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A Continuous Adjoint Approach to Shape Optimization for Navier Stokes Flow

Christian Brandenburg, Florian Lindemann, Michael Ulbrich and Stefan Ulbrich

Abstract. In this paper we present an approach to shape optimization which is based on continuous adjoint computations. If the exact discrete adjoint equation is used, the resulting formula yields the exact discrete reduced gradient. We first introduce the adjoint-based shape derivative computation in a Banach space setting. This method is then applied to the instationary Navier-Stokes equations. Finally, we give some numerical results.

Mathematics Subject Classification (2000). Primary 76D55; Secondary 49K20.

Keywords. shape optimization, Navier-Stokes equations, PDE-constrained optimization.

1. Introduction

In this paper, we consider the optimization of the shape of a body that is exposed to incompressible instationary Navier-Stokes flow in a channel. The developed techniques are quite general and can, without conceptual difficulties, be used to address a wide class of shape optimization problems with Navier-Stokes flow. The goal is to find the optimal shape of the body B , which is exposed to instationary incompressible fluid, with respect to some quantity of interest, e.g. drag, under constraints on the shape of B .

In a general setting, the shape optimization problem can be stated in the following way: Minimize an objective functional \bar{J} , depending on a domain Ω and a state $\tilde{y} = \tilde{y}(\Omega) \in Y(\Omega)$. The domain Ω is contained in a set of admissible domains \mathcal{O}_{ad} . Furthermore, \tilde{y} and Ω are coupled by the *state equation* $\bar{E}(\tilde{y}, \Omega) = 0$. Thus,

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the abstract shape optimization problem reads

$$\begin{aligned} \min \quad & \bar{J}(\tilde{y}, \Omega) \\ \text{s.t.} \quad & \bar{E}(\tilde{y}, \Omega) = 0, \quad \Omega \in \mathcal{O}_{\text{ad}}. \end{aligned}$$

The constraint $\bar{E}(\tilde{y}, \Omega) = 0$ is a partial differential equation defined on Ω , which in our case is given by the instationary incompressible Navier-Stokes equations.

Shape optimization is an important and active field of research with many engineering applications, especially in the areas of fluid dynamics and aerodynamics. Detailed accounts of the theory and applications of shape optimization can be found in, e.g., [1, 2, 3, 9, 15, 18]. We use the approach of transformation to a reference domain, as originally introduced by Murat and Simon [17], see also [8]. The domain is then fixed and the design is described by a transformation from a fixed domain to the domain Ω corresponding to the current design. This makes optimal control techniques readily applicable. Furthermore, as observed by Guillaume and Masmoudi [8] in the context of linear elliptic equations, discretization and optimization can be made commutable. This means that, if certain guidelines are followed, then the discrete analogue of the continuous adjoint representation of the derivative of the reduced objective function is the exact derivative of the discrete reduced objective function. This allows to circumvent the tedious differentiation of finite element code with respect to the position of the vertices of the mesh. We apply this approach to shape optimization problems governed by the instationary Navier-Stokes equations. On one hand we characterize the appropriate function space for domain transformation in this framework. On the other hand, we focus on the practical implementation of shape optimization methods based on shape derivatives. We show that existing solvers for the state and adjoint equation on the current computational domain Ω_k can be used to compute exact shape gradients conveniently for the continuous as well as for the discretized problem. Hence, although shape derivatives are defined through transformation to a reference domain, standard solvers on the transformed domain can be used for its computation.

The outline of this paper is as follows: In section 2, we will present our approach for the derivative computation in shape optimization in a general setting. These general results will be applied to the instationary incompressible Navier-Stokes equations in section 3. In section 4 we present the discretization and stabilization techniques we use to solve the Navier-Stokes equations numerically, which are based on the $cG(1)dG(0)$ variant of the G^2 -finite-element discretization by Eriksson, Estep, Hansbo, Johnson and others [4, 5]. Moreover, we explain how we apply the adjoint calculus to obtain conveniently exact shape gradients on the discrete level. We will then present numerical results obtained for a model problem in section 5, where we also briefly discuss the choice of shape transformations and parameterizations. Finally, in section 6, we will give conclusions and an outlook to future work.

2. The shape optimization problem

In this section, we present the framework that we will use for shape derivative computation in a functional analytical setting. We first transform the general shape optimization problem, which is defined on varying domains, into a problem that is defined on a fixed reference domain Ω_{ref} . Then, after introducing the reduced optimization problem on a space T of transformations of Ω_{ref} , we state optimality conditions and an adjoint based representation for the reduced gradient of the objective function.

2.1. Problem formulation on a reference domain

We consider the abstract shape optimization problem given by

$$\begin{aligned} \min \quad & \bar{J}(\tilde{y}, \Omega) \\ \text{s.t.} \quad & \bar{E}(\tilde{y}, \Omega) = 0, \quad \Omega \in \mathcal{O}_{\text{ad}}. \end{aligned}$$

Here, \mathcal{O}_{ad} denotes the set of admissible domains $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, \bar{J} is a real valued objective function defined on a Banach space $Y(\Omega)$ of functions defined on $\Omega \subset \mathbb{R}^d$,

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

and \bar{E} is an operator between function spaces $Y(\Omega)$ and $Z(\Omega)$ defined over Ω ,

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

with $\bar{E}(\tilde{y}, \Omega) \in Z(\Omega)$ for all $\tilde{y} \in Y(\Omega)$ and all $\Omega \in \mathcal{O}_{\text{ad}}$.

We now transform the shape optimization problem into a more convenient form. To this end, we consider a reference domain $\Omega_{\text{ref}} \in \mathcal{O}_{\text{ad}}$ and interpret admissible domains $\Omega \in \mathcal{O}_{\text{ad}}$ as images of Ω_{ref} under suitable transformations. This is done by introducing a Banach space $T(\Omega_{\text{ref}}) \subset \{\tau : \Omega_{\text{ref}} \rightarrow \mathbb{R}^d\}$ of bicontinuous transformations of Ω_{ref} . We select a suitable subset $T_{\text{ad}} \subset T(\Omega_{\text{ref}})$ of admissible transformations. The set \mathcal{O}_{ad} of admissible domains is then

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

We assume that

$$\left. \begin{aligned} Y(\Omega_{\text{ref}}) &= \{\tilde{y} \circ \tau : \tilde{y} \in Y(\tau(\Omega_{\text{ref}}))\} \\ \tilde{y} \in Y(\tau(\Omega_{\text{ref}})) &\mapsto y := \tilde{y} \circ \tau \in Y(\Omega_{\text{ref}}) \text{ is a homeomorphism} \end{aligned} \right\} \quad \forall \tau \in T_{\text{ad}}. \quad (\text{A})$$

Then, we can define the following equivalent optimization problem, which is entirely defined on the reference domain:

$$\begin{aligned} \min \quad & J(y, \tau) \\ \text{s.t.} \quad & E(y, \tau) = 0, \quad \tau \in T_{\text{ad}}. \end{aligned} \quad (2.1)$$

Here, the operator $E : Y(\Omega_{\text{ref}}) \times T(\Omega_{\text{ref}}) \rightarrow Z(\Omega_{\text{ref}})$ is defined such that for all $\tau \in T_{\text{ad}}$ and $\tilde{y} \in Y(\tau(\Omega_{\text{ref}}))$ it holds that

$$E(y, \tau) = 0 \iff \bar{E}(\tilde{y}, \tau(\Omega_{\text{ref}})) = 0,$$

where $y = \tilde{y} \circ \tau$. The objective function J is defined in the same fashion.

In the following, we will consequently denote by \tilde{y} the functions on the physical domain $\tau(\Omega_{\text{ref}})$ and by y the corresponding function on the reference domain Ω_{ref} , where

$$y = \tilde{y} \circ \tau.$$

Remark 2.1. Let $\Omega' \supset \bar{\Omega}_{\text{ref}}$ be open and bounded with Lipschitz boundary. If, which is the typical case for elliptic partial differential equations, $Y(\Omega) = H_0^1(\tau(\Omega_{\text{ref}}))$, $Z(\Omega) = H^{-1}(\tau(\Omega_{\text{ref}}))$ with $\tau \in T_{\text{ad}}$, then (A) holds if we choose $T(\Omega_{\text{ref}}) = W^{1,\infty}(\Omega')^d$ and if we require that all $\tau \in T_{\text{ad}} \subset W^{1,\infty}(\Omega')^d$ are such that $\tau : \bar{\Omega}_{\text{ref}} \rightarrow \tau(\bar{\Omega}_{\text{ref}})$ is a bi-Lipschitzian mapping.

For other spaces $Y(\Omega)$ and $Z(\Omega)$, it can be necessary to impose further requirements on T_{ad} .

If \bar{E} is given in variational form then the operator E can be obtained by using the transformation rule for integrals. This will be carried out for the instationary Navier-Stokes equations in section 3.

2.2. Reduced problem and optimality conditions

In the following, we will consider the optimization problem on the reference domain (2.1), which has the form

$$\begin{aligned} \min \quad & J(y, \tau) \\ \text{s.t.} \quad & E(y, \tau) = 0, \quad \tau \in T_{\text{ad}}. \end{aligned} \tag{2.1}$$

We denote by E_y and E_τ the partial derivatives of E with respect to y and τ .

In order to derive first order optimality conditions, we make the following assumptions:

- (A1) $T_{\text{ad}} \subset T(\Omega_{\text{ref}})$ is nonempty, closed, convex and assumption (A) holds.
- (A2) $J : Y(\Omega_{\text{ref}}) \times T(\Omega_{\text{ref}}) \rightarrow \mathbb{R}$ and $E : Y(\Omega_{\text{ref}}) \times T(\Omega_{\text{ref}}) \rightarrow Z(\Omega_{\text{ref}})$ are continuously Fréchet-differentiable.
- (A3) There exists an open neighborhood $T'_{\text{ad}} \subset T(\Omega_{\text{ref}})$ of T_{ad} and a unique solution operator $S : T'_{\text{ad}} \rightarrow Y(\Omega_{\text{ref}})$, assigning to each $\tau \in T'_{\text{ad}}$ a unique $y(\tau) \in Y(\Omega_{\text{ref}})$, such that $E(y(\tau), \tau) = 0$.
- (A4) The derivative $E_y(y(\tau), \tau) \in \mathcal{L}(Y(\Omega_{\text{ref}}), Z(\Omega_{\text{ref}}))$ is continuously invertible for all $\tau \in T'_{\text{ad}}$.

Under these assumptions $y(\tau)$ is continuously differentiable on $\tau \in T'_{\text{ad}} \supset T_{\text{ad}}$ by the implicit function theorem. Thus, it is reasonable to define the following reduced problem on the space of transformations $T(\Omega_{\text{ref}})$:

$$\begin{aligned} \min \quad & j(\tau) := J(y(\tau), \tau) \\ \text{s.t.} \quad & \tau \in T_{\text{ad}} \end{aligned},$$

where $y(\tau)$ is given as the solution of $E(y(\tau), \tau) = 0$.

In the following we will use the abbreviations

$$T_{\text{ref}} := T(\Omega_{\text{ref}}), \quad Y_{\text{ref}} := Y(\Omega_{\text{ref}}), \quad Z_{\text{ref}} := Z(\Omega_{\text{ref}}).$$

In order to derive optimality conditions and to compute the reduced gradient $j'(\tau)$, we introduce the Lagrangian function $\mathcal{L} : Y_{\text{ref}} \times T_{\text{ref}} \times Z_{\text{ref}}^* \rightarrow \mathbb{R}$,

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

with Lagrange multiplier $\lambda \in Z_{\text{ref}}^*$.

Under assumptions (A1)–(A4) a local solution $(y, \tau) \in Y_{\text{ref}} \times T_{\text{ad}}$ of (2.1) satisfies with an appropriate adjoint state $\lambda \in Z_{\text{ref}}^*$ the following first order necessary optimality conditions.

$$\mathcal{L}_\lambda(y, \tau, \lambda) = E(y, \tau) = 0 \quad (\text{state equation})$$

$$\mathcal{L}_y(y, \tau, \lambda) = J_y(y, \tau) + E_y^*(y, \tau)\lambda = 0 \quad (\text{adjoint equation})$$

$$\langle \mathcal{L}_\tau(y, \tau, \lambda), \tilde{\tau} - \tau \rangle_{T_{\text{ref}}^*, T_{\text{ref}}} = \langle J_\tau(y, \tau) + E_\tau^*(y, \tau)\lambda, \tilde{\tau} - \tau \rangle_{T_{\text{ref}}^*, T_{\text{ref}}} \geq 0 \quad \forall \tilde{\tau} \in T_{\text{ad}}.$$

2.2.1. Adjoint-based shape derivative computation on the reference domain. By using the adjoint equation the reduced gradient $j'(\tau)$ can be determined as follows:

1. For given τ , find $y(\tau) \in Y_{\text{ref}}$ by solving the state equation

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

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

$$\langle \lambda, E_y(y, \tau)\varphi \rangle_{Z_{\text{ref}}^*, Z_{\text{ref}}} = -\langle J_y(y, \tau), \varphi \rangle_{Y_{\text{ref}}^*, Y_{\text{ref}}} \quad \forall \varphi \in Y_{\text{ref}} \quad (2.2)$$

3. The reduced gradient with respect to τ is now given by

$$\langle j'(\tau), \cdot \rangle_{T_{\text{ref}}^*, T_{\text{ref}}} = \langle \lambda, E_\tau(y, \tau) \cdot \rangle_{Z_{\text{ref}}^*, Z_{\text{ref}}} + \langle J_\tau(y, \tau), \cdot \rangle_{T_{\text{ref}}^*, T_{\text{ref}}}. \quad (2.3)$$

2.2.2. Adjoint-based shape derivative computation on the physical domain. For the application of optimization algorithms it is convenient to solve, for a given iterate $\tau_k \in T(\Omega_{\text{ref}})$, an equivalent representation of the optimization problem on the domain $\Omega_k := \tau_k(\Omega_{\text{ref}})$. To this end, we introduce operators \tilde{E} , \tilde{J} and \tilde{j} , which differ from E , J and j only in that the function spaces Y , Z and T are defined on Ω_k instead of Ω_{ref} , i.e.,

$$\tilde{E}(\tilde{y}, \tilde{\tau}) = 0 \iff E(y, \tilde{\tau} \circ \tau_k) = 0, \text{ where } y = \tilde{y} \circ (\tilde{\tau} \circ \tau_k).$$

Then we have the relation

$$\tilde{j}(\tilde{\tau}) = j(\tilde{\tau} \circ \tau_k) = j(\tau) \quad \text{and therefore} \quad \tilde{\tau} \circ \tau_k = \tau, \text{ i.e., } \tilde{\tau} = \tau \circ \tau_k^{-1}.$$

We are thus led to the following procedure for computing the reduced gradient:

1. For $\text{id} : \Omega_k \rightarrow \Omega_k$, $\text{id}(\tau_k(x)) = \tau_k(x)$, $x \in \Omega_{\text{ref}}$, find $\tilde{y}_k \in Y(\Omega_k)$ by solving the state equation

$$\langle \tilde{E}(\tilde{y}_k, \text{id}), \varphi \rangle_{Z(\Omega_k), Z(\Omega_k)^*} = 0 \quad \forall \varphi \in Z(\Omega_k)^*,$$

where $\tilde{y}_k(\tau_k(x)) = y_k(x)$, $x \in \Omega_{\text{ref}}$. This corresponds to solving the standard state equation in variational form on the domain Ω_k , which in the abstract setting was denoted by $\tilde{E}(\tilde{y}_k, \Omega_k) = 0$.

2. Find the corresponding Lagrange multiplier $\tilde{\lambda}_k \in Z(\Omega_k)^*$ by solving the adjoint equation

$$\langle \tilde{\lambda}_k, \tilde{E}_{\tilde{y}}(\tilde{y}_k, \text{id})\varphi \rangle_{Z(\Omega_k)^*, Z(\Omega_k)} = -\langle \tilde{J}_{\tilde{y}}(\tilde{y}_k, \text{id}), \varphi \rangle_{Y(\Omega_k)^*, Y(\Omega_k)} \quad \forall \varphi \in Y(\Omega_k),$$

where $\tilde{\lambda}_k(\tau_k(x)) = \lambda_k(x)$, $x \in \Omega_{\text{ref}}$. This corresponds to the solution of the standard adjoint equation on Ω_k .

3. The reduced gradient applied to $V \in T(\Omega_{\text{ref}})$ is now given by

$$\begin{aligned} \langle j'(\tau_k), V \rangle_{T_{\text{ref}}^*, T_{\text{ref}}} &= \langle \tilde{j}'(\text{id}), \tilde{V} \rangle_{T(\Omega_k)^*, T(\Omega_k)} \\ &= \langle \tilde{\lambda}_k, \tilde{E}_{\tilde{\tau}}(\tilde{y}_k, \text{id})\tilde{V} \rangle_{Z(\Omega_k)^*, Z(\Omega_k)} + \langle \tilde{J}_{\tilde{\tau}}(\tilde{y}_k, \text{id}), \tilde{V} \rangle_{T(\Omega_k)^*, T(\Omega_k)} \end{aligned}$$

for $\tilde{V} \in T(\Omega_k)$, $\tilde{V} \circ \tau_k = V$, i.e., $\tilde{V} = V \circ \tau_k^{-1}$. If we define the linear operator

$$B_k \in \mathcal{L}(T(\Omega_{\text{ref}}), T(\Omega_k)), \quad B_k V = V \circ \tau_k^{-1} \quad (2.4)$$

then we have by our previous calculation

$$j'(\tau_k) = B_k^* \tilde{j}'(\text{id}) = B_k^* (\tilde{E}_{\tilde{\tau}}(\tilde{y}_k, \text{id})^* \tilde{\lambda}_k + \tilde{J}_{\tilde{\tau}}(\tilde{y}_k, \text{id})).$$

This procedure yields the exact gradient of the reduced objective function and has the advantage that we are able to use standard PDE-solvers for the state equation and adjoint equation on the domain Ω_k , since we evaluate at $\tilde{\tau} = \text{id}$.

2.3. Derivatives with respect to shape parameters

In practice, the shape of a domain is defined by design parameters $u \in U$ with a finite or infinite dimensional design space U . Thus, we have a map $\tau : U \rightarrow T(\Omega_{\text{ref}})$, $u \mapsto \tau(u)$ and a reference control $u_0 \in U$ with $\tau(u_0) = \text{id}$. Derivatives of the reduced objective function $j(\tau(u))$ at u_k are obtained using the chain rule. With $\tau_k = \tau(u_k)$ and B_k in (2.4) we have

$$\begin{aligned} \left\langle \frac{d}{du} j(\tau(u_k)), \cdot \right\rangle_{U^*, U} &= \langle j'(\tau(u_k)), \tau_u(u_k) \cdot \rangle_{T(\Omega_{\text{ref}})^*, T(\Omega_{\text{ref}})} \\ &= \langle \tilde{j}'(\text{id}), (\tau_u(u_k) \cdot) \circ \tau(u_k)^{-1} \rangle_{T(\Omega_k)^*, T(\Omega_k)} \\ &= \langle \tilde{j}'(\text{id}), B_k \tau_u(u_k) \cdot \rangle_{T(\Omega_k)^*, T(\Omega_k)} = \langle \tau_u(u_k)^* B_k^* \tilde{j}'(\text{id}), \cdot \rangle_{U^*, U}. \end{aligned}$$

Overall, this approach provides a flexible framework that can be used for arbitrary types of transformations (e.g. boundary displacements, free form deformation). The idea of using transformations to describe varying domains can be found, e.g., in Murat and Simon [17] and Guillaume and Masmoudi [8].

3. Shape optimization for the Navier-Stokes equations

We now apply this approach to shape optimization problems governed by the stationary Navier-Stokes equations for a viscous, incompressible fluid on a bounded domain $\Omega = \tau(\Omega_{\text{ref}})$ with Lipschitz boundary. According to our convention, we will denote all quantities on the physical domain by $\tilde{\cdot}$.

For $\Omega \subset \mathbb{R}^d$ with spatial dimension $d = 2$ or 3 , let $\Gamma_D \subset \partial\Omega$ be a nonempty Dirichlet boundary and $\Gamma_N = \partial\Omega \setminus \Gamma_D$. We consider the problem

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

where $\tilde{\mathbf{v}} : \Omega \times I \rightarrow \mathbb{R}^d$ denotes the velocity $\tilde{\mathbf{v}}(x, t)$ and $\tilde{p} : \Omega \times I \rightarrow \mathbb{R}$ the pressure $\tilde{p}(x, t)$ of the fluid at a point x at time t , $\tilde{\mathbf{n}} : \partial\Omega \rightarrow \mathbb{R}^d$ is the outer unit normal. Here $I = (0, T)$, $T > 0$ is the time interval and $\nu > 0$ is the kinematic viscosity; if the equations are written in dimensionless form, ν can be interpreted as $1/Re$ where Re is the Reynolds number.

We introduce the spaces

$$\begin{aligned} H_D^1(\Omega) &:= \{\tilde{\mathbf{v}} \in H^1(\Omega)^d : \tilde{\mathbf{v}}|_{\Gamma_D} = 0\}, \quad V := \{\tilde{\mathbf{v}} \in H_D^1(\Omega)^d : \operatorname{div} \tilde{\mathbf{v}} = 0\}, \\ H &:= \operatorname{cl}_{L^2}(V), \quad L_0^2(\Omega) := \{\tilde{p} \in L^2(\Omega) : \int_{\Omega} \tilde{p} = 0\}, \end{aligned}$$

the corresponding Gelfand triple $V \hookrightarrow H \hookrightarrow V^*$, and define

$$W_{2,q}(I; V) := \{\tilde{\mathbf{v}} \in L^2(I; V) : \tilde{\mathbf{v}}_t \in L^q(I; V^*)\}.$$

Now let

$$\tilde{\mathbf{v}}_D \in H^1(\Omega), \quad \operatorname{div} \tilde{\mathbf{v}}_D = 0, \quad \tilde{\mathbf{f}} \in L^2(I; V^*), \quad \tilde{\mathbf{v}}_0 \in H.$$

Under these assumptions the following results are known.

- If $\Gamma_D = \partial\Omega$, i.e. $\Gamma_N = \emptyset$, then for $d = 2$ there exists a unique weak solution $(\tilde{\mathbf{v}}, \tilde{p})$ with $\tilde{\mathbf{v}} - \tilde{\mathbf{v}}_D \in W_{2,2}(I; V)$ and $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$. For $d = 3$ there exists a weak solution $(\tilde{\mathbf{v}}, \tilde{p})$ with $\tilde{\mathbf{v}} - \tilde{\mathbf{v}}_D \in W_{2,4/3}(I; V) \cap L^\infty(I; H)$ and $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$, which is not necessarily unique. For the case $\tilde{\mathbf{v}}_D = 0$ the proofs can be found for example in [19, Ch. III]. These proofs can be extended to $\tilde{\mathbf{v}}_D \neq 0$ under the above assumptions on $\tilde{\mathbf{v}}_D$.
- If $\Gamma_N \neq \emptyset$ and Γ_D satisfies some geometric properties (for example, all $x \in \Omega$ can be connected in all coordinate directions by a line segment in Ω to a point in Γ_D) and if a sequence of Galerkin approximations exists that does not exhibit inflow on Γ_N then the same can be shown as for the Dirichlet case: For $d = 2$ there exists a unique weak solution $(\tilde{\mathbf{v}}, \tilde{p})$ with $\tilde{\mathbf{v}} - \mathbf{v}_D \in W_{2,2}(I; V)$ and $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$. For $d = 3$ there exists a weak solution (\mathbf{v}, \tilde{p}) with $\tilde{\mathbf{v}} - \tilde{\mathbf{v}}_D \in W_{2,4/3}(I; V) \cap L^\infty(I; H)$ and $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$, which is not necessarily unique. In fact, in the case without inflow on Γ_N all additional boundary terms have the correct sign such that the proofs in [19, Ch. III] for the Dirichlet case can be adapted.

In the case of possible inflow an existence and uniqueness result local in time and for small data global in time can be found in [10].

3.1. Weak formulation

In the following we consider the case $d = 2$ and $\Gamma_N = \emptyset$ to have a general global existence and uniqueness result at hand. Moreover, to avoid technicalities in formulating the equations, we consider homogeneous boundary data $\tilde{\mathbf{v}}_D \equiv 0$. Then we have $H_D^1(\Omega) = H_0^1(\Omega)^d$ with the above notations.

The classical weak formulation is now: Find $\tilde{\mathbf{v}} \in W_{2,2}(I; V)$ such that

$$\begin{aligned} \langle \tilde{\mathbf{v}}_t(\cdot, t), \tilde{\mathbf{w}} \rangle_{V^*, V} + \int_{\Omega} \tilde{\mathbf{v}}(x, t)^T \nabla \tilde{\mathbf{v}}(x, t) \tilde{\mathbf{w}}(x) dx + \int_{\Omega} \nu \nabla \tilde{\mathbf{v}}(x, t) : \nabla \tilde{\mathbf{w}}(x) dx \\ = \int_{\Omega} \tilde{\mathbf{f}}(x, t)^T \tilde{\mathbf{w}}(x) dx \quad \forall \tilde{\mathbf{w}} \in V \text{ for a.a. } t \in I \\ \tilde{\mathbf{v}}(\cdot, 0) = \tilde{\mathbf{v}}_0. \end{aligned} \quad (3.1)$$

As mentioned above, for $\tilde{\mathbf{f}} \in L^2(I; V^*)$ and $\tilde{\mathbf{v}}_0 \in H$ there exists a unique weak solution $\tilde{\mathbf{v}} \in W_{2,2}(I; V)$. The pressure $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$, is now uniquely determined, see [19, Ch. III].

The weak formulation (3.1) is equivalent to the following velocity-pressure formulation: Find $\tilde{\mathbf{v}} \in W_{2,2}(I; H_0^1(\Omega)^d)$ and $\tilde{p}(\cdot, t) \in L_0^2(\Omega)$, $t \in I$, such that

$$\begin{aligned} \langle \tilde{\mathbf{v}}_t(\cdot, t), \tilde{\mathbf{w}} \rangle_{H^{-1}, H_0^1} + \int_{\Omega} \tilde{\mathbf{v}}(x, t)^T \nabla \tilde{\mathbf{v}}(x, t) \tilde{\mathbf{w}}(x) dx + \int_{\Omega} \nu \nabla \tilde{\mathbf{v}}(x, t) : \nabla \tilde{\mathbf{w}}(x) dx \\ - \int_{\Omega} \tilde{p}(x, t) \operatorname{div} \tilde{\mathbf{w}}(x) dx = \int_{\Omega} \tilde{\mathbf{f}}(x, t)^T \tilde{\mathbf{w}}(x) dx \quad \forall \tilde{\mathbf{w}} \in H_0^1(\Omega) \text{ for a.a. } t \in I \\ \int_{\Omega} \tilde{q}(x) \operatorname{div} \tilde{\mathbf{v}}(x, t) dx = 0 \quad \forall \tilde{q} \in L_0^2(\Omega) \text{ for a.a. } t \in I \\ \tilde{\mathbf{v}}(\cdot, 0) = \tilde{\mathbf{v}}_0. \end{aligned}$$

To obtain a weak velocity-pressure formulation in space-time, which is convenient for adjoint calculations, we have to ensure that $\tilde{p} \in L^2(I; L_0^2(\Omega))$. To this end we assume that the data $\tilde{\mathbf{f}}$ and $\tilde{\mathbf{v}}_0$ are sufficiently regular, for example, see [19, Ch. III, Thm. 3.5],

$$\tilde{\mathbf{f}}, \tilde{\mathbf{f}}_t \in L^2(I; V^*), \tilde{\mathbf{f}}(\cdot, 0) \in H, \tilde{\mathbf{v}}_0 \in V \cap H^2(\Omega)^d. \quad (3.2)$$

Define the spaces

$$\begin{aligned} Y(\Omega) &:= W(I; H_0^1(\Omega)^d) \times L^2(I; L_0^2(\Omega)), \\ Z(\Omega) &:= L^2(I; H^{-1}(\Omega)^d) \times L^2(I; L_0^2(\Omega)). \end{aligned} \quad (3.3)$$

Then

$$Z^*(\Omega) := L^2(I; H_0^1(\Omega)^d) \times L^2(I; L_0^2(\Omega))$$

and the weak formulation (3.1) is equivalent to: Find $(\tilde{\mathbf{v}}, \tilde{p}) \in Y(\Omega)$, where $\Omega = \tau(\Omega_{\text{ref}})$ such that

$$\begin{aligned}
& \langle (\tilde{\mathbf{w}}, \tilde{q}), \bar{E}((\tilde{\mathbf{v}}, \tilde{p}), \Omega) \rangle_{Z^*(\Omega), Z(\Omega)} = \\
& = \int_{\Omega} \tilde{\mathbf{v}}(x, 0)^T \tilde{\mathbf{w}}(x, 0) \, dx - \int_{\Omega} \tilde{\mathbf{v}}_0^T \tilde{\mathbf{w}}(\cdot, 0) \, dx \\
& + \int_I \int_{\Omega} \tilde{\mathbf{v}}_t^T \tilde{\mathbf{w}} \, dx \, dt + \int_I \int_{\Omega} \nu \nabla \tilde{\mathbf{v}} : \nabla \tilde{\mathbf{w}} \, dx \, dt \\
& + \int_I \int_{\Omega} \tilde{\mathbf{v}}^T \nabla \tilde{\mathbf{w}} \, dx \, dt - \int_I \int_{\Omega} \tilde{p} \operatorname{div} \tilde{\mathbf{w}} \, dx \, dt \\
& - \int_I \int_{\Omega} \tilde{\mathbf{f}}^T \tilde{\mathbf{w}} \, dx \, dt + \int_I \int_{\Omega} \tilde{q} \operatorname{div} \tilde{\mathbf{v}} \, dx \, dt = 0 \quad \forall (\tilde{\mathbf{w}}, \tilde{q}) \in Z^*(\Omega).
\end{aligned} \tag{3.4}$$

This formulation defines now the state equation operator

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

3.2. Transformation to the reference domain

In the following we assume that

- (T) Ω_{ref} is a bounded Lipschitz domain and $\Omega' \supset \bar{\Omega}_{\text{ref}}$ is open and bounded with Lipschitz boundary. Moreover $T_{\text{ad}} \subset W^{2,\infty}(\Omega')^d$ is bounded such that for all $\tau \in T_{\text{ad}}$ the mappings $\tau : \bar{\Omega}_{\text{ref}} \rightarrow \tau(\bar{\Omega}_{\text{ref}})$ are bi-Lipschitzian and satisfy $\det(\tau') \geq \delta > 0$, with a constant $\delta > 0$. Here, $\tau'(x) = \nabla \tau(x)^T$ denotes the Jacobian of τ .

Moreover, the data $\tilde{\mathbf{v}}_0, \tilde{\mathbf{f}}$ are given such that

$$\tilde{\mathbf{f}} \in C^1(I; V(\Omega)), \quad \tilde{\mathbf{v}}_0 \in V(\Omega) \cap H^2(\Omega)^d \quad \forall \Omega \in \mathcal{O}_{\text{ad}} = \{\tau(\Omega_{\text{ref}}) : \tau \in T_{\text{ad}}\},$$

i.e. the data $\tilde{\mathbf{v}}_0, \tilde{\mathbf{f}}_0$ are used on all $\Omega \in \mathcal{O}_{\text{ad}}$.

Then assumption (T) ensures in particular (3.2) and assumption (A) holds in the following obvious version for time dependent problems, where the transformation acts only in space.

Lemma 3.1. *Let T_{ad} satisfy assumption (T). Then the state space $Y(\Omega)$ defined in (3.3) satisfies assumption (A), more precisely,*

$$\left. \begin{aligned}
Y(\Omega_{\text{ref}}) &= \{(\tilde{\mathbf{v}}, \tilde{p})(\tau(\cdot), \cdot) : (\tilde{\mathbf{v}}, \tilde{p}) \in Y(\tau(\Omega_{\text{ref}}))\} \\
(\tilde{\mathbf{v}}, \tilde{p}) \in Y(\tau(\Omega_{\text{ref}})) &\mapsto (\mathbf{v}, p) := (\tilde{\mathbf{v}}, \tilde{p})(\tau(\cdot), \cdot) \in Y(\Omega_{\text{ref}}) \text{ is a homeom.}
\end{aligned} \right\} \quad \forall \tau \in T_{\text{ad}}.$$

A proof of this result is beyond the scope of this paper and will be given elsewhere.

Given the weak formulation of the Navier-Stokes equations on a domain $\tau(\Omega_{\text{ref}})$ we can apply the transformation rule for integrals to obtain a variational formulation based on the domain Ω_{ref} . Using our convention to write $\tilde{\cdot}$ for a function that is defined on $\tau(\Omega_{\text{ref}})$ we use the identifications

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

etc. and the identity

$$\nabla_{\tilde{x}} \tilde{z}(\tau(x)) = \tau'(x)^{-T} \nabla_x z(x), \quad x \in \Omega_{\text{ref}}.$$

Using this formalism we get for example

$$\int_I \int_{\tau(\Omega_{\text{ref}})} \nu \nabla \tilde{\mathbf{v}} : \nabla \tilde{\mathbf{w}} \, dx \, dt = \int_I \sum_{i=1}^d \int_{\Omega_{\text{ref}}} \nu \nabla v_i^T \tau'^{-1} \tau'^{-T} \nabla w_i \det \tau' \, dx \, dt.$$

In this way and by using Lemma 3.1 we arrive at the following equivalent form of the weak formulation (3.4) on $\tau(\Omega_{\text{ref}})$, which is only based on the domain Ω_{ref} : Find $(\mathbf{v}, p) \in Y(\Omega_{\text{ref}})$ such that for all $(\mathbf{w}, q) \in Z^*(\Omega_{\text{ref}})$

$$\begin{aligned} & \langle (\mathbf{w}, q), E((\mathbf{v}, p), \tau) \rangle_{Z^*(\Omega_{\text{ref}}), Z(\Omega_{\text{ref}})} = \\ &= \int_{\Omega_{\text{ref}}} \mathbf{v}(x, 0)^T \mathbf{w}(x, 0) \det \tau' \, dx - \int_{\Omega_{\text{ref}}} \tilde{\mathbf{v}}_0(\tau(x))^T \mathbf{w}(x, 0) \det \tau' \, dx \\ &+ \int_I \int_{\Omega_{\text{ref}}} \mathbf{v}_t^T \mathbf{w} \det \tau' \, dx \, dt + \sum_{i=1}^d \int_I \int_{\Omega_{\text{ref}}} \nu \nabla v_i^T \tau'^{-1} \tau'^{-T} \nabla w_i \det \tau' \, dx \, dt \\ &+ \int_I \int_{\Omega_{\text{ref}}} \mathbf{v}^T \tau'^{-T} \nabla \mathbf{v} \, \mathbf{w} \det \tau' \, dx \, dt - \int_I \int_{\Omega_{\text{ref}}} p \, \text{tr}(\tau'^{-T} \nabla \mathbf{w}) \det \tau' \, dx \, dt \\ &- \int_I \int_{\Omega_{\text{ref}}} \tilde{\mathbf{f}}(\tau(x), t)^T \mathbf{w} \det \tau' \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} q \, \text{tr}(\tau'^{-T} \nabla \mathbf{v}) \det \tau' \, dx \, dt = 0. \end{aligned} \quad (3.5)$$

For $\tau = \text{id}$ we recover directly the weak formulation (3.4) on the domain $\Omega = \Omega_{\text{ref}}$, for general $\tau \in T_{\text{ad}}$ we obtain an equivalent form of (3.4) on the domain $\Omega = \tau(\Omega_{\text{ref}})$.

3.3. Objective function

We consider an objective functional \bar{J} defined on the domain $\tau(\Omega_{\text{ref}})$ of the type

$$\begin{aligned} \bar{J}((\tilde{\mathbf{v}}, \tilde{p}), \tau(\Omega_{\text{ref}})) &= \int_I \int_{\tau(\Omega_{\text{ref}})} f_1(x, \tilde{\mathbf{v}}(x, t), \nabla \tilde{\mathbf{v}}(x, t), \tilde{p}(x, t)) \, dx \, dt \\ &+ \int_{\tau(\Omega_{\text{ref}})} f_2(x, \tilde{\mathbf{v}}(x, T)) \, dx \end{aligned} \quad (3.6)$$

with $f_1 : \bigcup_{\tau \in T_{\text{ad}}} \tau(\Omega_{\text{ref}}) \times \mathbb{R}^2 \times \mathbb{R}^{2,2} \times \mathbb{R} \rightarrow \mathbb{R}$ and $f_2 : \bigcup_{\tau \in T_{\text{ad}}} \tau(\Omega_{\text{ref}}) \times \mathbb{R}^2 \rightarrow \mathbb{R}$. Again we transform the objective function to the reference domain Ω_{ref} .

$$\begin{aligned} \bar{J}((\tilde{\mathbf{v}}, \tilde{p}), \tau(\Omega_{\text{ref}})) &= \int_I \int_{\Omega_{\text{ref}}} f_1(\tau(x), \mathbf{v}(x, t), \tau'(x)^{-T} \nabla \mathbf{v}(x, t), p(x, t)) \det \tau' \, dx \, dt \\ &+ \int_{\Omega_{\text{ref}}} f_2(\tau(x), \mathbf{v}(x, T)) \det \tau' \, dx \\ &=: J^D((\mathbf{v}, p), \tau) + J^T(\mathbf{v}, \tau) = J((\mathbf{v}, p), \tau). \end{aligned}$$

3.4. Adjoint equation

We apply now the adjoint procedure of subsection 2.2.1 to compute the shape gradient. To this end, we have to compute the Lagrange multipliers $(\boldsymbol{\lambda}, \mu) \in Z^*(\Omega_{\text{ref}})$ by solving the adjoint system (2.2), which reads in this case

$$\begin{aligned} \langle (\boldsymbol{\lambda}, \mu), E_{(\mathbf{v}, p)}((\mathbf{v}, p), \tau)(\mathbf{w}, q) \rangle_{Z^*(\Omega_{\text{ref}}), Z(\Omega_{\text{ref}})} \\ = -\langle J_{(\mathbf{v}, p)}((\mathbf{v}, p), \tau), (\mathbf{w}, q) \rangle_{Y^*(\Omega_{\text{ref}}), Y(\Omega_{\text{ref}})} \quad \forall (\mathbf{w}, q) \in Y(\Omega_{\text{ref}}) \end{aligned}$$

with the given weak solution $(\mathbf{v}, p) \in Y(\Omega_{\text{ref}})$ of the state equation. In detail we seek $(\boldsymbol{\lambda}, \mu) \in Z^*(\Omega_{\text{ref}})$ with

$$\begin{aligned} & - \int_I \int_{\Omega_{\text{ref}}} \mathbf{w}^T \boldsymbol{\lambda}_t \det \tau' \, dt \, dx + \int_{\Omega_{\text{ref}}} \mathbf{w}(x, T)^T \boldsymbol{\lambda}(x, T) \det \tau' \, dx \\ & + \int_I \sum_{i=1}^d \int_{\Omega_{\text{ref}}} \nu \nabla w_i^T \tau'^{-1} \tau'^{-T} \nabla (\boldsymbol{\lambda})_i \det \tau' \, dx \, dt \\ & + \int_I \int_{\Omega_{\text{ref}}} (\mathbf{w}^T \tau'^{-T} \nabla \mathbf{v} + \mathbf{v}^T \tau'^{-T} \nabla \mathbf{w}) \boldsymbol{\lambda} \det \tau' \, dx \, dt \\ & - \int_I \int_{\Omega_{\text{ref}}} q \operatorname{tr}(\tau'^{-T} \nabla \boldsymbol{\lambda}) \det \tau' \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} \mu \operatorname{tr}(\tau'^{-T} \nabla \mathbf{w}) \det \tau' \, dx \, dt \\ & = -\langle J_{(\mathbf{v}, p)}((\mathbf{v}, p), \tau), (\mathbf{w}, q) \rangle_{Y^*(\Omega_{\text{ref}}), Y(\Omega_{\text{ref}})} \quad \forall (\mathbf{w}, q) \in Y(\Omega_{\text{ref}}). \end{aligned} \tag{3.7}$$

For $\tau = \text{id}$ this is the weak formulation of the usual adjoint system of the Navier-Stokes equations on Ω_{ref} , which reads in strong form

$$\begin{aligned} -\boldsymbol{\lambda}_t - \nu \Delta \boldsymbol{\lambda} - (\nabla \boldsymbol{\lambda})^T \mathbf{v} + (\nabla \mathbf{v}) \boldsymbol{\lambda} - \nabla \mu &= -J_v^D((\mathbf{v}, p), \text{id}) && \text{on } \Omega_{\text{ref}} \times I \\ -\operatorname{div} \boldsymbol{\lambda} &= -J_p^D((\mathbf{v}, p), \text{id}) && \text{on } \Omega_{\text{ref}} \times I \\ \boldsymbol{\lambda} &= 0 && \text{on } \partial \Omega_{\text{ref}} \times I \\ \boldsymbol{\lambda}(\cdot, T) &= -J_v^T(\mathbf{v}, \text{id}) && \text{on } \Omega_{\text{ref}} \end{aligned}$$

For general $\tau \in T_{\text{ad}}$ the adjoint system (3.7) is equivalent to the usual adjoint system of the Navier-Stokes equations on $\tau(\Omega_{\text{ref}})$. A detailed analysis of the adjoint equation of the Navier-Stokes equations can be found in [11, 21].

3.5. Calculation of the shape gradient

The derivative of the reduced objective $j(\tau) := J((\mathbf{v}(\tau), p(\tau)), \tau)$ is now given by (2.3), which reads in our case

$$\begin{aligned} \langle j'(\tau), \cdot \rangle_{T^*(\Omega_{\text{ref}}), T(\Omega_{\text{ref}})} &= \\ \langle (\boldsymbol{\lambda}, \mu), E_{\tau}((\mathbf{v}, p), \tau) \cdot \rangle_{Z^*(\Omega_{\text{ref}}), Z(\Omega_{\text{ref}})} &+ \langle J_{\tau}((\mathbf{v}, p), \tau), \cdot \rangle_{T^*(\Omega_{\text{ref}}), T(\Omega_{\text{ref}})}. \end{aligned} \tag{3.8}$$

To state this in detail, we have to compute the derivatives of E and J with respect to τ . Let (\mathbf{v}, p) and $(\boldsymbol{\lambda}, \mu)$ be the solution of the Navier-Stokes equations (3.5) and the corresponding adjoint equation (3.7) for given $\tau \in T_{\text{ad}}$. Using the formulation

(3.5) of E on the reference domain Ω_{ref} the first term can be expressed as

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

If $\tilde{\mathbf{v}}$ solves the state equation then the first term vanishes.

The part with the objective functional is given by

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

If $\tau = \text{id}$, i.e. $\tau(\Omega_{\text{ref}}) = \Omega_{\text{ref}}$ we obtain the following formula for the reduced gradient, where we omit the first term, since $\mathbf{v}(\cdot, 0) = \tilde{\mathbf{v}}_0(\tau(\cdot))$.

$$\begin{aligned}
\langle j'(\text{id}), V \rangle_{T^*(\Omega_{\text{ref}}), T(\Omega_{\text{ref}})} = & \\
& - \int_{\Omega_{\text{ref}}} V^T \nabla \tilde{\mathbf{v}}_0(x) \boldsymbol{\lambda}(x, 0) \, dx \\
& + \int_I \int_{\Omega_{\text{ref}}} \mathbf{v}_t^T \boldsymbol{\lambda} \operatorname{div} V \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} \nu \nabla \mathbf{v} : \nabla \boldsymbol{\lambda} \operatorname{div} V \, dx \, dt \\
& - \sum_{i=1}^d \int_I \int_{\Omega_{\text{ref}}} \nu \nabla \mathbf{v}_i^T (V' + V'^T) \nabla \boldsymbol{\lambda}_i \, dx \, dt \\
& - \int_I \int_{\Omega_{\text{ref}}} \mathbf{v}^T V'^T \nabla \mathbf{v} \boldsymbol{\lambda} \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} \mathbf{v}^T \nabla \mathbf{v} \boldsymbol{\lambda} \operatorname{div} V \, dx \, dt \\
& + \int_I \int_{\Omega_{\text{ref}}} p \operatorname{tr}(V'^T \nabla \boldsymbol{\lambda}) \, dx \, dt - \int_I \int_{\Omega_{\text{ref}}} p \operatorname{div} \boldsymbol{\lambda} \operatorname{div} V \, dx \, dt \\
& - \int_I \int_{\Omega_{\text{ref}}} \tilde{\mathbf{f}}^T \boldsymbol{\lambda} \operatorname{div} V \, dx \, dt - \int_I \int_{\Omega_{\text{ref}}} V^T \nabla \tilde{\mathbf{f}} \boldsymbol{\lambda} \, dx \, dt \tag{3.9} \\
& - \int_I \int_{\Omega_{\text{ref}}} \mu \operatorname{tr}(V'^T \nabla \mathbf{v}) \, dx \, dt + \int_I \int_{\Omega_{\text{ref}}} \mu \operatorname{div} \mathbf{v} \operatorname{div} V \, dx \, dt \\
& + \int_I \int_{\Omega_{\text{ref}}} f_1(x, \mathbf{v}, \nabla \mathbf{v}, p) \operatorname{div} V \, dx \, dt \\
& - \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial(\nabla \tilde{\mathbf{v}})} f_1(x, \mathbf{v}, \nabla \mathbf{v}, p) V'^T \nabla \mathbf{v} \, dx \, dt \\
& + \int_I \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_1(x, \mathbf{v}, \nabla \mathbf{v}, p) V \, dx \, dt \\
& + \int_{\Omega_{\text{ref}}} f_2(x, \mathbf{v}(x, T)) \operatorname{div} V \, dx \\
& + \int_{\Omega_{\text{ref}}} \frac{\partial}{\partial \tilde{x}} f_2(x, \mathbf{v}(x, T)) V \, dx.
\end{aligned}$$

Remark 3.2. As already mentioned in subsection 2.2.2, for computational purposes it is convenient for a given iterate τ_k to calculate the reduced gradient on the domain Ω_k . As described in detail in 2.2.2 we have to solve the Navier-Stokes equations and the adjoint system on Ω_k . Using $\langle j'(\tau_k), V \rangle_{T^*(\Omega_{\text{ref}}), T(\Omega_{\text{ref}})} = \langle \tilde{j}'(\text{id}), \tilde{V} \rangle_{T^*(\Omega_k), T(\Omega_k)}$ we can take the formula above replacing Ω_{ref} by Ω_k and using the corresponding functions defined on Ω_k .

Finally, if we assume more regularity for the state and adjoint, we can integrate by parts in the above formula and can represent the shape gradient as a functional on the boundary.

However, we prefer to work with the distributed version (3.8), since it is also appropriate for FE-Galerkin approximations, while the integration by parts

to obtain the boundary representation is not justified for FE-discretizations with H^1 -elements. In addition, (3.8) can also easily be transferred to a boundary representation by using the procedure of subsection 2.3 with a boundary displacement-to-domain transformation mapping $u \mapsto \tau(u) \in T_{\text{ad}}$. For Galerkin discretization the continuous adjoint calculus can then easily be applied on the discrete level.

4. Discretization

To discretize the instationary Navier-Stokes equations, we use the $cG(1)dG(0)$ space-time finite element method, which uses piecewise constant finite elements in time and piecewise linear finite elements in space. The $cG(1)dG(0)$ method is a variant of the General Galerkin G^2 -method developed by Eriksson, Estep, Hansbo, and Johnson [4, 5].

Let $\mathcal{I} = \{I_j = (t_{j-1}, t_j] : 1 \leq j \leq N\}$ be a partition of the time interval $(0, T]$ with a sequence of discrete time steps $0 = t_0 < t_1 < \dots < t_N = T$ and length of the respective time intervals $k_j := |I_j| = t_j - t_{j-1}$.

With each time step t_j , we associate a partition \mathcal{T}_j of the spatial domain Ω and the finite element subspaces V_h^j, P_h^j of continuous piecewise linear functions in space.

The $cG(1)dG(0)$ space-time finite element discretization with stabilization can be written as an implicit Euler scheme: $\mathbf{v}_h^0 = \mathbf{v}_0$ and for $j = 1 \dots N$, find $(\mathbf{v}_h^j, p_h^j) \in V_h^j \times P_h^j$ such that

$$\begin{aligned} (E^j(\mathbf{v}_h, p_h), (\mathbf{w}_h, q_h)) &:= \\ &:= \left(\frac{\mathbf{v}_h^j - \mathbf{v}_h^{j-1}}{k_j}, \mathbf{w}_h \right) + (\nu \nabla \mathbf{v}_h^j, \nabla \mathbf{w}_h) + (\mathbf{v}_h^j \cdot \nabla \mathbf{v}_h^j, \mathbf{w}_h) - (p_h^j, \operatorname{div} \mathbf{w}_h) \\ &+ (\operatorname{div} \mathbf{v}_h^j, q_h) + SD_\delta(\mathbf{v}_h^j, p_h^j, \mathbf{w}_h, q_h) - (f, \mathbf{w}_h) = 0 \quad \forall (\mathbf{w}_h, q_h) \in V_h^j \times P_h^j \end{aligned}$$

with stabilization

$$\begin{aligned} SD_\delta(\mathbf{v}_h^j, p_h^j, \mathbf{w}_h, q_h) &= \left(\delta_1 (\mathbf{v}_h^j \cdot \nabla \mathbf{v}_h^j + \nabla p_h^j - f), \mathbf{v}_h^j \cdot \nabla \mathbf{w}_h + \nabla q_h \right) \\ &+ (\delta_2 \operatorname{div} \mathbf{v}_h^j, \operatorname{div} \mathbf{w}_h). \end{aligned}$$

The stabilization parameters

$$\delta_1 = \begin{cases} \frac{1}{2}(k_j^{-2} + |\mathbf{v}_h^j|^2 h_j^{-2})^{-1/2} & \text{if } \nu < |\mathbf{v}_h^j| h_j \\ \kappa_1 h_j^2 & \text{otherwise} \end{cases}, \quad \delta_2 = \begin{cases} \kappa_2 h_j & \text{if } \nu < |\mathbf{v}_h^j| h_j \\ \kappa_2 h_j^2 & \text{otherwise} \end{cases}$$

act as a subgrid model in the convection-dominated case $\nu < |\mathbf{v}_h^j| h_j$, where h_j denotes the local (spatial) meshsize at time j and κ_1 and κ_2 are constants of unit size.

As discrete objective functional, we consider

$$\begin{aligned} J^h(\mathbf{v}_h, p_h) &= \sum_{j=1}^N k_j \int_{\Omega} f_1(x, \mathbf{v}_h^j, \nabla \mathbf{v}_h^j, p_h^j) dx + \int_{\Omega} f_2(x, \mathbf{v}_h^N) dx \\ &=: J^{D,h}(\mathbf{v}_h, p_h) + J^{T,h}(\mathbf{v}_h^N). \end{aligned}$$

This is exactly $J(\mathbf{v}_h, p_h)$, since \mathbf{v}_h, p_h are piecewise constant in time.

In order to obtain gradients which are exact on the discrete level, we consider the discrete Lagrangian functional based on the $cG(1)dG(0)$ finite element method, which is given by

$$\mathcal{L}_h(\mathbf{v}_h, p_h, \boldsymbol{\lambda}_h, \mu_h) = J^h(\mathbf{v}_h, p_h) + \sum_{j=1}^N k_j (E^j(\mathbf{v}_h, p_h), (\boldsymbol{\lambda}_h^j, \mu_h^j)).$$

Note again that this is exactly $\mathcal{L}(\mathbf{v}_h, p_h, \boldsymbol{\lambda}_h, \mu_h)$, since $\mathbf{v}_h, p_h, \boldsymbol{\lambda}_h, \mu_h$ are piecewise constant in time.

Now we take the derivatives of the discrete Lagrangian w.r.t. the state variables to obtain the discrete adjoint equation and w.r.t. the shape variables to obtain the reduced gradient.

The discrete adjoint system can be cast in the form of an implicit time-stepping scheme backward in time: For $j = N-1, \dots, 0$, find $(\boldsymbol{\lambda}_h^j, \mu_h^j) \in V_h^j \times P_h^j$ such that

$$\begin{aligned} &\frac{(\boldsymbol{\lambda}_h^j, \mathbf{w}_h)}{k_j} + (\nu \nabla \boldsymbol{\lambda}_h^j, \nabla \mathbf{w}_h) + (\mu_h^j, \operatorname{div} \mathbf{w}_h) - (q_h, \operatorname{div} \boldsymbol{\lambda}_h^j) \\ &+ (\mathbf{v}_h^j \cdot \nabla \mathbf{w}_h, \boldsymbol{\lambda}_h^j) + (\mathbf{w}_h \cdot \nabla \mathbf{v}_h^j, \boldsymbol{\lambda}_h^j) + SD_{\delta}^*(\mathbf{v}_h^j, p_h^j, \boldsymbol{\lambda}_h^j, \mu_h^j; \mathbf{w}_h, q_h) \\ &= \frac{(\boldsymbol{\lambda}_h^{j+1}, \mathbf{w}_h)}{k_j} - \frac{1}{k_j} \langle J_{\mathbf{v}_h^j}^{D,h}(\mathbf{v}_h, p_h), \mathbf{w}_h \rangle - \frac{1}{k_j} \langle J_{p_h^j}^{D,h}(\mathbf{v}_h, p_h), q_h \rangle \\ &\quad \forall (\mathbf{w}_h, q_h) \in V_h^j \times P_h^j, \end{aligned}$$

where the discrete initial adjoint $(\boldsymbol{\lambda}_h^N, \mu_h^N)$ solves the system

$$\begin{aligned} &\frac{\boldsymbol{\lambda}_h^N \cdot \mathbf{w}_h}{k_N} + (\nu \nabla \boldsymbol{\lambda}_h^N, \nabla \mathbf{w}_h) + (\mu_h^N, \operatorname{div} \mathbf{w}_h) + (\mathbf{v}_h^N \cdot \nabla \mathbf{w}_h, \boldsymbol{\lambda}_h^N) \\ &+ (\mathbf{w}_h \cdot \nabla \mathbf{v}_h^N, \boldsymbol{\lambda}_h^N) - (q_h, \operatorname{div} \boldsymbol{\lambda}_h^N) + SD_{\delta}^*(\mathbf{v}_h^N, p_h^N, \boldsymbol{\lambda}_h^N, \mu_h^N; \mathbf{w}_h, q_h) \\ &= -\frac{1}{k_N} \langle J_{\mathbf{v}_h^N}^{D,h}(\mathbf{v}_h, p_h), \mathbf{w}_h \rangle - \frac{1}{k_N} \langle J_{\mathbf{v}_h^N}^{T,h}(\mathbf{v}_h^N), \mathbf{w}_h \rangle - \frac{1}{k_N} \langle J_{p_h^N}^{D,h}(\mathbf{v}_h, p_h), q_h \rangle \end{aligned}$$

for all $(\mathbf{w}_h, q_h) \in V_h^N \times P_h^N$.

The adjoint stabilization term SD_δ^* is given by

$$\begin{aligned}
SD_\delta^*(\mathbf{v}_h^j, p_h^j, \boldsymbol{\lambda}_h^j, \mu_h^j; \mathbf{w}_h, q_h) &= \delta_1(\mathbf{w}_h \cdot \nabla \mathbf{v}_h^j, \mathbf{v}_h^j \cdot \nabla \boldsymbol{\lambda}_h^j) + \delta_1(\mathbf{v}_h^j \cdot \nabla \mathbf{w}_h, \mathbf{v}_h^j \cdot \nabla \boldsymbol{\lambda}_h^j) \\
&+ \delta_1(\mathbf{v}_h^j \cdot \nabla \mathbf{v}_h^j, \mathbf{w}_h \cdot \nabla \boldsymbol{\lambda}_h^j) + \delta_1(\nabla q_h, \nabla \mu_h^j) + \delta_2(\operatorname{div} \mathbf{w}_h, \operatorname{div} \boldsymbol{\lambda}_h^j) \\
&+ \delta_1(\mathbf{w}_h \cdot \nabla \mathbf{v}_h^j, \nabla \mu_h^j) + \delta_1(\mathbf{v}_h^j \cdot \nabla \mathbf{w}_h, \nabla \mu_h^j) \\
&+ \delta_1(\nabla q_h, \mathbf{v}_h^j \cdot \nabla \boldsymbol{\lambda}_h^j) + \delta_1(\nabla p_h^j, \mathbf{w}_h \cdot \nabla \boldsymbol{\lambda}_h^j) .
\end{aligned}$$

For simplicity, we have neglected the terms containing the right-hand-side f and the dependence of δ_1 on \mathbf{v}_h^h .

To compute shape derivatives on the discrete level we use a transformation space $T^h(\Omega_{\text{ref}})$ of piecewise linear continuous functions. Then a discrete version of assumption (A) holds, i.e., the finite element space remains after transformation the space of continuous piecewise linear functions in space. The same holds for higher order finite elements. Therefore, an analogue of (3.9) holds also on the discrete level if a Galerkin method is used and we obtain easily the exact shape derivative, if the adjoint state is computed by the exact discrete adjoint equation stated above. In this way we have obtained the exact shape derivative on the discrete level by using a continuous adjoint approach without the tedious task of computing mesh sensitivities.

5. Numerical results

In this section we demonstrate the adjoint shape derivative calculus on a numerical model problem. In particular, we consider an incompressible instationary flow around an object B for which the drag shall be minimized.

5.1. Problem description

The model problem is based on the DFG benchmark of a 2D instationary flow around a cylinder [20], see Figure 1. We prescribe a fixed parabolic inflow profile on the left boundary Γ_{in} with $v_{max} = 1.5m/s$, noslip boundary conditions on the top and bottom boundaries, as well as on the object boundary Γ_B , and a free outflow condition on the right boundary Γ_{out} . The flow is modeled by the instationary incompressible Navier-Stokes equations, with viscosity $\nu = 10^{-4}$. The Navier-Stokes equations are discretized with the $cG(1)dG(0)$ finite element method presented above, with a fixed time step size $k = 10^{-2}$ and a triangular spatial mesh with about 4100 vertices and 7900 elements.

The object boundary Γ_B is parameterized using a cubic B-Spline curve with 7 control points for the upper half of Γ_B , which is reflected at the $y = 0.2$ -axis to obtain a y-symmetric closed curve. This parameterization allows for apices at the front and rear of the object, while the remaining boundary is C^2 . We impose constraints on the volume of the object B as well as bound constraints on the control points. Using the coordinates of the control points as design parameters,

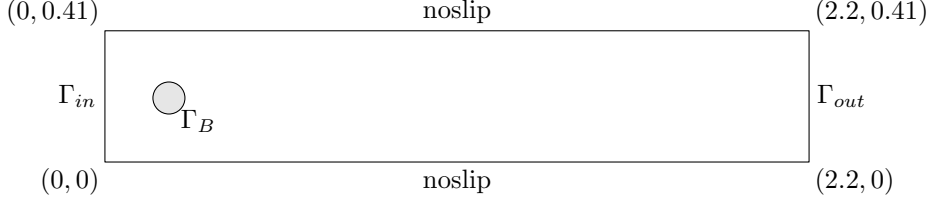


FIGURE 1. DFG-Benchmark flow around a cylinder; sketch of the geometry

we arrive at an optimization problem with 14 design variables, 12 of which are free (2 design parameters are fixed as we have to ensure that the y-coordinates of the first and last B-spline curve points equal 0.2 in order for the curve to be closed).

We compute the mean value of the drag on the object boundary Γ_B over the time interval $[0, T]$ by using the formula

$$J((\tilde{\mathbf{v}}, \tilde{p}), \Omega) = \frac{1}{T} \int_0^T \int_{\Omega} \left((\tilde{\mathbf{v}}_t + (\tilde{\mathbf{v}} \cdot \nabla) \tilde{\mathbf{v}} - \tilde{\mathbf{f}})^T \mathbf{\Phi} - \tilde{p} \operatorname{div} \mathbf{\Phi} + \nu \nabla \tilde{\mathbf{v}} : \nabla \mathbf{\Phi} \right) dx dt. \quad (5.1)$$

Here, $\mathbf{\Phi}$ is a smooth function such that with a unit vector ϕ pointing in the mean flow direction holds

$$\mathbf{\Phi}|_{\Gamma_B} \equiv \phi, \quad \mathbf{\Phi}|_{\partial\Omega \setminus \Gamma_B} \equiv 0 \quad \forall \Omega \in \mathcal{O}_{\text{ad}}.$$

This formula is an alternative formula for the mean value of the drag on Γ_B ,

$$c_d := \frac{1}{T} \int_0^T \int_{\Gamma_B} \mathbf{n} \cdot \sigma(\tilde{\mathbf{v}}, \tilde{p}) \cdot \phi dS,$$

with normal vector n and stress tensor $\sigma(\tilde{\mathbf{v}}, \tilde{p}) = \nu \frac{1}{2} (\nabla \tilde{\mathbf{v}} + (\nabla \tilde{\mathbf{v}})^T) - \tilde{p} I$, and can be obtained through integration by parts. For a detailed derivation, see [12]. Integration by parts in the time derivative shows that (5.1) can also be written as

$$\begin{aligned} J((\tilde{\mathbf{v}}, \tilde{p}), \Omega) &= \frac{1}{T} \int_0^T \int_{\Omega} \left(((\tilde{\mathbf{v}} \cdot \nabla) \tilde{\mathbf{v}} - \tilde{\mathbf{f}})^T \mathbf{\Phi} - \tilde{p} \operatorname{div} \mathbf{\Phi} + \nu \nabla \tilde{\mathbf{v}} : \nabla \mathbf{\Phi} \right) dx dt \\ &\quad + \frac{1}{T} \int_{\Omega} (\tilde{\mathbf{v}}(x, T) - \tilde{\mathbf{v}}_0(x))^T \mathbf{\Phi}(x) dx. \end{aligned} \quad (5.1)$$

Thus the drag functional (5.1) has the form (3.6). Moreover, using the well known embedding $Y(\Omega) \hookrightarrow C(I; L^2(\Omega)^d) \times L_0^2(\Omega)$ it is easy to see that $(\tilde{\mathbf{v}}, \tilde{p}) \in Y(\Omega) \mapsto J((\tilde{\mathbf{v}}, \tilde{p}), \Omega)$ is continuously differentiable if $\mathbf{\Phi} \in W^{1,\infty}(\mathbb{R}^2)^2$.

Computation of the state, adjoint and shape derivative equations is done using Dolfin [14], which is part of the FEniCS project [7]. The optimization is carried out using the interior point solver IPOPT [22], with a BFGS-approximation for the reduced Hessian.

5.2. Choice of shape parameters and shape deformation techniques

One aspect to consider in the implementation of shape optimization algorithms is the choice of the shape parameters and the shape deformation technique. Generally speaking, shape parameterizations and deformations fall into two classes. In the first case, a parameterization directly defines the whole domain, which can be accomplished by using, e.g., free form deformation. In the second case, the parameterization determines the shape of the surface Γ_B of the object B . Examples for this kind of parameterizations can be B-splines, NURBS, but also the set of boundary points Γ_B itself, if considered in an appropriate function space. Changes in the shape of the boundary Γ_B then have to be transferred to changes of the domain Ω_{ref} . This can be done in various ways, see, e.g., [2].

In our model problem, we have chosen a parameterization of the object boundary Γ_B based on closed cubic B-spline curves [16], where the B-spline control points act as design parameters u . The transformation of boundary displacements to displacements of the domain is done by solving an elasticity equation, where we prescribe the displacement of the object boundary as inhomogeneous Dirichlet boundary data [2]. The computational domains $\Omega_k := \Omega(\tau(u_k))$ are obtained as transformations of a triangulation of the domain shown in Figure 1. As described at the end of section 4 we use piecewise linear transformations to ensure a discrete analogue of assumption (A). Then by an analogue of (3.9) together with the discrete adjoint equation we obtained conveniently by a continuous adjoint calculus the exact shape derivative on the discrete level – which we have also checked numerically.

5.3. Results

The IPOPT-algorithm needs 15 interior-point iterations for converging to a tolerance of 10^{-3} , altogether needing 17 state equation solves and 16 adjoint solves. The drag value in the optimal shape is reduced by nearly one third in comparison to the initial shape. In the optimal solution, bound constraints for 8 of the design parameters are active, while 6 are inactive. The results of the optimization process are summarized in Table 1.

Figure 2 shows the velocity fields for the initial and optimal shape, with snapshots taken at end time, while Figure 3 shows the computational mesh both for the initial and the optimal shape. Both meshes are obtained by a transformation of the same reference mesh with a circular object, cf. Figure 1, by solving an elasticity equation with fixed displacement of the object boundary.

6. Conclusions and outlook

In this paper, we have presented a continuous adjoint approach that can easily be transferred in an exact way to the discrete level, if a Galerkin method in space is used. We use a domain representation of the shape gradient, since a boundary representation requires integration by parts, which is usually not justified on the

iteration	objective	dual infeasibility	linesarch-steps
0	1.2157690e-1	1.69e+0	0
1	1.0209697e-1	1.53e+0	2
2	9.7036722e-2	3.60e-1	1
3	8.7039312e-2	6.44e-1	1
4	8.4563185e-2	5.08e-1	1
5	8.3512670e-2	1.01e-1	1
6	8.2813890e-2	1.22e-1	1
7	8.2516118e-2	8.96e-2	1
8	8.2069666e-2	1.42e-1	1
9	8.2062288e-2	1.39e-1	1
10	8.1995990e-2	1.80e-2	1
11	8.1994727e-2	6.55e-3	1
12	8.1995485e-2	2.76e-3	1
13	8.1995822e-2	2.72e-3	1
14	8.1995966e-2	1.32e-3	1
15	8.1995811e-2	2.66e-5	1

TABLE 1. Optimization Results

discrete level. Nevertheless, adjoint based gradient representations can easily be derived from our gradient representation, e.g., for the boundary shape gradient in function space, but also for shape parameterizations, for example free form deformation or parameterized boundary displacement. The proposed approach allows the solution of the state equation and adjoint equation on the physical domain. Therefore existing solvers of the partial differential equation and its adjoint can be used.

We have applied our approach to the instationary incompressible Navier-Stokes equations. In the context of the stabilized $cG(1)dG(0)$ method – but also for other Galerkin schemes and other types of partial differential equations – we were able to derive conveniently the exact discrete shape derivative, since our calculus is exact on the discrete level, if some simple rules are followed.

The combination with error estimators and multilevel techniques is subject of current research. Our results indicate that these techniques can reduce the number of optimization iterations on the fine grids and the necessary degrees of freedom significantly. We leave these results to a future paper.

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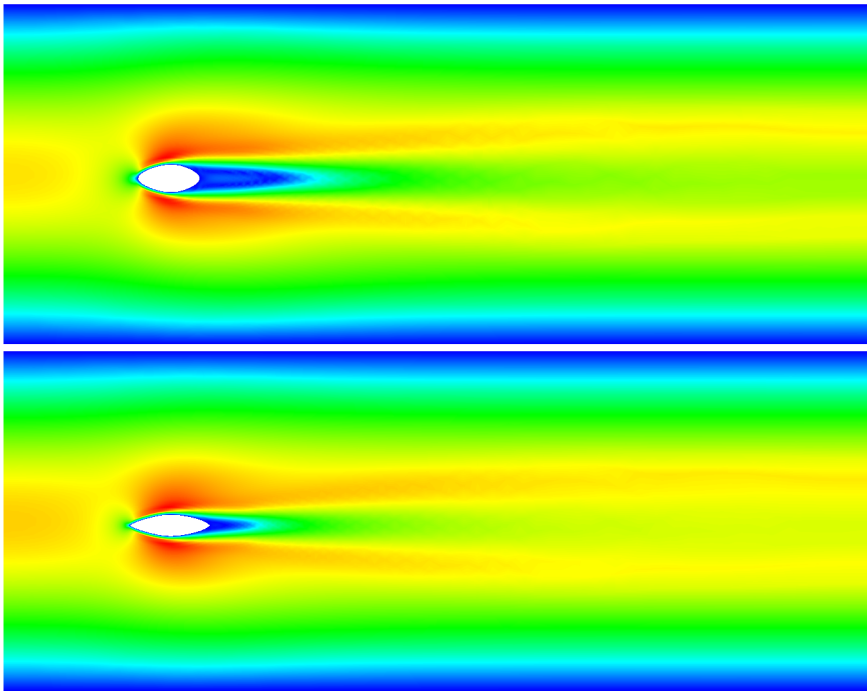


FIGURE 2. Comparison of the velocity fields for the initial and optimal shape

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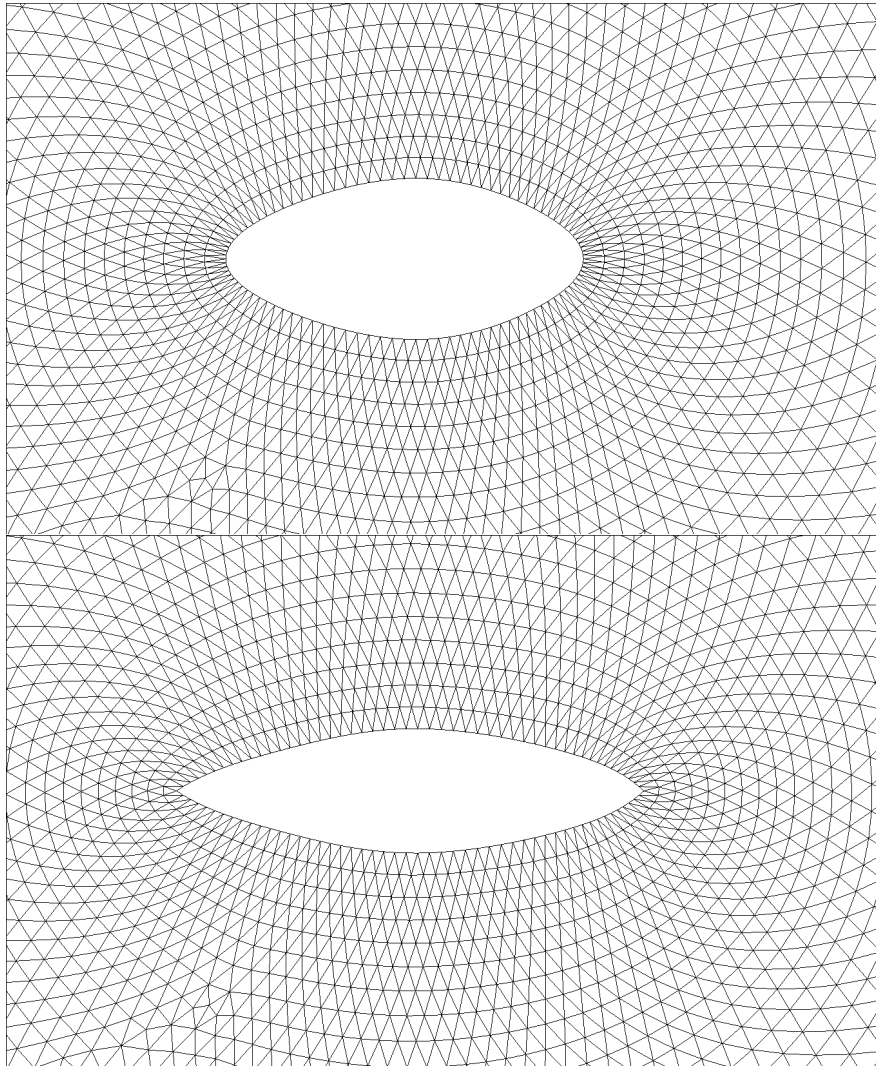


FIGURE 3. Comparison of the meshes for the initial and optimal shape

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