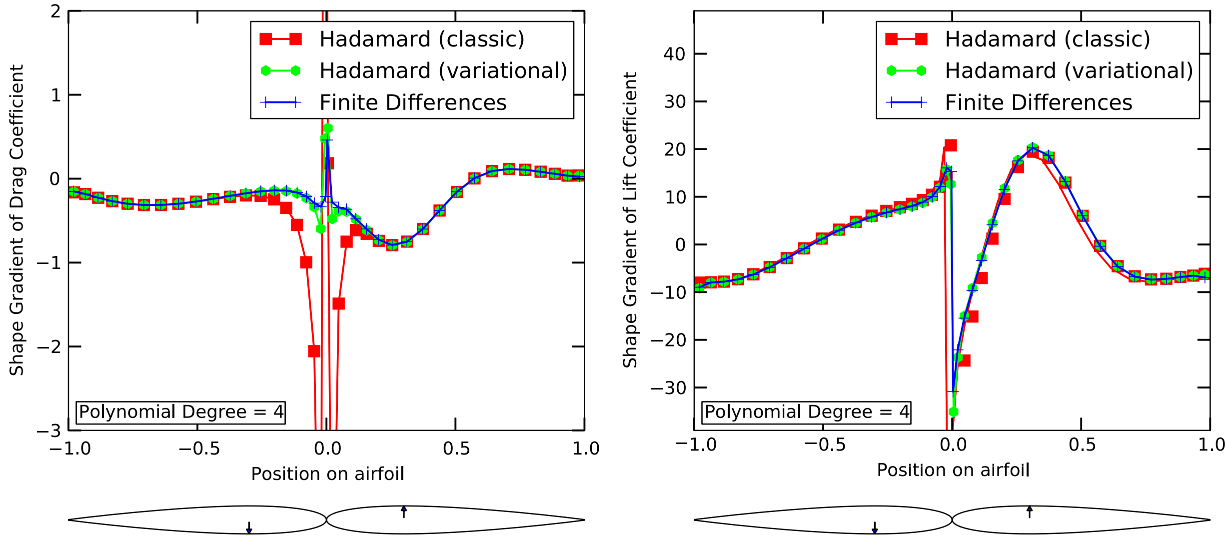

Fig. 4. Shape gradient of drag/lift coefficient to polynomial degree $p = 4$.

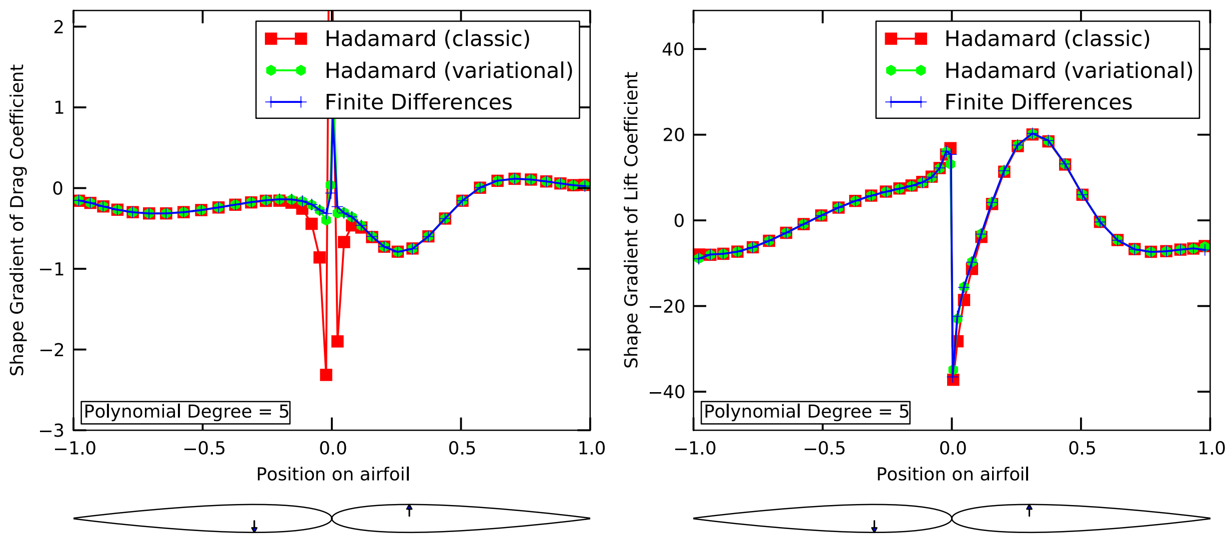

Fig. 5. Shape gradient of drag/lift coefficient to polynomial degree $p = 5$.

Despite the shortcomings in accuracy of the polynomial degree three solution, as shown in Fig. 3, it is well worth pointing out that the quality of the variational Hadamard form would most likely suffice to be used in a one-shot optimization without compunction. This can be justified, because the general manner of the shape derivative, especially in terms of sign, is captured. Contrary to this, the shape derivative of the pointwise approach shows a tremendous deviation over the whole profile, which questions its utility for optimization, which we intend to study as future work.

6. Conclusion

Shape optimization under PDE constraints very often follows the "function composition" approach, where the existence of local shape derivatives for each component in the whole chain containing mesh perturbation, PDE variation and the variation of the objective is assumed to exist. For elliptic problems, this approach is known to work very well [10], somewhat contrary to problems within aerodynamic design, where usually great care needs to be taken [16]. The main purpose of the present work was to circumvent this "step-by-step" differentiation and directly shape differentiate the weak form of the governing equations, similar to [24]. Here, however, we focus on the challenging task of shape optimization within compressible, viscous fluids, for which we also demonstrate the respective gain in accuracy numerically. Any approach based on the weak form is also much more inline with the actual flow solver. Thus, a variational methodology greatly benefits the alignment of the continuous shape differentiation process with the discrete implementation.

One aspect of the present work was the direct comparison between both approaches, which revealed extra terms arising if the variational form of the state equation is used as the governing model. Both shape derivatives were implemented into the DLR flow solver PADGE, a discontinuous Galerkin flow solver of variable order operating on fourth order curvilinear meshes. We conclude with numerical accuracy studies where we gauge both derivatives against a reference solution created by finite differences. Although the gap between the shape derivative based on the weak and strong form diminishes slightly with increasing order of the polynomial ansatz functions, we always found the weak form derivative to be of considerably higher accuracy. Finally, we found the general quality of this weak form shape derivative to be very promising for a future application within a one-shot optimization framework.

Acknowledgments

We wish to thank the BMBF for supporting this work as part of the project DGHPOPT BMBF 05M10PAB. We also wish to thank Dr. R. Hartmann, DLR Braunschweig, for his assistance with the flow solver PADGE.

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