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SHAPE SENSITIVITY ANALYSIS FOR STABILIZED NAVIER-STOKES EQUATIONS

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Summary: *The paper contributes to solving optimal flow 3D problems in the context of laminar incompressible flows of Newtonian fluid in rigid ducts. A stabilization of the finite element solution is required in case of problems of low viscosity (air) flows. Analytical sensitivity formulae for extra terms originating from the stabilization of the finite element discretized Navier-Stokes equations are presented, since the analysis of flow sensitivity to shape changes of a fluid domain has a crucial influence on efficiency of a shape optimization algorithm. Preliminary numerical examples are shown, employing our theoretical results within a steepest descent optimization algorithm.*

1. Introduction

Our aim is to find 3D optimal shapes of rigid ducts for problems involving laminar incompressible flows of Newtonian fluid. There are many industrial applications for this task, such as conduits for efficient cooling, exhaust piping, or related task concerning external flows, e.g. wing and blade profiles, or vehicle aerodynamics. Shapes of channels or obstacles placed in the stream influence important features of the flow, thus, present an important control handle for (bio)chemical processes, cooling, convected reaction-diffusion (e.g. catalysis, drug delivery), combustion, mixing, etc.

The option of analysing flow sensitivity to shape changes of a fluid domain allows for resorting to gradient-based optimization methods; then the quality of such analysis has a crucial influence on efficiency of the selected optimization algorithm. The sensitivities of the standard problem setting involve just standard terms of Navier-Stokes equations that were treated already in Rohan and Cimrman (2006). Since the stabilization of the finite element solution is required in case of problems of low viscosity (air) flows, in this paper *we present analytical sensitivity formulae for extra terms originating from stabilization of finite element discretized Navier-Stokes equations*, cf. Matthies and Lube (2007), describing laminar incompressible flows of Newtonian fluid.

The paper overview is as follows. In Section 2 we present the flow problem formulation, in Section 3 we introduce the Oseen iterations and record the stabilization technique, thereby modifying the state problem of the optimal shape problem which is defined in Section 4; therein

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also the sensitivity analysis is developed using the domain method involving the virtual design speed. Preliminary results obtained with the stabilized finite element approximation of the Navier-Stokes equation are presented in Section 5 and compared to the results of the standard Navier-Stokes equations for a moderate kinematic viscosity ($\sim 10^{-3}$). All numerical examples were computed using our software SfePy, see Cimrman et al. (2008).

2. Variational formulation of flow problem

The problem is defined in an open bounded domain $\Omega \subset \mathbb{R}^3$ with two (possibly overlapping) subdomains defined as

$$\overline{\Omega} = \overline{\Omega_D \cup \Omega_C} \quad \text{with} \quad \Gamma_C = \partial\Omega_D \cap \partial\Omega_C \;, \tag{1}$$

where Ω_C is the *control domain* and Ω_D is the *design domain*, see Fig. 1. The shape of Ω_D is modified exclusively through the *design boundary*, $\Gamma_D \subset \partial\Omega_D \setminus \Gamma_{\text{in-out}}$ where $\Gamma_{\text{in-out}} \subset \partial\Omega$ is the union of the "inlet-outlet" boundary of the channel; in general $\Gamma_{\text{in-out}}$ consists of two disjoint parts, $\Gamma_{\text{in-out}} = \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$.

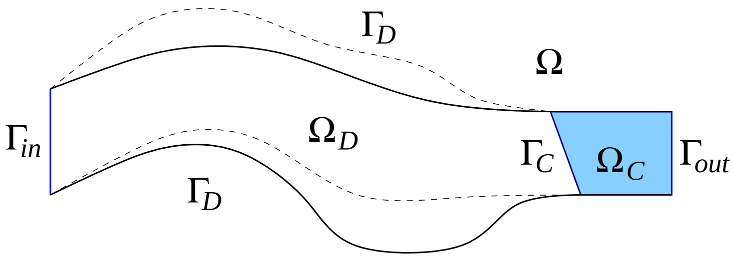

Fig. 1. The decomposition of domain Ω, control domain Ω_C at the outlet sector of the channel.

We seek a *steady state of an incompressible flow* in Ω by solving the following problem: find a velocity, $\boldsymbol{u}$, and pressure, p, fields in Ω such that (ν is the kinematic viscosity)

$$\begin{aligned} -\nu\nabla^2\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p = 0 \quad & \text{in } \Omega \;, \\ \nabla\cdot\boldsymbol{u} = 0 \quad & \text{in } \Omega \;, \end{aligned} \tag{2}$$

with the boundary conditions

$$\begin{aligned} \boldsymbol{u} = 0 \quad \text{on } \partial\Omega \setminus \Gamma_{\text{in-out}} \;, \quad & \boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \Gamma_{\text{in}} \;, \\ -p\boldsymbol{n} + \nu\frac{\partial\boldsymbol{u}}{\partial n} = -\bar{p}\boldsymbol{n} \quad & \text{on } \Gamma_{\text{out}} \;, \end{aligned} \tag{3}$$

where $\boldsymbol{n}$ is the unit outward-normal vector on Γ_{out}, $\frac{\partial}{\partial n} = \boldsymbol{n}\cdot\nabla$ and $\bar{\boldsymbol{u}}$ is a given inlet velocity profile. Note that by $(3)_2$ we prescribe the stress in the form of pressure $\bar{p}$, so that we enforce the condition of $\frac{\partial\boldsymbol{u}}{\partial n} = 0$, i.e. the flow is uniform in the normal direction w.r.t. Γ_{out}.

In the sequel we shall employ the following functional forms ($i = 1,2$ or $i = 1,2,3$, summation convention is employed):

$$\begin{aligned} a_\Omega(\boldsymbol{u}, \boldsymbol{v}) &:= \nu\int_\Omega \nabla\boldsymbol{u} : \nabla\boldsymbol{v} = \nu\int_\Omega \frac{\partial u_i}{\partial x_k}\frac{\partial v_i}{\partial x_k} \;, \\ c_\Omega(\boldsymbol{w}, \boldsymbol{u}, \boldsymbol{v}) &:= \int_\Omega (\boldsymbol{w}\cdot\nabla\boldsymbol{u})\cdot\boldsymbol{v} = \int_\Omega w_k\frac{\partial u_i}{\partial x_k}v_i \;, \\ b_\Omega(\boldsymbol{u}, p) &:= \int_\Omega p\,\nabla\cdot\boldsymbol{u} \;, \quad g_{\Gamma_{\text{out}}}(\boldsymbol{v}) := -\int_{\Gamma_{\text{out}}} \bar{p}\,\boldsymbol{v}\cdot\boldsymbol{n}\,dS \;, \end{aligned} \tag{4}$$

and the space of admissible velocities

$$\boldsymbol{V}_0 = \{\boldsymbol{v} \in \mathbf{H}^1(\Omega) \mid \boldsymbol{v} = 0 \text{ on } \partial\Omega \setminus \Gamma_{\text{out}}\} \ , \tag{5}$$

where $\mathbf{H}^1(\Omega) = [H^1(\Omega)]^3$. Using the forms (4) we obtain the following weak problem: find $\boldsymbol{u} \in \boldsymbol{V}_0(\Omega)$ and $p \in L^2(\Omega)$ such that

$$\begin{aligned} a_\Omega(\boldsymbol{u},\, \boldsymbol{v}) + c_\Omega(\boldsymbol{u},\, \boldsymbol{u},\, \boldsymbol{v}) - b_\Omega(\boldsymbol{v},\, p) = g_{\Gamma_{\text{out}}}(\boldsymbol{v}) \quad \forall \boldsymbol{v} \in \boldsymbol{V}_0 \ , \\ b_\Omega(\boldsymbol{u},\, q) = 0 \quad \forall q \in L^2(\Omega) \ . \end{aligned} \tag{6}$$

3. Stabilization of solution

In order to be able to solve low viscosity problems (air flow in a channel, $\nu \approx 10^{-5}$, a stabilization of the finite element solution is required. In Matthies and Lube (2007) a promising approach was published recently, combining both the inf-sup stable discretization (fulfilling the Babuška-Brezzi condition) and convection stabilization strategies. As our software implements those ideas, we recall here briefly the main results for the sake of paper completeness.

3.1. Generalized Oseen problem

The nonlinear Navier-Stokes equations (2) can be solved by a fixed-point or Newton-type iteration. This leads to a generalized Oseen problem, where the convective term $\boldsymbol{u} \cdot \nabla \boldsymbol{u}$ is replaced by $\boldsymbol{b} \cdot \nabla \boldsymbol{u}$ with the convection velocity $\boldsymbol{b}$ known (e.g. from the previous iteration step),

$$\begin{aligned} -\nu \nabla^2 \boldsymbol{u} + \boldsymbol{b} \cdot \nabla \boldsymbol{u} + \sigma \boldsymbol{u} + \nabla p = \boldsymbol{f} \quad & \text{in } \Omega \ , \\ \nabla \cdot \boldsymbol{u} = 0 \quad & \text{in } \Omega \ . \end{aligned} \tag{7}$$

The term $\sigma \boldsymbol{u}$ originates from time discretization of the nonstationary Navier-Stokes problem, $\sigma \sim \frac{1}{\Delta t}$, consequently $\boldsymbol{f}$ are "modified" volume forces incorporating also the approximated solution from the previous time (iteration); this is not present in our computations. In the stationary case $\sigma = 0$. Let us denote

$$\begin{aligned} A\left((\boldsymbol{u}, p), (\boldsymbol{v}, q)\right) &:= a_\Omega(\boldsymbol{u},\, \boldsymbol{v}) + c_\Omega(\boldsymbol{b},\, \boldsymbol{u},\, \boldsymbol{v}) - b_\Omega(\boldsymbol{v},\, p) + b_\Omega(\boldsymbol{u},\, q) + \sigma(\boldsymbol{u}, \boldsymbol{v})_\Omega \ , \\ L\left((\boldsymbol{v}, q)\right) &:= (\boldsymbol{f}, \boldsymbol{v})_\Omega + g_{\Gamma_{\text{out}}}(\boldsymbol{v}) \ , \\ (\boldsymbol{u}, \boldsymbol{v})_G &:= \int_G \boldsymbol{u} \cdot \boldsymbol{v} \quad \ldots L^2 \text{ inner product on } G \ . \end{aligned} \tag{8}$$

3.2. Grad-div, SUPG and PSPG stabilization

The weak form of the problem (7) is discretized by finite elements using inf-sup stable elements (for example Taylor-Hood P_2/P_1 elements on simplices) leading to the discrete weak formulation of the generalized Oseen problem: find $\boldsymbol{u}_h \in \boldsymbol{X}_h$ and $p \in M_h$ such that (subscript h indicates influence of the spatial discretization characterized by element size $h > 0$)

$$A\left((\boldsymbol{u}_h, p_h), (\boldsymbol{v}_h, q_h)\right) = L\left((\boldsymbol{v}_h, q_h)\right) \quad \forall (\boldsymbol{v}_h, q_h) \in (\boldsymbol{X}_{h0}, M_h) \ , \tag{9}$$

where $\boldsymbol{X}_h, M_h$ are appropriate finite element spaces and

$$\boldsymbol{X}_{h0} = \{\boldsymbol{v} \in \boldsymbol{X}_h \mid \boldsymbol{v} = 0 \text{ on } \partial\Omega \setminus \Gamma_{\text{out}}\} \ . \tag{10}$$

Following the authors in Matthies and Lube (2007), we now introduce modified forms involving parameters γ, κ_K and τ_K:

$$\begin{aligned} A_S\left((\boldsymbol{u},p),(\boldsymbol{v},q)\right) &:= A\left((\boldsymbol{u},p),(\boldsymbol{v},q)\right) + \gamma(\nabla\cdot\boldsymbol{u},\nabla\cdot\boldsymbol{v})_\Omega \\ &\quad + \sum_{K\in\mathcal{T}_h}\left(-\nu\nabla^2\boldsymbol{u}+\boldsymbol{b}\cdot\nabla\boldsymbol{u}+\sigma\boldsymbol{u}+\nabla p,\kappa_K(\boldsymbol{b}\cdot\nabla\boldsymbol{v})+\tau_K\nabla q\right)_K \\ L_S\left((\boldsymbol{v},q)\right) &:= L\left((\boldsymbol{v},q)\right) + \sum_{K\in\mathcal{T}_h}\left(\boldsymbol{f},\kappa_K(\boldsymbol{b}\cdot\nabla\boldsymbol{v})+\tau_K\nabla q\right)_K\ , \end{aligned} \tag{11}$$

where $\bigcup_{K\in\mathcal{T}_h}\overline{K}=\overline{\Omega}$ is a triangulation of Ω. Parameter γ controls the *grad-div* stabilization, the terms with κ_K correspond to the *streamline-diffusion (SUPG)* stabilization and the terms with τ_K mean the *pressure (PSPG)* stabilization.

3.3. Choice of stabilization parameters

Assuming scaling of the Oseen problem such that $b_\infty := ||\boldsymbol{b}||_\infty \sim 1$, and denoting $C_F \sim \mathrm{diam}(\Omega)$ the Friedrichs constant for Ω, the stabilization parameters are chosen as follows:

$$\gamma = \nu + b_\infty C_F\ , \tag{12}$$

τ_K and κ_K satisfy the following constraint where C is a suitable constant: and there exists a constant C such that

$$0 \le \tau_K \le \kappa_K \le C\frac{\min(1;\frac{1}{\sigma})h_K^2}{\nu+b_\infty C_F+\sigma C_F^2+b_\infty^2\min(\frac{C_F^2}{\nu};\frac{1}{\sigma})}\ . \tag{13}$$

The theoretical considerations in Matthies and Lube (2007) require σ to be a positive constant bounded away from zero. However, in practice, the stabilization may work even for stationary problems with $\sigma = 0$.

3.4. Simplifying assumptions

The stabilization makes possible to use even P_1/P_1 elements on simplices. This was also our choice, as it is the simplest case and the terms containing $\nabla^2\boldsymbol{u}$ disappear, simplifying thus the sensitivity formulae below in Section 4.3.1. We also assume a stationary solution with $\sigma = 0$, no volume forces, $\boldsymbol{f} = 0$, and zero pressure tractions, $\bar{p} = 0$. Using the following notation ($i = 1, 2$ or $i = 1, 2, 3$, summation convention is employed)

$$\begin{aligned} h_K\left(\boldsymbol{b}^1,\boldsymbol{b}^2,\boldsymbol{u},\boldsymbol{v}\right) &:= \left(\boldsymbol{b}^1\cdot\nabla\boldsymbol{u},(\boldsymbol{b}^2\cdot\nabla\boldsymbol{v})\right)_K = \int_K b_i^1\frac{\partial u_k}{\partial x_i}b_j^2\frac{\partial u_k}{\partial x_j}\ , \\ g_K\left(\boldsymbol{b},\boldsymbol{u},p\right) &:= \left(\nabla p,(\boldsymbol{b}\cdot\nabla\boldsymbol{u})\right)_K = \int_K\frac{\partial p}{\partial x_i}b_j\frac{\partial u_i}{\partial x_j}\ , \\ r_K\left(p,q\right) &:= \left(\nabla p,\nabla q\right)_K = \int_K\frac{\partial p}{\partial x_i}\frac{\partial q}{\partial x_i}\ , \end{aligned} \tag{14}$$

the stabilized Oseen problem for given convective velocity $\boldsymbol{b}$ is now given by (c.f. eq. (9))

$$A_S\left((\boldsymbol{u}_h,p_h),(\boldsymbol{v}_h,q_h)\right) = L_S\left((\boldsymbol{v}_h,q_h)\right) \quad \forall(\boldsymbol{v}_h,q_h)\in(\boldsymbol{X}_{h0},M_h)\ , \tag{15}$$

which reads as (omitting subscript $_h$):

$$
\begin{aligned}
a_\Omega(\boldsymbol{u}, \boldsymbol{v}) + c_\Omega(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{v}) - b_\Omega(\boldsymbol{v}, p) + \gamma(\nabla \cdot \boldsymbol{u}, \nabla \cdot \boldsymbol{v})_\Omega & \\
+ \sum_{K \in \mathcal{T}_h} \kappa_K \left(h_K(\boldsymbol{b}, \boldsymbol{b}, \boldsymbol{u}, \boldsymbol{v}) + g_K(\boldsymbol{b}, \boldsymbol{v}, p) \right) = 0 \quad & \forall \boldsymbol{v} \in \boldsymbol{X}_{h0} \;, \\
b_\Omega(\boldsymbol{u}, q) + \sum_{K \in \mathcal{T}_h} \tau_K \left(g_K(\boldsymbol{b}, \boldsymbol{u}, q) + r_K(p, q) \right) = 0 \quad & \forall q \in M_h \;.
\end{aligned}
\tag{16}
$$

Note that $\boldsymbol{b} = \boldsymbol{u}$ after convergence of the Oseen iteration, when the non-linear Navier-Stokes system is in mind. This is the system for which we are going to derive the sensitivity formulae.

4. Optimal flow problem

In this section we first introduce the basic ingredients of the optimization algorithm, cf. Haslinger and Mäkinen (2003), Rohan and Whiteman (2000). Then we define a shape optimization problem seeking an optimal flow, and describe a domain method of shape sensitivity analysis w.r.t. changes of the design domain Ω_D. Finally comes the core of this article — the sensitivity formulae for the additional stabilization terms introduced in (14) of Section 3..

4.1. Overview of the techniques used

We use a domain (volume) approach to the shape sensitivity analysis which is based on the material derivative idea of the continuum mechanics. From the computational point of view, the main ingredient of the method is a sufficiently smooth "design velocity" field defined in the whole fluid domain, which in the consequence defines the finite-element mesh perturbation. Such a design velocity field has the support only in those part of the fluid domain, where the mesh can be modified by changing the design, therefore it must vanish on the fixed part of the boundary. This field can be constructed in several ways differing each other in their complexity and universality of application. In Rohan and Cimrman (2006) we described a computational domain parametrization using the free-form deformation (FFD) approach, which provides the design velocity very efficiently and easily.

Given a design velocity field, partial sensitivities of the involved terms (e.g. diffusion, convection, stabilization terms) are derived by using partial shape derivatives in the direction of the design velocity. By virtue of the adjoint equation technique, these are used along with the adjoint state solution to define a gradient of an objective function of the optimization, which is subsequently used in a gradient-based minimization method. Relatively cheap computation of the shape sensitivities allows us to use efficiently the steepest descent algorithm to minimize the objective function.

4.2. Shape optimization problem

Our objective is to minimize the objective function $\Psi(\boldsymbol{u}, p)$ w.r.t. some criterion (see below) by means of varying Γ_D:

$$
\begin{aligned}
& \min_{\Gamma_D} \Psi(\boldsymbol{u}, p) \;, \\
\text{subject to: } & (\boldsymbol{u}, p) \text{ satisfy (16)} \;, \text{ with } \boldsymbol{b} = \boldsymbol{u} \;, \\
& \Gamma_D \text{ in } \mathcal{U}_{ad}(\Omega_0) \;.
\end{aligned}
\tag{17}
$$

Above $(17)_2$ imposes the admissibility of the velocity and pressure fields, whereas $(17)_3$ restricts shape variation of Γ_D w.r.t. some "initial" shape inherited from the reference domain Ω_0 which defines the associated *set of admissible shapes*, $\mathcal{U}_{ad}(\Omega_0)$, given by the parametrization of Ω_D shape, see Rohan and Cimrman (2006).

We can use, for example, the following objective functions (possibly their mutual combinations) targetted to:

1. Achieve most uniform as possible flow in control region:

$$\Psi_1(\boldsymbol{u}) = \frac{\nu}{2} \int_{\Omega_C} |\nabla \boldsymbol{u}|^2 = \frac{1}{2} a_{\Omega_C} (\boldsymbol{u}, \boldsymbol{u}) \ . \tag{18}$$

   Here we wish to enhance flow uniformity by reducing the gradients of flow velocities in Ω_C. The objective function does not depend on the pressure p. Moreover, if $\Gamma_D \subset \partial\Omega_D \setminus (\Gamma_{\text{in}-\text{out}} \cup \partial\Omega_C)$, the control domain Ω_C does not depend on design modifications, which simplifies the sensitivity formulae.

2. Minimize inlet-outlet pressure difference:

$$\Psi_2(p) = \int_{\Gamma_{\text{in}}} p - \int_{\Gamma_{\text{out}}} \bar{p} \ . \tag{19}$$

   In this case the pressure loss is minimized. Recall that $\bar{p}$ is a given outlet pressure.

4.3. Sensitivity analysis – domain method

The aim of this section is to introduce the sensitivity formulae which describe how the quantities of interest change when the design domain is being modified. More precisely, we follow the approach of the material derivative associated with the so-called design velocity field $\vec{\mathcal{V}} : \overline{\Omega_D} \to \mathbb{R}^3$ representing an artificial flux of material particles. Thus, for any (feasible) infinitesimal design change in the direction of velocity field $\vec{\mathcal{V}}$ we shall be able to predict the associated sensitivity as the directional domain derivative. In what follows, by δf we refer to the total (directional) derivative of a function, or functional f, whereas notation $\delta_D f$ is reserved for the *partial derivative w.r.t. domain perturbation* (infinitesimal) in the direction $\vec{\mathcal{V}}$. Let $u : \Omega \to \mathbb{R}$ be a real valued function and $f_\Omega(u)$ a real valued functional depending on domain Ω. The total sensitivity of f is given by

$$\delta f_\Omega(u) = \delta_D f_\Omega(u) + \delta_u f_\Omega(u) \circ \delta u \ , \tag{20}$$

where $\delta_u F(u) \circ v$ means the Gateaux differential of $F(u)$ w.r.t. u in the direction v. In the optimal shape problems, quantity u is typically the solution of a *state problem* considered, thus depending on the design of Ω, so that δu is the (total) material derivative of u w.r.t. the domain perturbation.

First we introduce the *feasible design velocity fields* in the context of our problem (17): $\vec{\mathcal{V}}$ is a feasible w.r.t. Ω_D if and only if the following holds:

$$\begin{aligned} &\text{supp}\vec{\mathcal{V}} \subset \overline{\Omega_D} \text{ and } \vec{\mathcal{V}} = 0 \text{ on } \Gamma_{\text{in}-\text{out}} \cup \Gamma_C \ , \\ &\vec{\mathcal{V}} \text{ is differentiable in } \Omega_D. \end{aligned} \tag{21}$$

4.3.1. Sensitivity formula and optimality conditions

In this section we present the sensitivity formula for computing $\delta\Psi(\boldsymbol{u})$ in the sense of (20). We consider the Lagrangian associated with (17)

$$\begin{aligned}\mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) = {} & \Psi(\boldsymbol{u}, p) \\ & + a_\Omega(\boldsymbol{u}, \boldsymbol{w}) + c_\Omega(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - b_\Omega(\boldsymbol{w}, p) + \gamma(\nabla\cdot\boldsymbol{u}, \nabla\cdot\boldsymbol{w})_\Omega \\ & + \sum_{K\in\mathcal{T}_h} \kappa_K \left(h_K(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + g_K(\boldsymbol{u}, \boldsymbol{w}, p)\right) \\ & + b_\Omega(\boldsymbol{u}, q) + \sum_{K\in\mathcal{T}_h} \tau_K \left(g_K(\boldsymbol{u}, \boldsymbol{u}, q) + r_K(p, q)\right) ,\end{aligned} \tag{22}$$

where $\boldsymbol{w} \in \boldsymbol{X}_{h0}$ and $q \in M_h$ are the Lagrange multipliers associated with the state problem constraint imposed in (17). The desired sensitivity formula can be obtained using the KKT conditions concerning the “inf-sup” problem

$$\inf_{\Gamma_D, \boldsymbol{u}, p} \sup_{\boldsymbol{w}, q} \mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) . \tag{23}$$

We shall now consider only such paths in the set of all primary-variable states $(\Gamma_D, \boldsymbol{u}, p)$, that for each design Γ_D we find its associated admissible state $(\boldsymbol{u}, p)$. With restriction to such paths we compute the sensitivity of $\mathcal{L}$, and remembering (20):

$$\begin{aligned} & \delta\mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) \circ (\mathcal{V}, \delta\boldsymbol{u}, \delta p) \\ & = \delta_D a_\Omega(\boldsymbol{u}, \boldsymbol{w}) + \delta_D c_\Omega(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - \delta_D b_\Omega(\boldsymbol{w}, p) + \gamma\delta_D(\nabla\cdot\boldsymbol{u}, \nabla\cdot\boldsymbol{w})_\Omega \\ & \quad + \sum_{K\in\mathcal{T}_h} \kappa_K \left(\delta_D h_K(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + \delta_D g_K(\boldsymbol{u}, \boldsymbol{w}, p)\right) \\ & \quad + \delta_D b_\Omega(\boldsymbol{u}, q) + \sum_{K\in\mathcal{T}_h} \tau_K \left(\delta_D g_K(\boldsymbol{u}, \boldsymbol{u}, q) + \delta_D r_K(p, q)\right) \\ & \quad + \delta_D\Psi(\boldsymbol{u}, p) \\ & \quad + a_\Omega(\delta\boldsymbol{u}, \boldsymbol{w}) + c_\Omega(\delta\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + c_\Omega(\boldsymbol{u}, \delta\boldsymbol{u}, \boldsymbol{w}) - b_\Omega(\boldsymbol{w}, \delta p) + \gamma(\nabla\cdot\delta\boldsymbol{u}, \nabla\cdot\boldsymbol{w})_\Omega \\ & \quad + \sum_{K\in\mathcal{T}_h} \kappa_K \left(h_K(\delta\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + h_K(\boldsymbol{u}, \delta\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + h_K(\boldsymbol{u}, \boldsymbol{u}, \delta\boldsymbol{u}, \boldsymbol{w})\right) \\ & \quad + \sum_{K\in\mathcal{T}_h} \kappa_K \left(g_K(\delta\boldsymbol{u}, \boldsymbol{w}, p) + g_K(\boldsymbol{u}, \boldsymbol{w}, \delta p)\right) \\ & \quad + b_\Omega(\delta\boldsymbol{u}, q) + \sum_{K\in\mathcal{T}_h} \tau_K \left(g_K(\delta\boldsymbol{u}, \boldsymbol{u}, q) + g_K(\boldsymbol{u}, \delta\boldsymbol{u}, q) + r_K(\delta p, q)\right) \\ & \quad + \delta_u\Psi(\boldsymbol{u}, p) \circ \delta\boldsymbol{u} + \delta_p\Psi(\boldsymbol{u}, p) \circ \delta p \\ & = \delta\Psi(\boldsymbol{u}, p) ,\end{aligned} \tag{24}$$

where the last equality follows from the state admissibility; indeed, for a given design Γ_D, the state admissibility conditions (16) hold, so that except of $\Psi(\boldsymbol{u}, p)$ all terms in (22) vanish.

Expressing the KKT optimality conditions $\delta_{\boldsymbol{u},p}\mathcal{L} = 0$, we obtain the *adjoint state problem*:

$$
\begin{aligned}
\delta_{\boldsymbol{u}}\mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) \circ \delta\boldsymbol{u} = 0 = {} & \delta_u \Psi(\boldsymbol{u}, p) \circ \boldsymbol{v} \\
& + a_\Omega(\boldsymbol{v}, \boldsymbol{w}) + c_\Omega(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{w}) + c_\Omega(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) + \gamma(\nabla \cdot \boldsymbol{v}, \nabla \cdot \boldsymbol{w})_\Omega \\
& + \sum_{K \in \mathcal{T}_h} \kappa_K \left(h_K(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + h_K(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{u}, \boldsymbol{w}) + h_K(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) \right) \\
& + \sum_{K \in \mathcal{T}_h} \kappa_K \left(g_K(\boldsymbol{v}, \boldsymbol{w}, p) \right) \\
& + b_\Omega(\boldsymbol{v}, q) + \sum_{K \in \mathcal{T}_h} \tau_K \left(g_K(\boldsymbol{v}, \boldsymbol{u}, q) + g_K(\boldsymbol{u}, \boldsymbol{v}, q) \right) , \\
\delta_p\mathcal{L}(\Gamma_D, \boldsymbol{u}, p, \boldsymbol{w}, q) \circ \delta p = 0 = {} & \delta_p \Psi(\boldsymbol{u}, p) \circ \eta \\
& - b_\Omega(\boldsymbol{w}, \eta) + \sum_{K \in \mathcal{T}_h} \kappa_K \left(g_K(\boldsymbol{u}, \boldsymbol{w}, \eta) \right) + \sum_{K \in \mathcal{T}_h} \tau_K \left(r_K(\eta, q) \right) ,
\end{aligned}
\tag{25}
$$

for all $\boldsymbol{v} \in \boldsymbol{X}_{h0}$ and for all $\eta \in M_h$. The adjoint state problem allows eliminating the total derivatives $\delta\boldsymbol{u}$, δp from sensitivity formula (24). It is readily seen that, on substituting in (25) the test functions $\boldsymbol{v} = \delta\boldsymbol{u}$, $\eta = \delta p$, in (24) we may cancel all terms except the partial design sensitivities $\delta_D *$. Therefore, the sensitivity analysis with restriction to the admissible states is performed, as follows: Given a design Γ_D, adjust domain Ω_D and

- compute the admissible state $(\boldsymbol{u}, p)$ by solving (16),
- compute the adjoint state $(\boldsymbol{w}, q)$ by solving (25),
- compute the sensitivity w.r.t. given design velocity field $\vec{\mathcal{V}}$ using

$$
\begin{aligned}
\delta\Psi(\boldsymbol{u}) = {} & \delta_D a_\Omega(\boldsymbol{u}, \boldsymbol{w}) + \delta_D c_\Omega(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) - \delta_D b_\Omega(\boldsymbol{w}, p) + \delta_D(\gamma(\nabla \cdot \boldsymbol{u}, \nabla \cdot \boldsymbol{w})_\Omega) \\
& + \sum_{K \in \mathcal{T}_h} \kappa_K \left(\delta_D h_K(\boldsymbol{u}, \boldsymbol{u}, \boldsymbol{u}, \boldsymbol{w}) + \delta_D g_K(\boldsymbol{u}, \boldsymbol{w}, p) \right) \\
& + \delta_D b_\Omega(\boldsymbol{u}, q) + \sum_{K \in \mathcal{T}_h} \tau_K \left(\delta_D g_K(\boldsymbol{u}, \boldsymbol{u}, q) + \delta_D r_K(p, q) \right) \\
& + \delta_D \Psi(\boldsymbol{u}, p) .
\end{aligned}
\tag{26}
$$

Often $\delta_D \Psi(\boldsymbol{u}, p) = 0$: for example in (18), where $\Psi(\boldsymbol{u}, p)$ is evaluated over Ω_C that does not depend on design modifications.

Below we shall derive the particular partial design sensitivities employed in (26), which depend on $\vec{\mathcal{V}}$. We also repeat, for the sake of completeness, the formulae for the standard Navier-Stokes problem (6) already presented in Rohan and Cimrman (2006).

4.3.2. Partial shape derivatives

Once the design velocity field is defined, the design domain can be parametrized by means of a scalar parameter τ: let $\vec{\mathcal{V}}$ is feasible according to (21), we introduce

$$
\overline{\Omega_D}(\tau) = \{y\} \qquad \text{where} \qquad y_i(x, \tau) = x_i + \tau \mathcal{V}_i(x) , \quad x \in \overline{\Omega_D},\ \tau \in \mathbb{R} . \tag{27}
$$

Above and in what follows by Ω_D we denote the fixed domain, whereas $\Omega_D(\tau)$ is the perturbed one. Recalling the general sensitivity relation (20), we define the *partial shape derivative* of $f_\Omega(u)$

$$\delta_D f_\Omega(u) = \frac{\mathrm{d}}{\mathrm{d}\,\tau}\left(f_{\Omega_D(\tau)}(u)\right)_{\tau=0} \ . \tag{28}$$

In order to compute the partial shape derivative involved in (26), we need the following preliminaries, which are easy to verify ($J(y(x,\tau)) = \det[\partial y_i(x,\tau)/\partial x_j]$):

$$\begin{aligned} \delta_D\left(\frac{\partial y_i}{\partial x_j}\right) &= \frac{\mathrm{d}}{\mathrm{d}\,\tau}\left(\frac{\partial y_i(x,\tau)}{\partial x_j}\right)_{\tau=0} = \frac{\partial \mathcal{V}_i(x)}{\partial x_j} \ , \\ \delta_D\left(\frac{\partial x_k}{\partial y_j}\right) &= \frac{\mathrm{d}}{\mathrm{d}\,\tau}\left(\frac{\partial x_k}{\partial y_j(x,\tau)}\right)_{\tau=0} = -\frac{\partial \mathcal{V}_k(x)}{\partial x_j} \ , \\ \delta_D\left(J(y)\right) &= \frac{\mathrm{d}}{\mathrm{d}\,\tau}\left(J(y(x,\tau))\right)_{\tau=0} = \frac{\partial \mathcal{V}_i(x)}{\partial x_i} = \mathrm{div}\vec{\mathcal{V}} \ . \end{aligned} \tag{29}$$

We are now ready to apply (28) to variation of $a_\Omega\left(\boldsymbol{u},\, \boldsymbol{w}\right)$; note that only Ω_D is being perturbed because of restricted support of $\vec{\mathcal{V}}$, so that $\delta_D a_\Omega\left(\boldsymbol{u},\, \boldsymbol{w}\right) = \delta_D a_{\Omega_D}\left(\boldsymbol{u},\, \boldsymbol{w}\right)$. Therefore, we consider

$$\begin{aligned} a_{\Omega_{D(\tau)}}\left(\boldsymbol{u},\, \boldsymbol{w}\right) &= \nu\int_{\Omega_D(\tau)} \frac{\partial u_i}{\partial y_k(\tau)}\frac{\partial w_i}{\partial y_k(\tau)}\,dy \\ &= \nu\int_{\Omega_D} \frac{\partial u_i(x)}{\partial x_j}\frac{\partial x_j}{\partial y_k(x,\tau)}\,\frac{\partial w_i(x)}{\partial x_l}\frac{\partial x_l}{\partial y_k(x,\tau)}\,J(y(x,\tau))\,dx \ . \end{aligned} \tag{30}$$

On differentiating above w.r.t. τ, using (29) we get the desired expression

$$\delta_D a_\Omega\left(\boldsymbol{u},\, \boldsymbol{w}\right) = \nu\int_{\Omega_D}\left[\frac{\partial u_i}{\partial x_k}\frac{\partial w_i}{\partial x_k}\mathrm{div}\mathcal{V} - \frac{\partial \mathcal{V}_j}{\partial x_k}\frac{\partial u_i}{\partial x_j}\frac{\partial w_i}{\partial x_k} - \frac{\partial u_i}{\partial x_k}\frac{\partial \mathcal{V}_l}{\partial x_k}\frac{\partial w_i}{\partial x_l}\right] \ . \tag{31}$$

In much the same way one finds the formulae for other sensitivities involved in (26):

$$\delta_D c_\Omega\left(\boldsymbol{u},\, \boldsymbol{u},\, \boldsymbol{w}\right) = \int_{\Omega_D}\left[u_k\frac{\partial u_i}{\partial x_k}\,w_i\,\mathrm{div}\mathcal{V} - u_k\frac{\partial \mathcal{V}_j}{\partial x_k}\frac{\partial u_i}{\partial x_j}\,w_i\right] \ , \tag{32}$$

$$\delta_D b_\Omega\left(\boldsymbol{u},\, q\right) = \int_{\Omega_D} q\,\left[\mathrm{div}\boldsymbol{u}\,\mathrm{div}\mathcal{V} - \frac{\partial \mathcal{V}_k}{\partial x_i}\frac{\partial u_i}{\partial x_k}\right] \ , \tag{33}$$

$$\delta_D(\nabla\cdot\boldsymbol{u},\nabla\cdot\boldsymbol{w})_\Omega = \int_{\Omega_D}\left[\mathrm{div}\boldsymbol{u}\mathrm{div}\boldsymbol{w}\mathrm{div}\mathcal{V} - \frac{\partial \mathcal{V}_k}{\partial x_i}\frac{\partial u_i}{\partial x_k}\mathrm{div}\boldsymbol{w} - \mathrm{div}\boldsymbol{u}\,\frac{\partial \mathcal{V}_k}{\partial x_i}\frac{\partial w_i}{\partial x_k}\right] \ , \tag{34}$$

$$\begin{aligned} \delta_D h_K\left(\boldsymbol{b}^1,\, \boldsymbol{b}^2,\, \boldsymbol{u},\, \boldsymbol{v}\right) = \int_K \Big[&(\boldsymbol{b}^1\cdot\nabla)u_k(\boldsymbol{b}^2\cdot\nabla)v_k\mathrm{div}\mathcal{V} \\ &- \boldsymbol{b}^1\cdot\nabla\mathcal{V}_i\frac{\partial u_k}{\partial x_i}(\boldsymbol{b}^2\cdot\nabla)v_k - (\boldsymbol{b}^1\cdot\nabla)u_k\boldsymbol{b}^2\cdot\nabla\mathcal{V}_i\frac{\partial v_k}{\partial x_i}\Big] \ , \end{aligned} \tag{35}$$

$$\delta_D g_K\left(\boldsymbol{b},\, \boldsymbol{u},\, p\right) = \int_K\left[\frac{\partial p}{\partial x_i}\boldsymbol{b}\cdot\nabla u_i\mathrm{div}\mathcal{V} - \frac{\partial \mathcal{V}_k}{\partial x_i}\frac{\partial p}{\partial x_k}\boldsymbol{b}\cdot\nabla u_i - \frac{\partial p}{\partial x_i}\boldsymbol{b}\cdot\nabla\mathcal{V}_k\frac{\partial u_i}{\partial x_k}\right] \ , \tag{36}$$

$$\delta_D r_K\left(p,\, q\right) = \int_K\left[\nabla p\cdot\nabla q\mathrm{div}\mathcal{V} - \nabla\mathcal{V}_k\frac{\partial p}{\partial x_k}\cdot\nabla q - \nabla p\cdot\nabla\mathcal{V}_k\frac{\partial q}{\partial x_k}\right] \ . \tag{37}$$

We may conclude that using (31)-(37) (plus possibly $\delta_D\Psi(\boldsymbol{u},p)$ for some particular objective functions) applied in (26), the total shape derivative can be recovered for any feasible $\vec{\mathcal{V}}$; construction of such $\vec{\mathcal{V}}$ for our specific design parametrization was addressed in Rohan and Cimrman (2006).

5. Examples

Here we present some preliminary results obtained with the *stabilized finite element approximation* of the Navier-Stokes equation (16). Other examples can be found in Cimrman and Rohan (2007).

In the examples presented below we use $\nu = 1.25 \cdot 10^{-3}$. A consistent unit set {m, s, kg} is used. Concerning the boundary conditions, the velocity component in the tube direction is set to 1 on the inlet part of the boundary. On the walls we assume no-slip condition $\boldsymbol{u} = 0$. On the outlet we specify $\bar{p} = 0$. The boundary of the control domain Ω_C does not depend on design changes: $\Gamma_D \cap \partial\Omega_C = \emptyset$. The results are summarized in figures which show the domain shape and the fluid flow within, as well as control boxes that govern the FFD parametrization of the domain and hence the domain shape.

5.1. Numerical solution

The solution strategy differs for the standard system (6) and the stabilized one (16):

- The weak problem (6) is discretized by an inf-sup stable finite element discretization (fulfilling the Babuška-Brezzi condition), namely by P1B/P1 elements (piecewise-linear velocities enriched by a bubble function and piecewise-linear pressures). The resulting system on nonlinear algebraic equations can be solved by the Newton iteration.

- The weak problem (16) is discretized using the simplest P1/P1 elements, violating the Babuška-Brezzi condition; this is compensated by the extra stabilization terms. The resulting system of nonlinear algebraic equations is solved using the Oseen iterations, see Section 3.1..

All computations were performed by our software which can be found at http://sfepy.kme.zcu.cz, cf. Cimrman et al. (2008).

5.2. Results of numerical simulations

First, the classical problem formulation was used, see Rohan and Cimrman (2006). In Fig. 2 a flow pattern is shown on a twisted tube geometry (diameter: 1 cm) prior to the shape optimization. Enhancing the flow uniformity in Ω_C, denoted by two grey planes in the figure, was the objective, $\Psi(\boldsymbol{u}) = \Psi_1(\boldsymbol{u})$, recall (18). The final design is shown in Fig. 3 — the objective was improved by straightening the tube. The optimization algorithm needed 10 iterations with 40 objective function evaluations in 161 s (i.e. solving the direct problem (6)) and 11 objective function gradient evaluations in 611 s.

Then the stabilized formulation proposed in Section 4. was employed. The stabilization parameters were set according to (13), with the constant $C = 0.1$. The flow in the initial design (same as in Fig. 2) is in Fig. 4. The final design is shown in Fig. 5 — here the objective improvement resulted in"necking" the tube. The optimization algorithm needed 10 iterations with 35 objective function evaluations in 197 s (i.e. solving the direct problem (16)) and 11 objective function gradient evaluations in 1223 s.

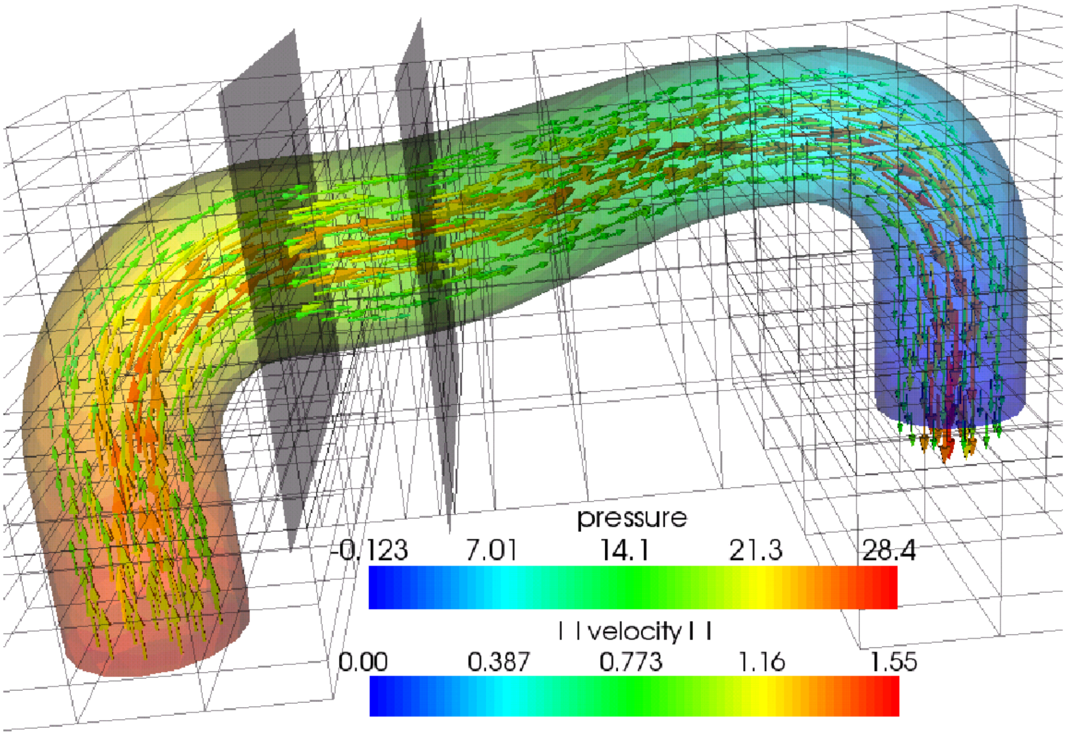

Fig. 2. Classical unstabilized formulation – *initial design*. Flow and domain control boxes. Control domain Ω_C between two grey planes.

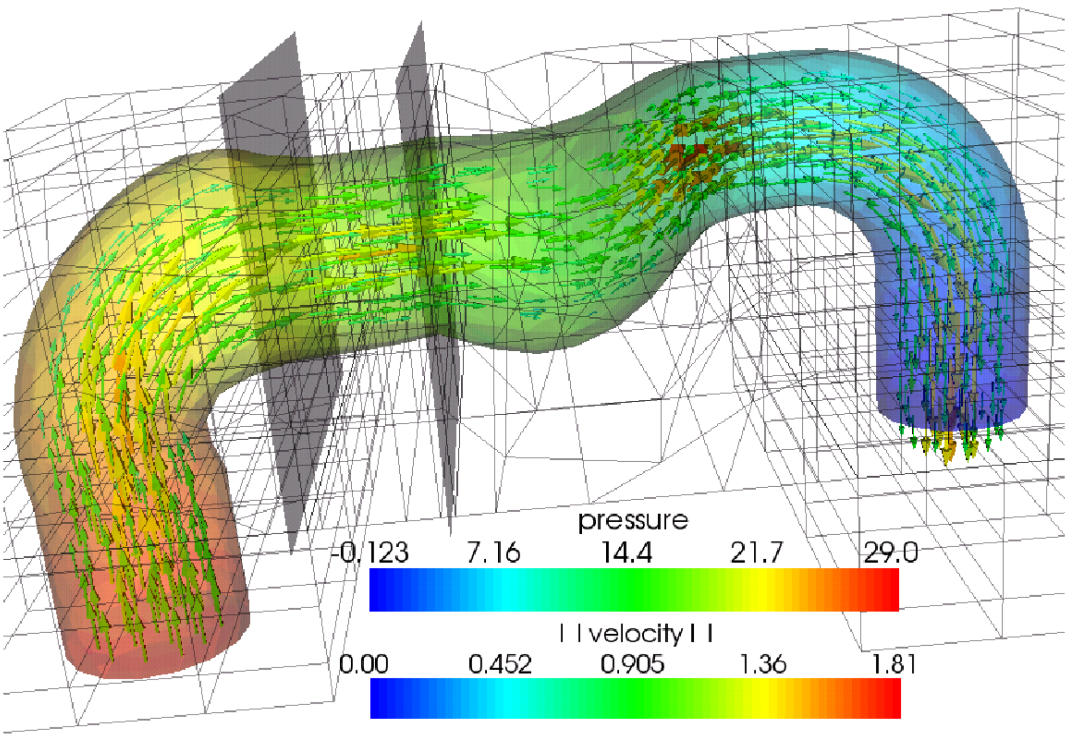

Fig. 3. Classical unstabilized formulation – *optimized design*. Flow and domain control boxes. Control domain Ω_C between two grey planes.

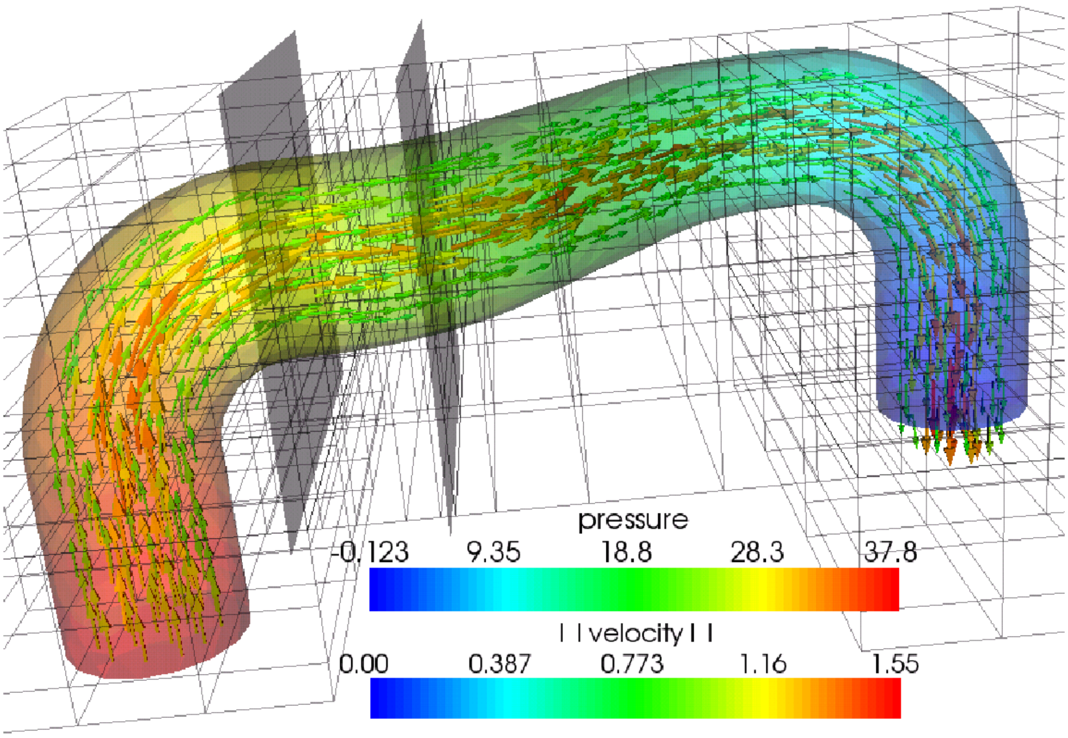

Fig. 4. Stabilized formulation – *initial design*. Flow and domain control boxes. Control domain Ω_C between two grey planes.

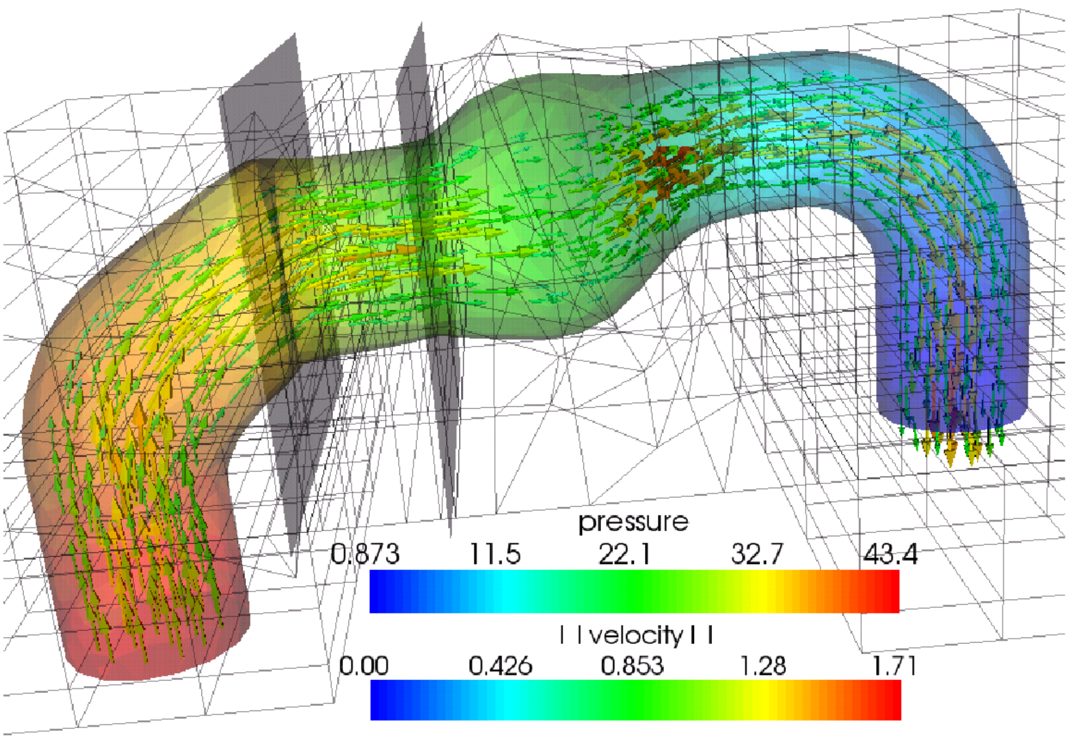

Fig. 5. Stabilized formulation – *optimized design*. Flow and domain control boxes. Control domain Ω_C between two grey planes.

Note that in both cases the shape changes of the domain are local — only the control boxes relevant to the objective improvement move. In both examples the final designs were better than the initial designs w.r.t. the objective functions used, see Fig. 6. In practice, however, more constraints need to be added to the FFD control boxes to enforce, e.g. higher degree of smoothness of the boundary, to prevent excessive deformation as in Fig. 4. It is also clear that the stabilization terms influence the solution as well as the optimization procedure. The crucial question is the choice of the stabilization parameters γ, τ_k and κ_K, which will be a topic of our future research. The point is to stabilize sufficiently to allow solving high Reynolds number flows and at the same time not to spoil the solution by an over-stabilization.

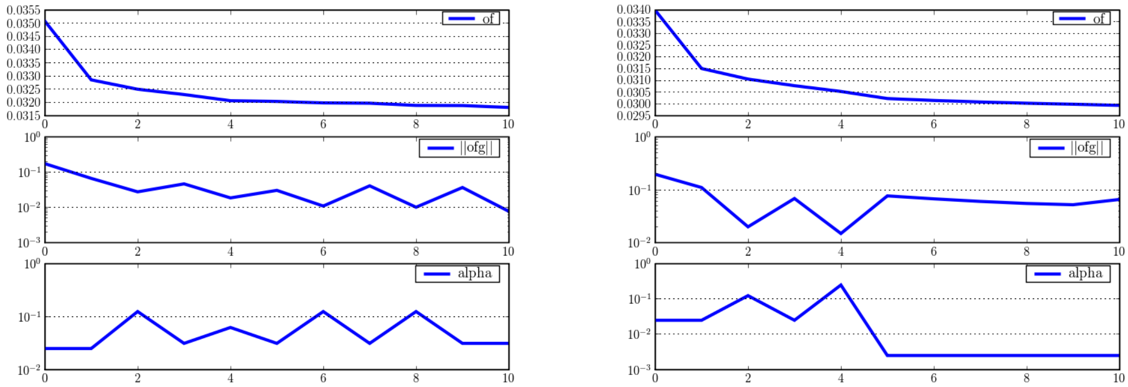

Fig. 6. Convergence of the steepest descent optimization algorithm, left: classical formulation, right: stabilized formulation. Notation: `of` objective function, `||ofg||` norm of objective function gradient, `alpha` line-search step.

6. Conclusions

In this paper we developed the sensitivity analysis for the stabilized optimal flow problem. The adjoint technique of the analytical sensitivity analysis is very efficient and accurate comparing to finite-difference based differentiation, especially when large number of design parameters is considered. According to the numerical tests performed for the so-called spline-box parametrization (reported in Rohan and Cimrman (2006)) there is an evident need for involving further optimization constraints concernig a required flow capacity and some enhanced smoothness requirements imposed on the design geometry.

Acknowledgement

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