Shape Sensitivity Analysis and Optimization in Fluid Dynamics

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1 Introduction

In this paper we are interested in developing methodologies for the sensitivity analysis of boundary (shape) functionals and the optimal shape design of bodies immersed in a fluid. Under the terminology of optimal control theory, when a shape functional depends on the solution of a boundary value problem (BVP) it is said to be *constrained.* In the same spirit, the BVP is the *state*, the domain is the *control* and the geometric/topological constraints on the domain are the *control constraints*. The above notions are found in problems concerned with the optimal control of domain boundaries, commonly referred to as *shape optimization* methods. Shape optimization methods have found widespread application in aerodynamics, aeroacoustics, structural mechanics, electromagnetics and many other engineering and physical disciplines where one is interested in finding an optimal shape given a desired function. For instance, classical examples are the drag minimization of an aerodynamic body, design of magnets producing prescribed magnetic fields and the optimal locomotion of microswimmers in Stokes flow.

In engineering sciences and applied mathematics one usually refers to adjoint-based shape optimization methods owing to the following central idea: treating the state equation as an equality constraint for a shape functional, and through the use of Lagrange multipliers, we naturally obtain a dual (adjoint) variable associated with a dual (adjoint) problem which, in fact, is the adjoint equation of the linearized state. The importance of this realization will be made clearer in the following chapters, as the methodology will be described in detail. This work builds upon the Euler equations whilst only a brief description is provided for the extension of the method to boundary value problems described by the Navier-Stokes equations.

1.1 Preliminaries of shape sensitivity analysis

The main mathematical tools of shape optimization are outlined in the following subsections. Upon these notions, a methodology for shape optimization in fluid dynamics is described in sections 2 and 3.

1.1.1 Domain transformations

Let $\Omega \subset \mathbb{R}^n$ be a domain of class C^k with $k \geq 1$ and disjoint boundaries $\partial\Omega = \{\Gamma_\infty, \Gamma\}$ where Γ_∞ can be termed as the *farfield* boundary and Γ the *obstacle boundary*. Let also both the convex, bounded domain B and the domain Σ be simply connected and of the same class, such that $\Omega = B \setminus \Sigma$ and $\partial B = \Gamma_\infty \subset \partial\Omega$, $\partial\Sigma = \Gamma \subset \partial\Omega$. Later on, we will see that there will be a BVP defined on Ω and from now on, we set our *control* to be the boundary Γ of the obstacle Σ, where every boundary functional will be defined. Therefore, to perform the shape sensitivity analysis of boundary functionals we consider a transformation (flow map) that acts on Ω. This transformation is based on the concept of an artificial velocity vector.

Definition 1.1. *(Speed method) The admissible artificial velocity (speed) fields $\mathscr{V}$ are elements of $\mathscr{D}(B, \mathbb{R}^n)$. For $\mathscr{V} \in \mathscr{D}(B, \mathbb{R}^n)$ we define the perturbation of the identity mapping $T_\tau(\Omega)(\mathscr{V}) \in C([0,\epsilon], \mathscr{D}(B, \mathbb{R}^n))$ by*

$$T_\tau(\Omega)(\mathscr{V}) := x \mapsto x + \tau\mathscr{V}(x) : \Omega \to \Omega_\tau \quad \textit{for every} \quad x \in \Omega \subset B \tag{1}$$

and for $\tau \in [0,\epsilon], \epsilon > 0$. For sufficiently small $\tau > 0$, $T_\tau(\Omega)(\mathscr{V})$ is a diffeomorphism [1] that maps Ω onto Ω_τ.

Subsequently, $T_\tau : \Omega \to \Omega_\tau$ generates a one-parameter family of perturbed domains

$$\mathcal{O} := \{\Omega_\tau := T_\tau(\Omega) : 0 \leq \tau \leq \epsilon, \partial\Omega_\tau = \{\Gamma_\tau, \Gamma_\infty\}, \Gamma_\tau \cap \Gamma_\infty = \varnothing\}$$

that share the same topological and regularity properties[1] and are always contained in the compact set $\overline{B}$.

A convenient artificial velocity field, that we will be using in the following sections, was proposed by Hadamard [2], having the following definition.

Definition 1.2. *(Hadamard parameterization) Consider the extension $\mathcal{V} \in \mathscr{D}(B, \mathbb{R}^n)$ of the unit normal vector field $\nu \in C^\infty(\Gamma)$. The Hadamard parameterization is recovered using the aforementioned speed method with $\mathscr{V}(x) = \hat{\zeta}(x)\mathcal{V}(x)$ for $x \in \Omega$, where $\hat{\zeta} \in C^\infty(\mathbb{R}^n)$ is defined as the extension of a function $\zeta \in C^\infty(\Gamma)$.*

Remark 1. *It is possible to enforce additional conditions on the admissible class of artificial velocity fields in order to satisfy certain geometric constraints. For instance, to preserve the volume of Ω_τ for every $\tau \in [0, \epsilon]$ we can set $\mathscr{V}$ to be divergence-free*

$$\mathscr{V} \in \mathscr{V}_C := \{u \in \mathscr{D}(B, \mathbb{R}^n) : \int_\Omega \nabla \cdot u = \int_\Gamma u \cdot \nu = 0\}$$

1.1.2 The structure of the shape derivative

Functionals defined in the domain Ω or on the boundary Γ are referred to as shape functionals. In the present context, we define the mapping $\mathscr{J} : \mathcal{O} \to \mathscr{D}'(B)$ taking domains from the one-parameter family $\mathcal{O}$ to the space of distributions $\mathscr{D}'(B)$. Subsequently, $\mathscr{J}(V) : \mathscr{D}(B) \to \mathbb{R}^n$ for $V \in \mathcal{O}$. The simplest examples of shape functionals are the measures

$$\mathscr{J}_1 = \int_{\mathbb{R}^n} \chi_\Omega \, \mathrm{d}^n x \qquad , \qquad \mathscr{J}_2 = \int_\Gamma \mathrm{d}\Gamma$$

where χ_Ω is the characteristic function of Ω. Based on the above, we define the shape (Gateaux) derivative of the functional $\mathscr{J}(\Omega)$ by

$$d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = \frac{\mathrm{d}}{\mathrm{d}\tau} \mathscr{J}(\Omega)(\mathscr{V}) \Big|_{\tau=0^+} = \lim_{\tau \to 0} \frac{\mathscr{J}(\Omega_\tau) - \mathscr{J}(\Omega)}{\tau} \tag{2}$$

where the limit is to be understood in the topology of $\mathscr{D}'$.

Definition 1.3. *(Shape differentiable functional) The functional $\mathscr{J}(\Omega) : \mathscr{D} \to \mathbb{R}$ is shape differentiable in Ω if*

i) the shape derivative $d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V})$ exists for all admissible directions $\mathscr{V} \in \mathscr{D}(B, \mathbb{R}^n)$,

ii) the mapping $T_\tau(\Omega)(\mathscr{V}) \mapsto d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) : \Omega_\tau \to \mathbb{R}$ is linear and continuous.

[1] The regularity is preserved for $\mathscr{V} \in \mathscr{D}(B, \mathbb{R}^n)$.

For example, we have that

$$\mathscr{J}(\Omega_\tau) = \int_{\mathbb{R}^n} \chi_{\Omega_\tau} = \int_{\mathbb{R}^n} \chi_\Omega \, \gamma(\tau)$$

where $\tau \mapsto \gamma(\tau) \equiv \det(\nabla T_\tau)$ can be shown to be differentiable in $\mathscr{D}$ with [3]

$$\frac{\gamma(\tau)-1}{\tau} \to \nabla \cdot \mathscr{V} \qquad \text{as} \quad \tau \to 0$$

Then

$$d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = \int_\Omega \nabla \cdot \mathscr{V} = \langle \chi_\Omega, \nabla \cdot \mathscr{V} \rangle_{\mathscr{D}'(\mathbb{R}^n) \times \mathscr{D}(\mathbb{R}^n)} = \langle -\nabla \chi_\Omega, \mathscr{V} \rangle_{(\mathscr{D}'(\mathbb{R}^n))^n \times (\mathscr{D}(\mathbb{R}^n))^n}$$

with $\langle \cdot, \cdot \rangle_{\mathscr{D}' \times \mathscr{D}}$ denoting the duality pairing. Thus, there exists distribution $\mathcal{G} \in \mathscr{D}'(\Omega, \mathbb{R}^n)$ such that

$$d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = \langle \mathcal{G}, \mathscr{V} \rangle_{\mathscr{D}' \times \mathscr{D}} = \langle -\nabla \chi_\Omega, \mathscr{V} \rangle_{\mathscr{D}' \times \mathscr{D}} \qquad \text{for all} \qquad T_\tau \in C([0, \epsilon], \mathscr{D}(B, \mathbb{R}^n))$$

Furthermore, for $\Gamma \in C^1$, using Stoke's theorem we can write

$$d_{\mathscr{V}} \mathscr{J} = \int_\Omega \nabla \cdot \mathscr{V} = \int_\Gamma \mathscr{V} \cdot \nu$$

The next result follows from the above definitions.

Proposition 1.1. *Let V be an open and bounded set in $\mathbb{R}^n$ and suppose that for every set $\Omega_\tau \in \mathcal{O}$ we have that $\Omega_\tau \subset \overline{B} \subset V$. If a shape functional $\mathscr{J}(\Omega_\tau) : \mathscr{D} \to \mathbb{R}$ is shape differentiable in Ω_τ, then there exists a distribution $\mathcal{G} \in \mathscr{D}'(\Omega, \mathbb{R}^n)$ such that*

$$d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = \langle \mathcal{G}, \mathscr{V} \rangle_{\mathscr{D}'(B) \times \mathscr{D}(B)} \qquad \textit{for all} \qquad T_\tau \in C([0, \epsilon], \mathscr{D}(B, \mathbb{R}^n)) \tag{3}$$

It is easy to see that artificial velocity fields producing nontrivial transformations $T_\tau(\Omega)(\mathscr{V})$ must be supported on Γ.

Proposition 1.2. *For $\mathscr{V} \in \mathscr{D}(\Omega)$ and for shape differentiable $\mathscr{J}(\Omega_\tau) : \mathscr{D} \to \mathbb{R}$ we have that*

$$\mathscr{J}(\Omega_\tau)(\mathscr{V}) = \mathscr{J}(\Omega)(\mathscr{V}) \implies d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = 0$$

for any $\tau \in [0, \epsilon]$.

Proof. The above result immediately follows from the definition of the shape derivative and the fact that for compactly supported speed fields in Ω one obtains $\Omega_\tau \equiv \Omega$. $\square$

Proposition 1.3. *Let Ω be a domain of class C^k with $\partial\Omega = \{\Gamma, \Gamma_\infty\}$ and $\mathscr{J}(\Omega) : \mathscr{D}(B) \to \mathbb{R}$ be shape differentiable with $d_{\mathscr{V}} \mathscr{J} = \langle \mathcal{G}, \mathscr{V} \rangle_{\mathscr{D}' \times \mathscr{D}}$. Then*

$$\langle \mathscr{V}\big|_\Gamma, \nu \rangle_{\mathbb{R}^n} \equiv 0 \implies d_{\mathscr{V}} \mathscr{J}(\Omega)(\mathscr{V}) = 0$$

Proof. Assume that $\langle \mathscr{V}\big|_\Gamma, \nu\rangle_{\mathbb{R}^n} \equiv 0$. Then, for any $x \in \Gamma$ we have that $T_\tau(x, \mathscr{V}) \in \Gamma$. That means that the boundary Γ is globally invariant to the transformation induced by $T_\tau(\Omega)(\mathscr{V})$ and consequently $\Omega_\tau \equiv \Omega$, implying that $d_{\mathscr{V}}\mathscr{J}(\Omega)(\mathscr{V}) = 0$. □

The collection of the above results leads to the structure theorem of the shape gradient.

Theorem 1.4. *(Hadamard-Zolesio structure theorem) Let $\mathscr{J}(\Omega_\tau) : \mathscr{D}(B) \to \mathbb{R}$ be a shape differentiable functional in any $\Omega_\tau \in C^\infty$ with $\partial\Omega \in C^\infty$. Then, there exists a scalar distribution $g \in \mathscr{D}'(\Gamma)$ such that the gradient $\mathcal{G} \in \mathscr{D}(\Omega, \mathbb{R}^n)$ is given by*

$$\mathcal{G}(x) = \gamma_\Gamma^*(g\nu) \qquad , \qquad x \in \Omega \tag{4}$$

where $\gamma_\Gamma : \mathscr{D}(\Omega, \mathbb{R}^n) \to \mathscr{D}(\Gamma, \mathbb{R}^n)$ is the trace operator and γ_Γ^* denotes its adjoint operator. Hence, a general formula for the shape gradient is obtained.

$$d_{\mathscr{V}}\mathscr{J}(\Omega)(\mathscr{V}) = \langle \mathcal{G}, \mathscr{V}\rangle_{\mathscr{D}'(B,\mathbb{R}^n)\times\mathscr{D}(B,\mathbb{R}^n)} = \langle g, \mathscr{V}\big|_\Gamma \cdot \nu\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)} = d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}) \tag{5}$$

Proof. We can prove that for a distribution $u \in \mathscr{D}'(\Omega)$ of order k and with compact support on Γ, it holds that [4, Thm. 2.3.5]

$$\begin{aligned}\langle u, \varphi\rangle_{\mathscr{D}'\times\mathscr{D}} &= \sum_{|\alpha|\le k} u_\alpha \left(\partial^\alpha \varphi\big|_\Gamma\right) = \sum_{|\alpha|\le k} u_\alpha\, \gamma_\Gamma\big(\partial^\alpha\varphi\big) \\ &= \sum_{|\alpha|\le k} \Big(\big(-1\big)^{|\alpha|}\partial^\alpha\big(\gamma_\Gamma^* u_\alpha\big)\Big)\, \varphi\end{aligned} \tag{6}$$

where u_α is a distribution of compact support on Γ and of order $k - |\alpha|$. Thus,

$$u = \big(-1\big)^{|\alpha|}\partial^\alpha\big(\gamma_\Gamma^* u_\alpha\big)$$

where we have defined the adjoint of the trace operator as

$$\langle \gamma_\Gamma^* u_\alpha, \varphi\rangle_{\mathscr{D}'(\mathbb{R}^n)\times\mathscr{D}(\mathbb{R}^n)} := \langle u_\alpha, \gamma_\Gamma\varphi\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)}$$

From propositions 1.1 and 1.2 it immediately follows that $\operatorname{supp}\mathcal{G} \subset \Gamma$ which in turn implies that there exists distribution $\hat{g} \in \mathscr{D}'(\Gamma, \mathbb{R}^n)$ such that

$$d_{\mathscr{V}}\mathscr{J}(\Omega)(\mathscr{V}) = \langle \mathcal{G}, \mathscr{V}\rangle_{\mathscr{D}'(B,\mathbb{R}^n)\times\mathscr{D}(B,\mathbb{R}^n)} = \langle \hat{g}, \gamma_\Gamma\mathscr{V}\rangle_{\mathscr{D}'(\Gamma,\mathbb{R}^n)\times\mathscr{D}(\Gamma,\mathbb{R}^n)}$$

Now define $\mathscr{B} = \{u \in \mathscr{D}(B, \mathbb{R}^n) : \langle u, \nu\rangle_{\mathbb{R}^n} = 0 \text{ on } \Gamma\}$ and observe that proposition 1.3 infers that $\mathscr{B} \subset \ker\big(\, d_{\mathscr{V}}(\cdot)(\Omega)(\mathscr{V})\big)$. This suggests that without loss of generality we can select $\mathscr{V}$ from the quotient space $\mathscr{D}(B, \mathbb{R}^n)/\mathscr{B}$ where two elements $\mathscr{V}_1, \mathscr{V}_2 \in \mathscr{D}(B, \mathbb{R}^n)/\mathscr{B}$ having different tangential components on Γ are identified. Based on this, we obtain the final form

$$d_{\mathscr{V}}\mathscr{J}(\Omega)(\mathscr{V}) = \langle \hat{g}, \gamma_\Gamma\mathscr{V}\rangle_{\mathscr{D}'(\Gamma,\mathbb{R}^n)\times\mathscr{D}(\Gamma,\mathbb{R}^n)} = \langle g, \nu\cdot\gamma_\Gamma\mathscr{V}\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)} = \langle \gamma_\Gamma^*(g\nu), \mathscr{V}\rangle_{\mathscr{D}'(B)\times\mathscr{D}(B)}$$

for scalar distribution $g \in \mathscr{D}'(\Gamma)$. □

Remark 2. *This important result implies that the shape derivative of a distribution defined over the domain Ω can be reduced to a distribution defined only on the boundary Γ.*

Furthermore, if g is integrable, e.g. $g \in L^1(\Gamma)$, then

$$d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}) = \langle g, \nu\cdot\gamma_\Gamma\mathscr{V}\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)} = \int_\Gamma g\, \mathscr{V}\cdot\nu \tag{7}$$

In the sections to follow we will work out a methodology where an augmenented (constrained) shape functional defined on the domain Ω is reduced to a functional on the boundary by the use of the adjoint state of the boundary value problem acting on Ω. To this end, we first need to develope the notions of material and shape derivative for functions living in Ω.

1.1.3 Shape derivatives of domain and boundary functionals

Definition 1.4. *(Material derivative) Let $u_\tau : \Omega_\tau \to \mathbb{R}$ be a function in $C^k(\Omega_\tau)$ that depends smoothly on the parameter $\tau \in [0, \epsilon]$ and $u_0 \equiv u$. The material derivative of u with respect to the transformation T_τ is defined as*

$$\dot{u}(x) := D_{\mathscr{V}} u(x) := \lim_{\tau \to 0} \frac{(u_\tau \circ T_\tau)(x) - u(x)}{\tau} \quad , \quad x \in \Omega \tag{8}$$

with the subscript $\mathscr{V}$ denoting the artificial velocity field associated to $T_\tau(x)(\mathscr{V})$.

Remark 3. *The operator $D_{\mathscr{V}}$ satisfies the classical rules of differential operators such as the chain rule, product rule, etc. but does not commute with time and space derivatives. It is also identified with the Lie derivative for scalar functions f, i.e. $D_{\mathscr{V}} f \equiv \mathcal{L}_{\mathscr{V}} f$.*

A more explicit form of the material derivative can be obtained by extending $u_\tau(x) : \Omega_\tau \to \mathbb{R}$ to $\widetilde{u}(x, \tau) : \overline{B} \times [0, \epsilon] \to \mathbb{R}$. Then for $x \in \Omega$ and $\widetilde{u}(x, 0) \equiv u(x)$, we can write

$$\begin{aligned} D_{\mathscr{V}} u(x) = \frac{\mathrm{d}}{\mathrm{d}\tau} \Big(\widetilde{u}(x, \tau) \circ T_\tau(\mathscr{V})(x) \Big) \Big|_{\tau=0} &= \partial_\tau \widetilde{u}(x, 0) + \nabla \widetilde{u}(x, 0) \, \frac{\mathrm{d}}{\mathrm{d}\tau} T_\tau(\mathscr{V})(x) \Big|_{\tau=0} \\ &= \partial_\tau \widetilde{u}(x, 0) + \big(\mathscr{V}(x) \cdot \nabla \big) \widetilde{u}(x, 0) \\ &= \partial_\tau u(x) + \big(\mathscr{V}(x) \cdot \nabla \big) u(x) \end{aligned} \tag{9}$$

It can be seen from the above expression that the material derivative can be decomposed in two parts: the rate of change of u due to its dependence on τ, and the convective effect which is due to the artificial velocity field $\mathscr{V}(x)$. Given the vector field $\mathscr{V}(x)$, the convective term can be easily computed for known u. On the other hand the term $\partial_\tau u(x)$ is trickier to compute since u is usually the solution of a BVP evolving with the pseudotime τ on the domains $\mathcal{O}$.

Definition 1.5. *(Shape derivative) In the above context, the derivative $\partial_\tau u(x) \equiv u'(x)$ for $x \in \Omega$ is called the shape derivative of u with respect to the transformation $T_\tau(x)(\mathscr{V})$. Also, assuming that the material derivative exists, we can define the shape derivative in explicit form as*

$$u'(x) = D_{\mathscr{V}} u(x) - \big(\mathscr{V}(x) \cdot \nabla \big) u(x) \quad , \quad x \in \Omega \tag{10}$$

Remark 4. *The shape derivative operator obeys the classical rules of differential operators and also commutes with time and space derivatives.*

Using the above notions and some basic differential geometry we can now calculate the shape derivatives of functionals depending on the transforming domain Ω.

Lemma 1.5. *Let $C^k(\Omega_\tau) \ni u_\tau : \Omega_\tau \to \mathbb{R}$ and consider the distributed and the boundary functionals $\mathscr{E}$ and $\mathscr{J}$ respectively, defined by*

$$\mathscr{E}_\tau = \int_{\Omega_\tau} u_\tau(x) \quad , \quad \mathscr{J}_\tau = \int_{\Gamma_\tau} u_\tau(x) \quad \textit{for all} \quad x \in \Omega_\tau, \tau \in [0, \epsilon] \tag{11}$$

The shape derivatives of $\mathscr{E}$, $\mathscr{J}$ with respect to the transformation $T_\tau(\Omega)(\mathscr{V})$ read

$$d_{\mathscr{V}} \mathscr{E} := \frac{\mathrm{d}}{\mathrm{d}\tau} \mathscr{E}_\epsilon \Big|_{\tau=0} = \int_\Omega u' + \int_\Gamma u \langle \mathscr{V}, \nu \rangle_{\mathbb{R}^n} \tag{12a}$$

$$d_{\mathscr{V}} \mathscr{J} := \frac{\mathrm{d}}{\mathrm{d}\tau} \mathscr{J}_\epsilon \Big|_{\tau=0} = \int_\Gamma u' + \big(\langle \nu, \nabla \rangle_{\mathbb{R}^n} + \kappa \big) u \langle \mathscr{V}, \nu \rangle_{\mathbb{R}^n} \tag{12b}$$

where ν is the normal unit vector on Γ, κ the mean curvature of Γ and $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ denotes the inner product in $\mathbb{R}^n$. Also, the manifold Γ is considered closed, i.e. $\partial \Gamma = \varnothing$.

Proof. For the former functional, we first transform it in the reference domain Ω as

$$\mathscr{E}_\tau = \int_{\Omega_\tau} u_\tau(y)\,\mathrm{d}y = \int_\Omega (u_\tau \circ T_\tau)(x)\,\det(\nabla T_\tau)\,\mathrm{d}x$$

Differentiating with respect to the pseudotime τ

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\int_{\Omega_\tau} u_\tau(y)\,\mathrm{d}y\Big)\Big|_{\tau=0} &= \frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\int_\Omega (u_\tau \circ T_\tau)(x)\,\det(\nabla T_\tau)\,\mathrm{d}x\Big)\Big|_{\tau=0} \\
&= \int_\Omega D_{\mathscr{V}} u(x) + u(x)\frac{\mathrm{d}}{\mathrm{d}\tau}\det(\nabla T_\tau)\,\mathrm{d}x \\
&= \int_\Omega u'(x) + \big(\mathscr{V}(x)\cdot\nabla\big)u(x) + u(x)\big(\nabla\cdot\mathscr{V}(x)\big)\,\mathrm{d}x \\
&= \int_\Omega u'(x) + \nabla\cdot\big(\mathscr{V}(x)u(x)\big)\,\mathrm{d}x
\end{aligned}$$

where we have used the formulas $\frac{\mathrm{d}}{\mathrm{d}\tau}\det(\nabla T_\tau) = \nabla\cdot\mathscr{V}$ and $D_{\mathscr{V}} u = u' + \big(\mathscr{V}(x)\cdot\nabla\big)u(x)$. Since $\mathscr{V}$ has compact support in B, $\mathscr{V}$ vanishes on Γ_∞. Thus, the divergence theorem for $\partial\Omega = \{\Gamma, \Gamma_\infty\}$ asserts that

$$d_{\mathscr{V}}\mathscr{E}(\Omega)(\mathscr{V}) = \int_\Omega u' + \int_\Gamma (\mathscr{V}\cdot\nu)u$$

For the latter case, we will be using without proof the following transformation formulas [3, Sec. 2.17]

$$\int_{\Gamma_\tau} u_\tau(y)\,\mathrm{d}y = \int_{\Gamma_\tau} \big(u_\tau \circ T_\tau\big)(x)\,\gamma_\tau\,\mathrm{d}x$$

where $\gamma_\tau = \det(\nabla T_\tau)\,\big\|(\nabla T_\tau^\top)^{-1}\cdot\nu\big\|_{\mathbb{R}^n}$ and

$$\gamma_\tau' := \frac{\mathrm{d}}{\mathrm{d}\tau}\gamma_\tau\Big|_{\tau=0} = \nabla_\Gamma\cdot\mathscr{V} \tag{13}$$

where ∇_Γ denotes the tangential derivative. Also [5, Sec. 4.4],

$$\int_\Gamma \nabla_\Gamma u = \int_\Gamma u\kappa\nu \quad \text{for any} \quad u\in C^k(\Gamma) \tag{14}$$

for a smooth manifold Γ with $\partial\Gamma = \varnothing$ and mean curvature κ. Using the above formulas and working as before we find

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\int_{\Gamma_\tau} u_\tau(y)\,\mathrm{d}y\Big)\Big|_{\tau=0} &= \frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\int_\Gamma (u_\tau \circ T_\tau)(x)\,\gamma_\tau\,\mathrm{d}x\Big)\Big|_{\tau=0} \\
&= \int_\Gamma D_{\mathscr{V}} u(x) + u(x)\frac{\mathrm{d}}{\mathrm{d}\tau}\gamma_\tau\,\mathrm{d}x \\
&= \int_\Gamma u'(x) + \big(\mathscr{V}(x)\cdot\nabla\big)u(x) + u(x)\nabla_\Gamma\cdot\mathscr{V}(x)\,\mathrm{d}x \\
&= \int_\Gamma u'(x) + \big(\mathscr{V}\cdot\nu\big)\partial_\nu u(x) + \big(\mathscr{V}(x)\cdot\nabla_\Gamma\big)u(x) + u(x)\nabla_\Gamma\cdot\mathscr{V}(x)\,\mathrm{d}x \\
&= \int_\Gamma u'(x) + \big(\mathscr{V}\cdot\nu\big)\partial_\nu u(x) + \nabla_\Gamma\cdot\big(u(x)\mathscr{V}(x)\big)\,\mathrm{d}x
\end{aligned}$$

where in the last two lines we decomposed the term $\big(\mathscr{V}(x)\cdot\nabla\big)u(x)$ in normal and tangential components. Finally, using formula (14) one obtains

$$d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}) = \int_\Gamma u' + (\mathscr{V}\cdot\nu)\big(\partial_\nu + \kappa\big)u$$

$\square$

2 Optimal control of the boundary for the Euler equations

This section contains the main material of the present work where the shape optimization method is formulated as an optimal control problem for the boundary Γ.

2.1 Linearized Euler equations

Let $\Omega \subset \mathbb{R}^3$ with disjoint boundaries $\partial\Omega = \{\Gamma_\infty, \Gamma\}$ be the set that was defined in the previous section and define the *primitive* and the *conservative* variables as the vectors $U_p, U_c \in C^1(\Omega, \mathbb{R}^5)$ respectively, having the form

$$U_{p_i} = \big(\rho, u_1, u_2, u_3, p\big)^\top(x) \quad , \quad U_i \equiv U_{c_i} = \big(\rho, \rho u_1, \rho u_2, \rho u_3, E\big)^\top(x) \quad , \quad x \in \Omega \tag{15}$$

Definition 2.1. *(Euler equations) The nonlinear system of conservation laws for the mass continuity, momentum balance and energy conservation that describes the dynamics of an inviscid compressible fluid is fully described by the convective flux vector $F_{c_{ij}} \in C^1(\Omega, \mathbb{R}^5)$ given by*

$$F_{c_{ij}} = \big(\rho u_1, \rho u_i u_1 + p\delta_{i1}, \rho u_i u_2 + p\delta_{i2}, \rho u_i u_3 + p\delta_{i3}, \rho u_i H\big)^\top \quad , \quad i = 1, \ldots, 3\,, \tag{16}$$

the vector of conservative variables U_i and the constitutive equations of the fluid. For ideal gases, the constitutive equations take the form

$$p = (\gamma - 1)\rho\big(E - \frac{1}{2}u_i u_i\big) \quad , \quad H = E + \frac{p}{\rho} \quad , \quad \gamma \simeq 1.4 \quad (\textit{atm. air}) \tag{17}$$

Finally, ρ represents the density, p the pressure, $V = (u_1, u_2, u_3)$ the velocity vector, E the total energy, H the enthalpy and γ the heat capacity ratio.

We are interested in BVP problems of the Euler equations for domains that contain a smooth (streamlined) obstacle Σ. Consequently, Γ is the boundary of the obstacle and the farfield boundary Γ_∞ is placed at a sufficient distance from the body, where freestream flow conditions can be considered. For the steady Euler equations, i.e. $\partial_t U \equiv 0$ after a transient period, the BVP reads

$$\begin{cases} \partial_i\big(F_{c_{ij}}(U)\big) = 0 & \text{in} \quad \Omega \\ V\cdot\nu = 0 & \text{on} \quad \Gamma \\ W^+ = W_\infty & \text{on} \quad \Gamma_\infty \end{cases} \tag{18}$$

where ν is the unit normal vector on Γ and W is the vector of characteristic variables[2].

[2] At the farfield, boundary conditions are prescribed according to the propagation direction of characteristics.

The linearized Euler equations can then be expressed according to first order perturbations around a base state U_0. Defining the perturbation vector δU we write $U = U_0 + \delta U$ and thus

$$F_{c_{ij}}(U) = F_{c_{ij}}(U_0) + \frac{\partial F_{c_{ij}}}{\partial U_k}\bigg|_{U_{0k}} \delta U_k = F_{c_{i0}} + A^c_{ijk}\Big|_{U_{0k}} \delta U_k \qquad i = 1, \dots, 3,\ j, k = 1, \dots, 5 \tag{19}$$

The third order tensor A^c_{ijk} is known as convective flux Jacobian and takes the compact form

$$A^c_{ijk} = \begin{pmatrix} 0 & \delta_{i1} & \delta_{i2} & \delta_{i3} & 0 \\ -u_i u_1 + \delta_{i1}\phi & u_1 - (\gamma-2)u_1\delta_{i1} & u_1\delta_{i2} - (\gamma-1)u_2\delta_{i1} & u_1\delta_{i3} - (\gamma-1)u_3\delta_{i1} & (\gamma-1)\delta_{i1} \\ -u_i u_2 + \delta_{i2}\phi & u_2\delta_{i1} - (\gamma-1)u_1\delta_{i2} & u_2 - (\gamma-2)u_i\delta_{i2} & u_2\delta_{i3} - (\gamma-1)u_3\delta_{i2} & (\gamma-1)\delta_{i2} \\ -u_i u_3 + \delta_{i3}\phi & u_3\delta_{i1} - (\gamma-1)u_1\delta_{i3} & u_3\delta_{i2} - (\gamma-1)u_2\delta_{i3} & u_1 - (\gamma-2)u_i\delta_{i3} & (\gamma-1)\delta_{i3} \\ u_i(\phi - H) & -(\gamma-1)u_i u_1 + H\delta_{i1} & -(\gamma-1)u_1 u_2 + H\delta_{i2} & -(\gamma-1)u_i u_3 + H\delta_{i3} & \gamma u_i \end{pmatrix} \tag{20}$$

where $\phi = (\gamma - 1)/2\ u_i u_i$. Consequently, the linearized BVP for the Euler equations reads

$$\begin{cases} \partial_i\big(A^c_{ijk}\delta U_k\big) = 0 & \text{in} \quad \Omega \\ \delta u_i\ \nu_i = 0 & \text{on} \quad \Gamma \\ \delta W^+ = 0 & \text{on} \quad \Gamma_\infty \end{cases} \tag{21}$$

2.2 Shape derivatives of the Euler equations

Now we want to control the boundary Γ in such a way that the Euler equations are satisfied in the domain Ω_τ for every $\tau \in [0, \epsilon]$, $\Omega \equiv \Omega_{\tau=0}$. To this end, we derive a BVP problem for the shape derivatives of the Euler system. The Euler equations (18) in weak form read

$$\int_{\Omega_\tau} \partial_i\big(F_{c_{ij}}(U)\big)\ \varphi_j = 0 \quad , \quad \varphi_j \in \mathscr{D}(\Omega_\tau, \mathbb{R}^5)$$

Taking the shape derivative (Lemma 1.5)

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\int_{\Omega_\tau} \partial_i\big(F_{c_{ij}}(U)\big)\ \varphi_j\Big)\Big|_{\tau=0} = 0$$

$$\int_\Omega \Big(\partial_i\big(F_{c_{ij}}(U)\big)\ \varphi_j\Big)' + \int_\Gamma \Big(\partial_i\big(F_{c_{ij}}(U)\big)\ \varphi_j\Big)\langle \mathscr{V}, \nu\rangle_{\mathbb{R}^3} = 0$$

and since $\varphi_j \in \mathscr{D}(\Omega_\tau, \mathbb{R}^5)$ does not depend on the pseudotime τ we get

$$\int_\Omega \Big(\partial_i\big(F_{c_{ij}}(U)\big)\Big)'\ \varphi_j = \int_\Omega \partial_i\big(F'_{c_{ij}}(U)\big)\ \varphi_j = \int_\Omega \partial_i\big(A^c_{ijk}\big|_U U'_k\big)\ \varphi_j = 0$$

because the shape derivative commutes with the time and space derivatives. Subsequently,

$$\partial_i\big(A^c_{ijk} U'_k\big) = 0 \qquad \text{in} \quad \Omega \tag{22}$$

where U'_k is the vector of shape derivatives of the conservative variables. To work out the boundary condition at the deforming boundary Γ_τ we observe that we need to satisfy the no-penetration boundary condition on Γ_τ for every $\tau \in [0, \epsilon]$. Thus, we impose $u_\tau \cdot \nu_\tau = 0$ for all τ and $x \in \Omega_\tau$ or $(u_\tau \cdot \nu_\tau) \circ T_\tau = 0$ for all τ and $x \in \Omega$. More specifically,

$$(u_\tau \cdot \nu_\tau) \circ T_\tau = (u_\tau \cdot \nu_\tau) \circ T_\tau - u \cdot \nu = 0 \qquad , \qquad \tau > 0$$

because $u \cdot \nu = 0$ (at $\tau = 0$). For small τ, and up to the limit, this is equivalent to

$$D_{\mathscr{V}}(u \cdot \nu) = 0 \qquad \text{on} \quad \Gamma \tag{23}$$

For $\mathscr{V}(x) = \zeta(x)\nu(x)$ with $x \in \Gamma$, the above condition can be also written as

$$D_{\mathscr{V}}(u \cdot \nu) = u' \cdot \nu + u \cdot \nu' + \zeta\big(\partial_\nu u \cdot \nu\big) = 0 \tag{24}$$

Lastly, since the boundary Γ_∞ is fixed for all τ we simply obtain

$$(W^+)' = W'_\infty = 0 \qquad \text{on} \quad \Gamma_\infty$$

Thus, the BVP describing the shape derivatives U'_i of (18) takes the form

$$\begin{cases} \partial_i\big(A^c_{ijk} U'_k\big) = 0 & \text{in} \quad \Omega \\ u' \cdot \nu = -u \cdot \nu' - \zeta\big(\partial_\nu u \cdot \nu\big) & \text{on} \quad \Gamma \\ (W^+)' = 0 & \text{on} \quad \Gamma_\infty \end{cases} \tag{25}$$

which closely resembles the linearized Euler equations (21) but with a modified boundary condition on Γ to account for the deforming boundary.

2.3 Boundary functionals depending on pressure

When the Euler equations are involved in aerodynamic shape optimization problems it is reasonable to study boundary functionals that depend on the pressure. Quantities of interest that are functions of the pressure alone are the lift, drag and moment coefficients. Since viscous phenomena are absent in the Euler equations, one can only optimize a shape with respect to its pressure drag, e.g. reduce the drag penalty due to shock-waves in transonic flows. This can result in an automatic and precise way for the design of shock-free airfoils.

Therefore, from now on we work with functionals defined on the boundary Γ having the form

$$\mathscr{J}(\Gamma)(p) = \int_\Gamma g(p, \nu) \tag{26}$$

where $g \in C^k$ for $k \geq 1$ is a function of the pressure p and the outward normal unit vector ν on Γ. For instance, the pressure drag coefficient on an airfoil is given by

$$c_d = \int_\Gamma g(p, \nu) = \int_\Gamma c_p(\nu \cdot \frac{V_\infty}{\|V_\infty\|}) \quad \text{where} \quad c_p = \frac{p - p_\infty}{q_\infty}$$

with V_∞ the freestream velocity vector in $\mathbb{R}^3$, p_∞ the freestream pressure and $q_\infty = \frac{1}{2}\rho_\infty V_\infty$ the freestream dynamic pressure. Using Lemma 1.5 the shape derivative of the above functional is expressed by

$$d_{\mathscr{V}} \mathscr{J}(\Gamma)(\mathscr{V}) = \int_\Gamma g'(p, \nu) + \big((\nu \cdot \nabla) + \kappa\big) g(p, \nu) \big(\mathscr{V} \cdot \nu\big) \tag{27}$$

$$\text{with} \quad g'(p, \nu) = \frac{\partial g}{\partial p}\, p' + \frac{\partial g}{\partial \nu} \cdot \nu' \tag{28}$$

It is insightful to rewrite the above functional in the form

$$d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}) = \int_\Gamma \underbrace{\frac{\partial g}{\partial p}\,p' + \frac{\partial g}{\partial \nu}\cdot\nu'}_{\text{flow and geometric shape derivatives}} + \underbrace{\big((\nu\cdot\nabla)+\kappa)g(p,\nu)\big(\mathscr{V}\cdot\nu\big)}_{\text{geometry and Euler flow solution}} \tag{29}$$

which immediately suggest that the shape derivative $d_{\mathscr{V}}\mathscr{J}$ is composed by two main terms: one depending on the sensitivity of the pressure field and the normal unit vector to the transformation T_τ and the other depending on known geometric properties, the transformation $T_\tau(\Omega)(\mathscr{V})$ and the solution of the Euler equations (18).

Note that, given a speed vector field $\mathscr{V}\in\mathscr{D}(B,\mathbb{R}^n)$ and the solution to equation (18), we can subsequently solve the BVP (25) for the shape derivatives to compute $d_{\mathscr{V}}\mathscr{J}(\Omega)(\mathscr{V})\in\mathbb{R}$. But this is not exactly what we wish to obtain. Instead, we are searching for the scalar distribution $\mathcal{G}\in\mathscr{D}'(\Gamma)$ such that

$$d_{\mathscr{V}}\mathscr{J} := \langle\mathcal{G},\mathscr{V}\big|_\Gamma\cdot\nu\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)}$$

holding for all speed vectors $\mathscr{V}\in\mathscr{D}(B,\mathbb{R}^n)$ with $\mathscr{V}\big|_\Gamma\in\mathscr{D}(\Gamma)$. This scalar distribution is the gradient defined over the boundary Γ that we will later use to perform the shape optimization.

However, it is worth mentioning that the gradient $\mathcal{G}\in\mathscr{D}'(\Gamma)$ can still be approximated by the above method. For example, we can consider the restriction of a normalized artificial velocity field $\mathscr{V}\in\mathscr{D}(B,\mathbb{R}^n)$ in a region $\mathscr{N}(x_0):=B_\rho(x_0)\cap\Gamma$ for $x_0\in\Gamma$. For sufficiently small $\rho>0$

$$d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}\big|_{\mathscr{N}(x_0)})\simeq\mathcal{G}(x_0) \tag{30}$$

Intuitevely speaking, it is as if we were taking the Dirac delta function as the artificial velocity field $\mathscr{V}$, even though we cannot exactly do that. Hence, to approximate the gradient over the boundary Γ at $n\in\mathbb{N}$ neighborhoods $\{\mathscr{N}(x_n)\}$ of Γ using (30), we would require n solutions of the shape derivative boundary value problem (25), one for every $\mathscr{V}\big|_{\mathscr{N}(x_n)}$.

It turns out that this can be avoided by the use of the adjoint Euler equations, so that only one BVP needs to be solved to obtain the exact gradient, as it will be shown in the next section.

2.4 Adjoint Euler equations

Let $\varphi\in H^1(\Omega,\mathbb{R}^5)$ and take the integration by parts of the shape derivative equation (22) for the Euler system to obtain

$$\int_\Omega \partial_i\big(A^c_{ijk}U'_k\big)\,\varphi_j = \int_\Omega U'_k\,\big(-A^c_{ijk}\partial_i\varphi_j\big) + \int_{\Gamma\cup\Gamma_\infty} U'_k\,A^c_{ijk}\nu_i\,\varphi_j = 0 \quad , \quad \varphi\in H^1(\Omega,\mathbb{R}^5)$$

For the above relation to hold, we first demand that

$$-A^c_{ijk}\partial_i\varphi_j = 0 \qquad \text{in} \quad \Omega \tag{31}$$

The above linear homogeneous equations are known as the *adjoint equations* or the *adjoint state* to the system of Euler equations (18). To make the term associated to the boundary Γ vanish we work in terms of the shape derivatives of the primitive variables U_{p_i}. Knowing that the product rule holds for the shape derivative, e.g. $\big(\rho u_i\big)' = \rho' u_i + \rho u_i'$, the shape derivative of pressure computes

$$
\begin{aligned}
p' = \Big((\gamma-1)\rho\Big(E - \frac{1}{2}u_i u_i\Big)\Big)' &= (\gamma-1)\Big(\big(\rho E\big)' - \frac{\rho'}{2}u_i u_i - \rho u_i u_i'\Big) \\
p' = (\gamma-1)\Big(\big(\rho E\big)' - \rho u_i u_i'\Big) - \rho'\phi \quad &, \quad \phi = (\gamma-1)\frac{1}{2}u_i u_i
\end{aligned} \tag{32}
$$

Taking the formula (20) of the convective flux Jacobian A^c_{ijk} and regrouping the terms, we observe that many terms vanish due to the boundary condition on Γ, i.e. $u_i\nu_i = 0$. After computations we obtain

$$
\begin{aligned}
\int_\Gamma U_k' \, A^c_{ijk}\nu_i \, \varphi_j &= \int_\Gamma \big(\rho u_i'\nu_i\big)\varphi_1 + \big(\rho u_i'\nu_i H\big)\varphi_5 + \rho u_i'\nu_i(u_i\varphi_{i+1}) + p'\big(\nu_i\varphi_{i+1}\big) = 0 \\
\int_\Gamma \big(\rho u_i'\nu_i\big)&\big(\varphi_1 + u_i\varphi_{i+1} + H\varphi_5\big) + p'\big(\nu_i\varphi_{i+1}\big) = 0 \quad \text{for} \quad i = 1,\dots,3
\end{aligned} \tag{33}
$$

On the farfield boundary Γ_∞ it is possible to set $\varphi_j \equiv 0$. However, this may overconstrain the system and a better choice could be to apply boundary conditions depending on the characteristic variables [6]. Here, for simplicity it is assumed that $\varphi_j \equiv 0$ on Γ_∞. Observing the structure of the pressure functional (29), we see that the unknown pressure shape derivative term can be replaced if we select suitable boundary conditions on Γ. Taking (33) with $\nu_i\varphi_{i+1} = \frac{\partial g}{\partial p}$ we obtain

$$
\int_\Gamma \frac{\partial g}{\partial p}\, p' = -\int_\Gamma \big(\rho u_i'\nu_i\big)\big(\varphi_1 + u_i\varphi_{i+1} + H\varphi_5\big) \tag{34}
$$

Hence, setting $\Phi = \rho\varphi_1 + \rho u_i\varphi_{i+1} + \rho H\varphi_5$, formula (29) can be recast to the form

$$
\begin{aligned}
d_{\mathscr{V}}\mathscr{J} &= \int_\Gamma \frac{\partial g}{\partial p}\, p' + \frac{\partial g}{\partial \nu}\cdot\nu' + \big((\nu\cdot\nabla)+\kappa\big)g\big(\mathscr{V}\cdot\nu\big) \\
&= \int_\Gamma -(u'\cdot\nu)\;\Phi + \frac{\partial g}{\partial \nu}\cdot\nu' + \big(\partial_\nu g + \kappa g\big)\big(\mathscr{V}\cdot\nu\big)
\end{aligned} \tag{35}
$$

The shape derivative of the velocity u' on the boundary Γ is defined by the boundary condition (23) and $\nu' = -\nabla_\Gamma(\mathscr{V}\cdot\nu)$. Proceeding with integration by parts we obtain

$$
\begin{aligned}
d_{\mathscr{V}}\mathscr{J} &= \int_\Gamma \big(u\cdot\nu' + \mathscr{V}\cdot\nabla(u\nu)\big)\;\Phi + \frac{\partial g}{\partial \nu}\cdot\nu' + \big(\partial_\nu g + \kappa g\big)\big(\mathscr{V}\cdot\nu\big) \\
&= \int_\Gamma -\big(u\cdot\nabla_\Gamma(\mathscr{V}\cdot\nu)\big)\;\Phi - \frac{\partial g}{\partial \nu}\cdot\nabla_\Gamma(\mathscr{V}\cdot\nu) + \big(\partial_\nu g + \kappa g\big)\big(\mathscr{V}\cdot\nu\big) \\
&= \int_\Gamma \Big(\nabla_\Gamma\cdot(\Phi u) - \nabla_\Gamma\cdot\frac{\partial g}{\partial \nu} + \big(\partial_\nu g + \kappa g\big)\Big)\big(\mathscr{V}\cdot\nu\big) \\
&= \int_\Gamma \mathcal{G}\big(\mathscr{V}\cdot\nu\big)
\end{aligned} \tag{36}
$$

which is the form of the shape gradient that we would expect to find according to the structure theorem 1.4. Taking the Hadamard parameterization (Definition 1.2), we find the distribution that is identified with the shape gradient in terms of the solution of the Euler system and its adjoint state

$$d_{\mathscr{V}}\mathscr{J}(\Gamma)(\mathscr{V}) = \int_{\Gamma} \mathcal{G}\,\zeta = \langle \mathcal{G}, \zeta\rangle_{\mathscr{D}'(\Gamma)\times\mathscr{D}(\Gamma)} \qquad , \qquad \zeta \in \mathscr{D}(\Gamma)$$

$$\mathcal{G} = \nabla_\Gamma \cdot (\Phi u) - \nabla_\Gamma \cdot \frac{\partial g}{\partial \nu} + (\partial_\nu g + \kappa g) \tag{37}$$

where ζ is a smooth function that describes the displacement of the boundary Γ. To compute Φ the solution of the adjoint BVP is required

$$\begin{cases} -A^c_{ijk}\partial_i \varphi_j = 0 & \text{in} \quad \Omega \\ \varphi_{i+1}\nu_i = \frac{\partial g}{\partial p} & \text{on} \quad \Gamma \\ \varphi_j = 0 & \text{on} \quad \Gamma_\infty \end{cases} \tag{38}$$

for $i = 1, \ldots, 3$ and $k, j = 1, \ldots, 5$. Observe that (38) incorporates the adjoint Euler equations, which is a system of linear hyperbolic equations with variable coefficients, and a boundary condition on the deforming boundary Γ that depends on the cost functional $\mathscr{J}$.

2.5 An algorithm for optimal shape design of aerodynamic bodies

To summarize the above procedures, the basic sketch of a shape optimization algorithm is presented, generating airfoils of minimal drag subject to the given constraints.

Algorithm 1: Pressure drag minimization of obstacle immersed in inviscid fluid.

Input:

Initial geometry: Initial domain $\Omega = B \setminus \Sigma$.

Flow conditions: Freestream Mach number M_∞, velocity vector V_∞ etc.

Optimization parameters: Marching step $\delta_s > 0$ and tolerance $\varepsilon > 0$.

Pick $\mathscr{V} \in \mathscr{V}_C$ and choose the Hadamard parameterization (Definition 1.2).

Set $i \leftarrow 0$ and $\Omega_i \leftarrow \Omega$.

begin

1. Solve Euler equations (18) in Ω_i to obtain the flow solution

$$U_{p_i} = \left(\rho, u_1, u_2, u_3, p\right)^\top(x) \qquad \text{for every} \qquad x \in \Omega_i$$

and compute the convective flux Jacobian $A^c_{ijk}(U_p)$ in Ω_i.

2. Solve adjoint Euler equations (38) in Ω_i to obtain the adjoint state

$$(\varphi_1, \varphi_2, \varphi_3, \varphi_4, \varphi_5)^\top(x) \qquad \text{for every} \qquad x \in \Omega_i$$

3. Compute the shape gradient (37) on Γ_i with suitable $\zeta \in \mathscr{D}(\Gamma)$ to account for the volume preserving contraint of the set $\mathscr{V}_C$ (see Remark 1).

4. Perturb the current boundary Γ_i to create the new domain Ω_{i+1} using the transformation

$$x \mapsto x + \delta_s \mathscr{V}_C^* \quad \text{with} \quad \mathscr{V}_C^*(x) = (\zeta\mathcal{G})\,\nu \quad \text{for} \quad x \in \Gamma$$

or by perturbing the control points of a B-spline curve that parameterizes the boundary Γ_i in the direction of $\mathcal{G}$ and with step δ_s.

Stop if reduction in drag coefficient c_d is below the given tolerance ε.

Otherwise set $i \leftarrow i + 1$ and go to **1**.

end

Output: Boundary shape Γ^* that minimizes the drag coefficient c_d (according to the Euler equations) for prescribed flow conditions and geometric constraints.

3 Optimal control of the boundary for the Navier-Stokes equations

The shape optimization method that is described in section 2 is carried out using the Euler equations. To introduce the effect of viscous phenomena and turbulence on the optimization, the method must build upon the Navier-Stokes equations. However, the shape optimization method is not to be developed from scratch. To the contrary, the Euler equations and the adjoint Euler equations are the 'convective' part of the Navier-Stokes equations and their adjoint state respectively. More specifically, looking at the equations as a conservation law, the Navier-Stokes equations are the Euler equations with the addition of new terms to account for the viscous momentum and thermal stresses. Considering drag minimization applications, the objective function $\mathscr{J}$ given by (26) is augmented to account for friction (momentum stress component parallel to the boundary Γ) and the boundary conditions on the wall are modified to account for the no-slip (zero wall velocity) condition instead of the no-penetration condition of the Euler equations.

In this section a very brief overview is given regarding the extension of the Euler shape optimization method to a method based on the Navier-Stokes equations.

3.1 Compressible Navier-Stokes equations

In section 2.1 the Euler equations along with their linearized form were given. In the present section the steady compressible Reynolds-Averaged Navier-Stokes (RANS) equations are presented in conservative form.

Definition 3.1. *(Compressible RANS equations) The nonlinear system of conservation laws for the mass continuity, momentum balance and energy conservation that describes the mean dynamics of a viscous compressible fluid is fully described by the flux functions $F_{c_{ij}}, F_{v1_{ij}}, F_{v2_{ij}} \in C^1(\Omega, \mathbb{R}^5)$ and the following boundary value problem for adiabatic boundary Γ.*

$$\begin{cases} \nabla \cdot F_c - \nabla \cdot (\mu_d F_{v1} + \mu_h F_{v2}) = 0 & \textit{in } \Omega \\ \quad V = 0 & \textit{on } \Gamma \\ \partial_\nu T = 0 & \textit{on } \Gamma \\ W^+ = W_\infty & \textit{on } \Gamma_\infty \\ \textit{Turbulence model for } \mu_t \textit{ and B.C.} \end{cases} \tag{$\dagger$}$$

where $\mu_d = \mu + \mu_t$ with μ (μ_t) the dynamic (turbulent) viscosity, $\mu_h = \mu/Pr + \mu_t/Pr_t$ with Pr (Pr_t) the classical (turbulent) Prandtl coefficient. The convective fluxes $F_{c_{ij}}$ and the viscous fluxes $F_{v1_{ij}}, F_{v2_{ij}}$ are given by

$$F_c = \begin{Bmatrix} \rho u_i \\ \rho u_i u_1 + p\delta_{i1} \\ \rho u_i u_2 + p\delta_{i2} \\ \rho u_i u_3 + p\delta_{i3} \\ \rho u_i H \end{Bmatrix} \qquad F_{v1} = \begin{Bmatrix} \cdot \\ \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ u_j \tau_{ij} \end{Bmatrix} \qquad F_{v2} = \begin{Bmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ c_p \partial_i T \end{Bmatrix} \qquad i = 1, 3$$

where $V = (u_1, u_2, u_3)$, $\tau_{ij} = \partial_j u_i + \partial_i u_j - \frac{2}{3}\delta_{ij}\nabla \cdot V$ the stress tensor, H the enthalpy, T the temperature, $c_p = R\gamma/(\gamma - 1)$ the heat capacity at constant pressure and R is the gas constant. The dynamic viscosity μ is given by Sutherland's Law as a function of temperature and $Pr \simeq 0.71$ for air. The turbulent Prandtl number Pr_t can be taken $\simeq 0.91$ owing to Reynold's *analogy. Otherwise an additional model is required when Reynold's analogy is violated. Finally, an appropriate turbulence model is required for closure because of the assumption that turbulence manifests itself as an increase in viscosity ($\mu_d = \mu + \mu_t$).*

The linearized RANS equations are obtained in the same fashion as the Euler equations but with some additional effort. The convective flux fuction was already linearized and given by the formula (20). The linearization of the viscous flux function can be found in [7]. There are two classical ways to proceed on this: i) the turbulent viscosity μ_t is considered constant in the linearization (frozen-viscosity assumption), ii) the turbulent viscosity is nonconstant and one should proceed with also linearizing the turbulence model.

3.2 Augmenting the pressure functional

The pressure functional (26) which served as the cost function for the Euler-based shape optimization is augmented to account for the viscous forces on drag. The new functional reads

$$\mathscr{I}(p, \tau_{ij}, \nu) = \int_\Gamma g(p, \tau_{ij}, \nu) = \int_\Gamma \big(p\nu_i - (\mu + \mu_t)\tau_{ij}\nu_j\big)\, d_i \qquad i, j = 1, \ldots, 3 \tag{39}$$

where d_i is a nondimensional vector denoting the direction where the force is projected and takes the direction of the freestream velocity when drag minimization is considered.

The same shape derivative formula that was used to obtain (29) can be used and new shape derivatives associated with the momentum stress tensor will appear leading to a modified boundary condition for the adjoint RANS boundary value problem.

3.3 Adjoint Navier-Stokes equations

The adjoint RANS boundary value problem shares the same form as its Euler analogue, given by (38), but with the addition of the viscous Jacobian tensors. The same farfield boundary condition on Γ_∞ can be used but the boundary condition on the airfoil boundary Γ must be reevaluated according the the procedure described in section 2.4 since the cost function $\mathscr{I}$ contains new terms depending on the stress tensor τ_{ij}.

Since the Navier-Stokes shape optimization method is only an extension of the present work, the complete derivation of the method for the RANS equations is left for future work.

4 Numerical treatment for the primal and adjoint Euler equations

To conclude this work, the numerical treatment of the primal and the adjoint Euler equations is discussed and numerical solutions are provided for three distinct flow regimes: subsonic, transonic and supersonic.

4.1 Numerical scheme

The Euler system (18) and its adjoint state (38) can be numerically solved using a finite volume method. Finite volume and finite element methods occur naturally for linear and nonlinear systems of conservation laws and are thus usually preferred to the finite difference method. In this section the numerical schemes are presented in brevity for the one-dimensional case, but they immediately extend to $\mathbb{R}^2$ and $\mathbb{R}^3$.

In the context of the finite volume method, the domain $\Omega \subset \mathbb{R}$ is partitioned in *grid cells* or *finite volumes* $\{\mathcal{C}_i\}$, with $\bigcup_i \mathcal{C}_i = \Omega$, $i \in \mathbb{N}$. A grid cell is defined as a subinterval of Ω such that

$$\mathcal{C}_i = (x_{i-1/2}, x_{i+1/2}) \subset \Omega$$

with volume $\Delta x = |x_{i-1/2} - x_{i+1/2}|$. Subsequently, for $u(x,t)$ defined in $\Omega \times \mathbb{R}_+$ we have the local approximation

$$U_i^n \simeq \fint_{\mathcal{C}_i} u(x, t_n)\,\mathrm{d}x = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} u(x, t_n)\,\mathrm{d}x \tag{40}$$

at the timestep $n \in \mathbb{N}$. Also, the value U_i^n is usually referred to as *cell-center value* while values with indeces $(\cdot)_{(\cdot)\pm 1/2}$ are named *face-centered* values. Considering the general form of a scalar conservation law in $\Omega \times \mathbb{R}_+$

$$\partial_t u + \partial_x F(u) = 0$$

with flux function F as in (16) and u the vector of conservative variables (15), we can work out to find the following explicit approximation

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\big(F_{i+1/2}^n - F_{i-1/2}^n\big) \tag{41}$$

for $\Delta t = t^{n+1} - t^n$ and with $F_{i+1/2}^n$ denoting the approximation of the flux on the face $i + 1/2$, given by

$$F_{i+1/2}^n \simeq \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} F\big(u(x_{i+1/2}, t)\big)\,\mathrm{d}t \tag{42}$$

We would like to approximate the flux $F_{i+1/2}^n$in terms of the values of U^n. To this end, knowing that the Euler system and its adjoint state exhibit hyperbolic behavior and thus finite propagation speed, it sounds reasonable to approximate the flux by a formula of the form

$$F_{i-1/2}^n = \mathcal{F}(U_{i-1}^n, U_i^n) \qquad , \qquad F_{i+1/2}^n = \mathcal{F}(U_i^n, U_{i+1}^n)$$

where $\mathcal{F}(\cdot)$ is the *numerical flux function*. Consequently, the numerical scheme (41) takes the form

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\big(\mathcal{F}(U_{i-1}^n, U_i^n) - \mathcal{F}(U_i^n, U_{i+1}^n)\big) \tag{43}$$

which in general describes a three-point stencil explicit discretization that preserves the conservative nature of the original equation. In the present work, the central-difference scheme of Jameson-Schmidt-Turkel (JST) [8] is employed, for which the numerial flux function takes the form

$$F_{i\pm 1/2}^n = \mathcal{F}(\mathcal{S}_5) = F(U_{i\pm 1/2}^n) - \mathcal{D}_{i\pm 1/2} \tag{44}$$

with $U_{i-1/2}^n = \frac{1}{2}\big(U_{i-1}^n + U_i^n\big)$ and $\mathcal{S}_5 = \big(U_{i-2}^n, U_{i-1}^n, U_i^n, U_{i+1}^n, U_{i+2}^n\big)$ denoting the five-point stencil of the scheme. The term $\mathcal{D}_{i-1/2}$ is the artificial dissipative flux, used to correct for odd-even decoupling and stabilize the central scheme, which is given by

$$\mathcal{D}_{i-1/2} = \epsilon_{i-1/2}^{(2)}\,\Delta u_{i-1/2} + \epsilon_{i-1/2}^{(4)}\big(\Delta u_{i-3/2} - 2\Delta u_{i-1/2} + \Delta u_{i+1/2}\big) \tag{45}$$

with $\Delta u_{i-1/2} = u_i - u_{i-1}$ and dissipation coefficients

$$\epsilon^{(2)}_{i-1/2} = \kappa_2 s_{i-1/2}\rho_{i-1/2} \qquad , \qquad \epsilon^{(4)}_{i-1/2} = \max(0, \kappa_4\rho_{i-1/2} - \kappa_4'\epsilon^{(2)}_{i-1/2}) \tag{46}$$

where

$$s_{i-1/2} = \max(s_i, s_{i-1}) \qquad , \qquad s_i = \left|\frac{p_{i+1} - p_j + p_{i-1}}{p_{i+1} + p_i + p_{i-1}}\right| \tag{47}$$

is a *pressure sensor* that activates in the presence of shock-waves to increase the first order artificial dissipation term so that oscillations are avoided. Also,

$$\rho_{i-1/2} = \max(\rho_i, \rho_{i-1}) \qquad , \qquad \rho_i = \max|\lambda_\ell| \quad , \quad \ell = 1, \ldots, 3 \tag{48}$$

with ρ_i being the spectral radius and λ_ℓ the eigenvalues of the convective Jacobian (20), which in one dimension is given by truncating the matrix A^c_{ijk} to A^c_{1jk} for $j, k = 1, 2, 5$. Finally, the constant coefficients $\kappa_2, \kappa_4, \kappa_4' \in \mathbb{R}_+$ depend on the flow regime. Some typical values for transonic flows are

$$\kappa_2 = \frac{1}{2} \quad , \quad \kappa_4 = \frac{1}{64} \quad , \quad \kappa_4' = 1 \qquad\qquad \text{(Euler equations)} \tag{49}$$

The JST scheme, described by the numerical flux function (44), was originally devised for the Euler equations and is a second-order accurate scheme. Since the adjoint Euler equations share many similar properties with the primal Euler equations, the same scheme is used for the adjoint state for both simplicity and consistency. Previous studies have shown that the adjoint variables are continuous along the shock-waves of the flow solution [9] while discontinuities may arise near the wall (airfoil) boundaries for transonic and supersonic flows. For this reason, in the present study, first order dissipation terms have been dropped from the scheme in the case of the adjoint Euler equations. This is also reflected on the following choice of the dissipation coefficients

$$\kappa_2 = 0 \quad , \quad \kappa_4 = \frac{1}{128} \quad , \quad \kappa_4' = 1 \qquad\qquad \text{(Adjoint Euler equations)} \tag{50}$$

For the numerical solution, the unsteady form of the equations is actually solved by marching in time in order to reach a steady-state (if it exists). To accelerate the convergence to a steady-state, a local time-step is used along with implicit residual smoothing and multigrid. Residual smoothing increases the support of the discretization and allows for greater times-steps (increased CFL numbers) while multigrid is effective in making errors of different frequency scales vanish faster. The system is finally solved using a five-stage Runge-Kutta method. Additional numerical details are omitted from this paper.

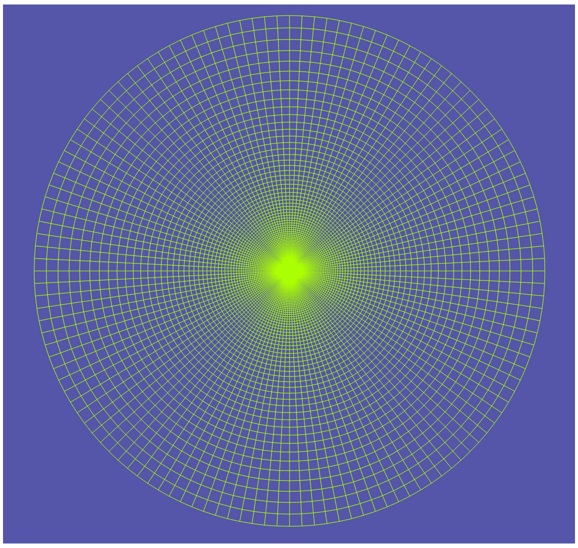
4.2 Numerical solution

This paper concludes with the numerical solution of the primal (18) and the adjoint (38) Euler boundary value problem. In figure 1 the discretization (mesh) of the solution domain Ω is depicted for a NACA0012 airfoil (boundary Γ). The farfield boundary Γ_∞ extends at a distance of ~ 150 chords[3] and the mesh contains ~ 260 million cells. The numerical solution for subsonic, transonic and supersonic flow is presented in figure 2 for the same angle of attack

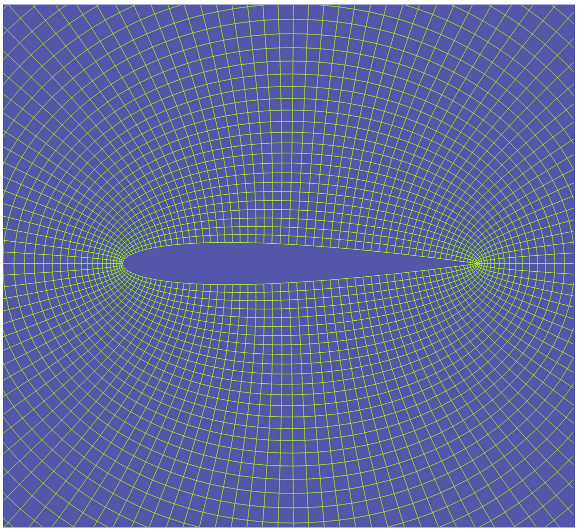
[3]Chord refers to the airfoil characteristic length, i.e. the distance between the leading and the trailing edge.

of $1.25°$ for all the cases.

It is worth mentioning that outgoing characteristics of the primal equations correspond to incoming characteristics for the adjoint state and vice-versa (characteristics change sign). In other words, information propagates backwards in time. For the subsonic case, the adjoint solution closely resembles the primal solution. More interesting are the adjoint solutions for the transonic and supersonic cases, where shocks appear in the primal solutions. For the transonic case, the flow accelerates over the airfoil where it becomes supersonic until it reaches adverse pressure gradients that decelerate it to the point that a shock-wave appears (figure 2c). Consequently, a sonic bubble formes over the upper (suction) surface. The appearance of the 'lambda shape' in the corresponding adjoint solution (figure 2d) can be interpreted in the following way: variations in density along the characteristics that impinge on the sonic point and the shock-foot will produce large changes to the surface pressure distribution. In general, the adjoint solution shows quantitavely and quantitative how the surface pressure will change depending on density field perturbations. In similar fashion, for the supersonic case with bow-shock (figures 2e and 2f), the flow is particularly sensitive near the leading edge of the airfoil which dictates the formation of the bow-shock. Also, the change of sign of the characteristics is evident.



(a) Discretized domain Ω



(b) Close-up of airfoil (boundary $\Gamma \subset \partial\Omega$)

Figure 1: Discretization of the domain Ω.

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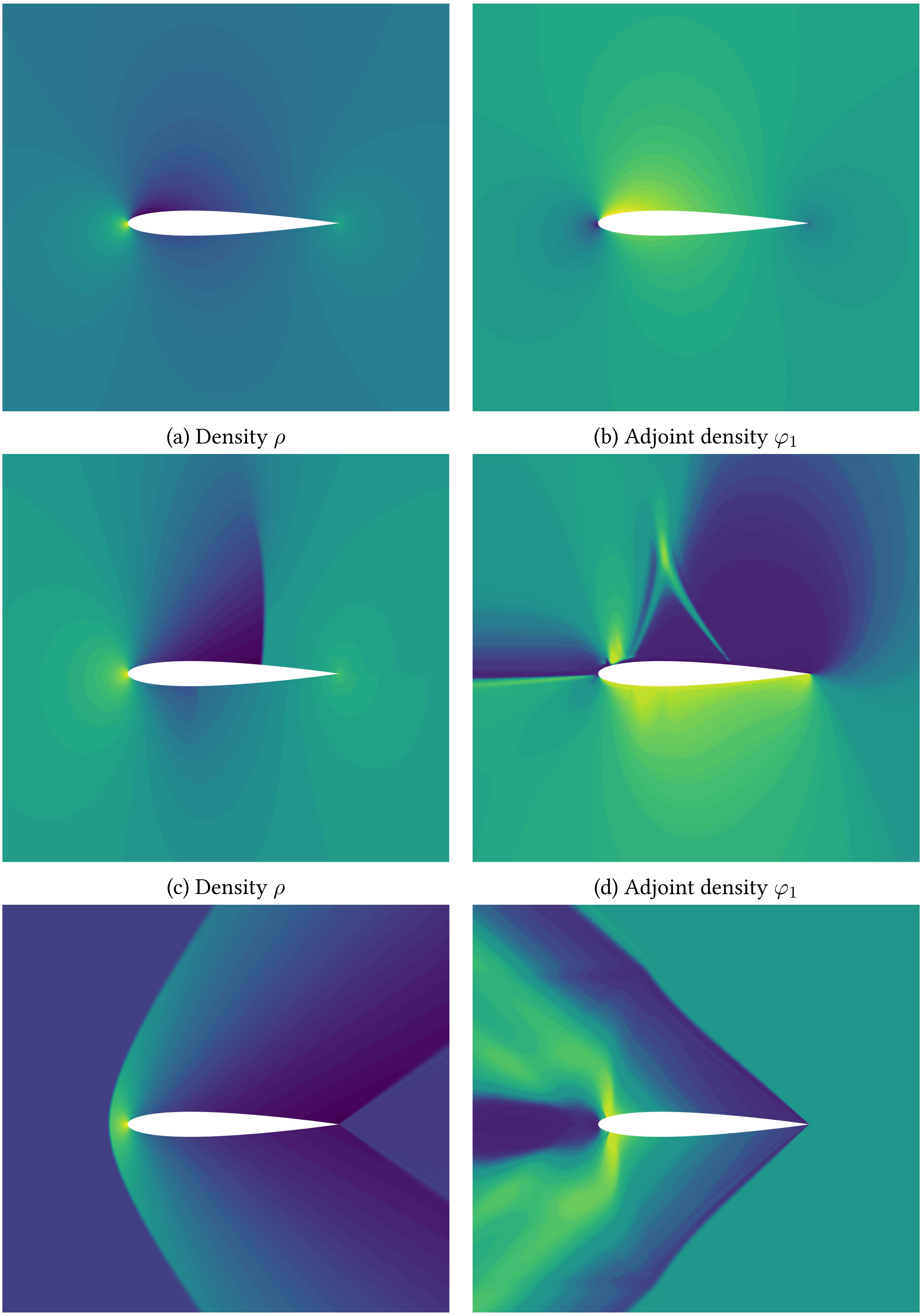

(a) Density ρ (b) Adjoint density φ_1

(c) Density ρ (d) Adjoint density φ_1

(e) Density ρ (f) Adjoint density φ_1

Figure 2: Numerical solution for the NACA0012 airfoil at $M_\infty = 0.5$ (subsonic) (a,b), $M_\infty = 0.8$ (transonic) (c,d) and $M_\infty = 1.5$ (supersonic) (e,f) with angle of attack $\alpha = 1.25°$.